



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:05 PM UTC

PDB ID : 5TB0 / pdb_00005tb0
EMDB ID : EMD-8391
Title : Structure of rabbit RyR1 (EGTA-only dataset, all particles)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;
Frank, J.
Deposited on : 2016-09-10
Resolution : 4.40 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

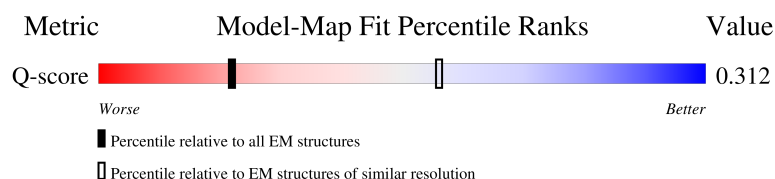
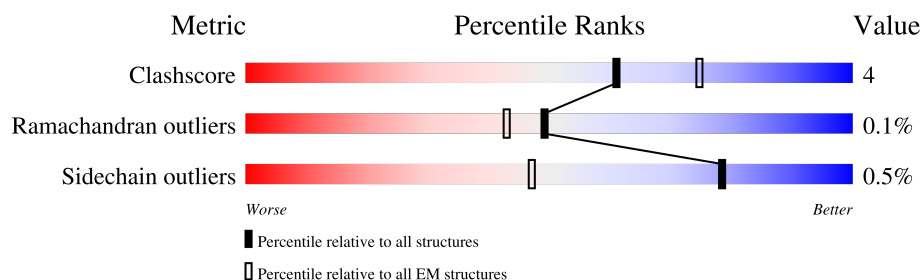
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3132 (3.91 - 4.90)

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

Mol	Chain	Length	Quality of chain
1	A	108	55% 89% 10%
1	F	108	55% 90% 9%
1	H	108	52% 91% 8%
1	J	108	54% 90% 9%

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Mol	Chain	Length	Quality of chain
2	B	4416	52% 85% 10% 5%
2	E	4416	52% 85% 10% 5%
2	G	4416	51% 84% 10% 5%
2	I	4416	52% 84% 10% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 121272 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 Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	A	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	J	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

- Molecule 2 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

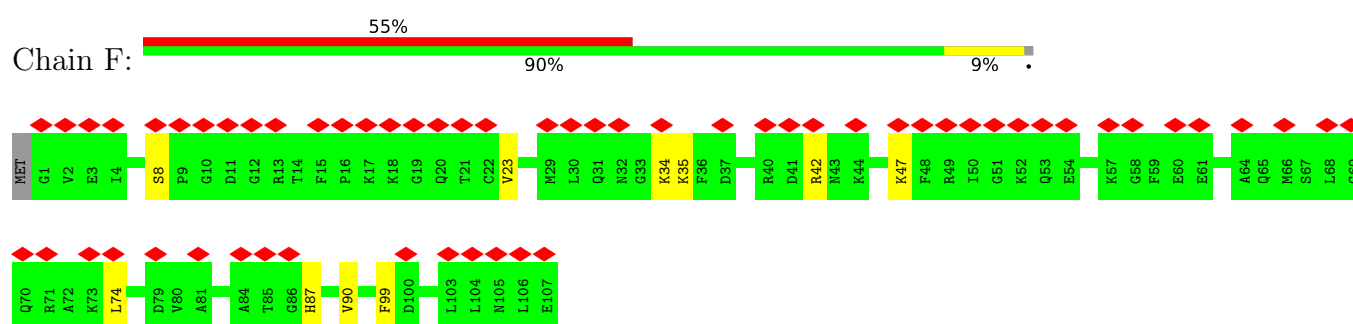
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	B	1	Total	Zn	0
			1	1	
3	G	1	Total	Zn	0
			1	1	
3	E	1	Total	Zn	0
			1	1	
3	I	1	Total	Zn	0
			1	1	

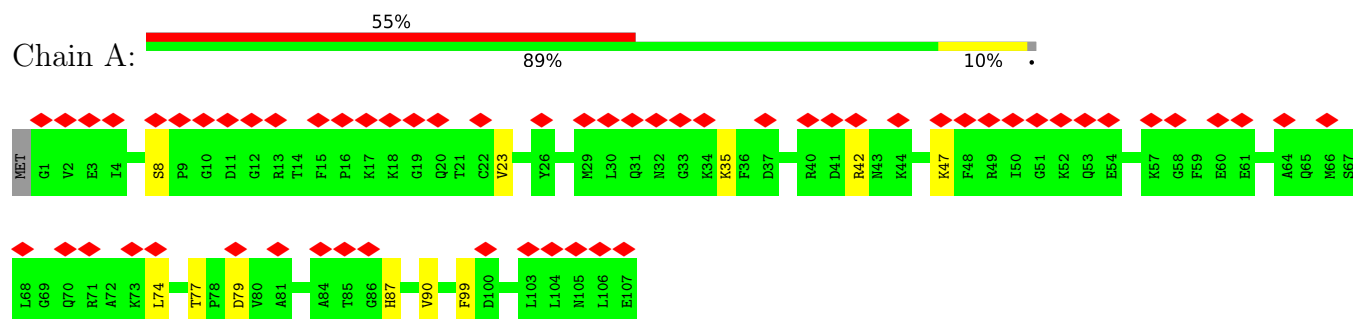
3 Residue-property plots [i](#)

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.

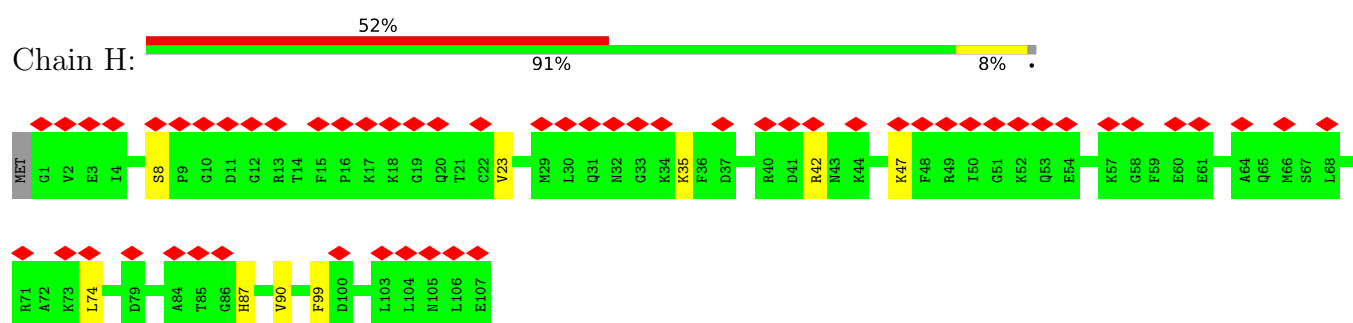
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



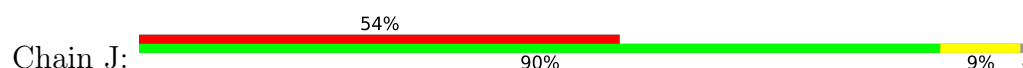
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

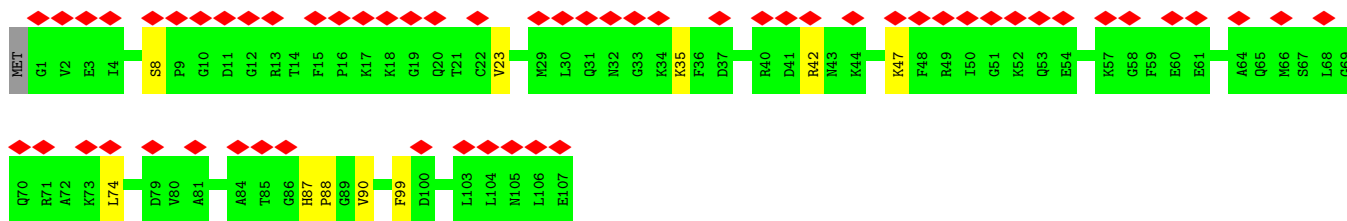


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

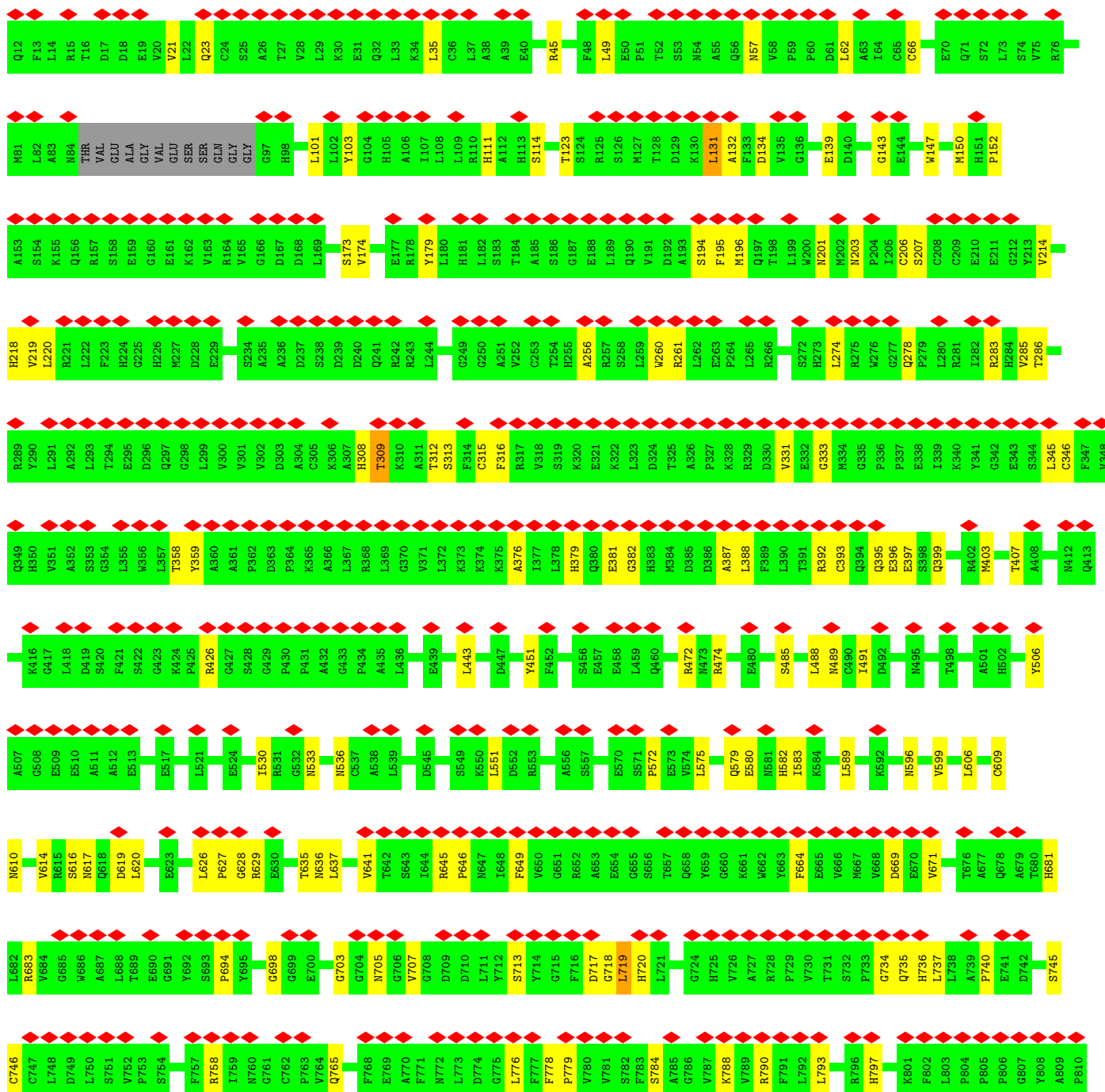
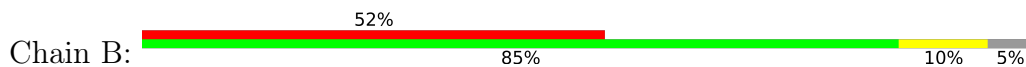


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B





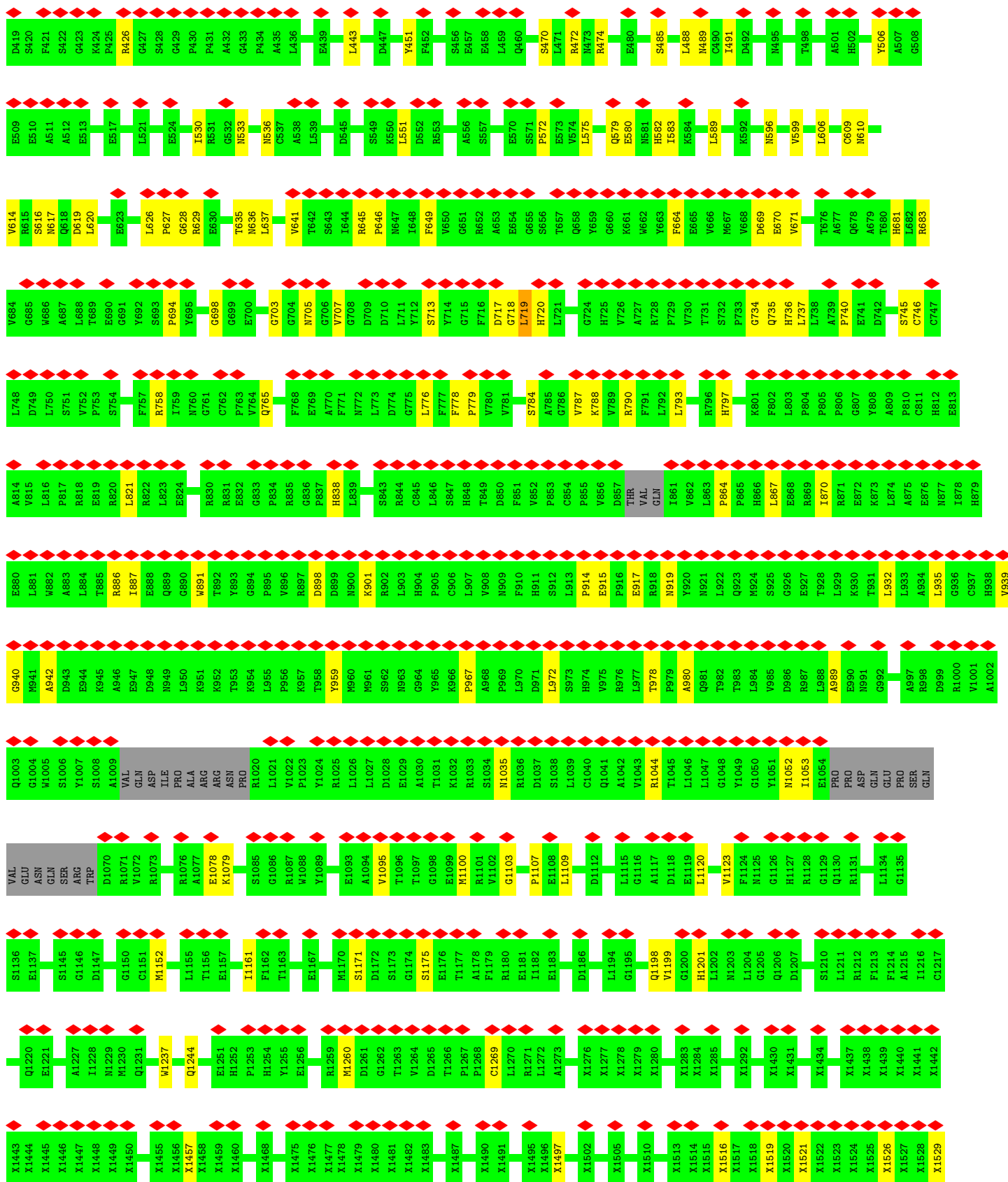
• Molecule 2: Ryanodine receptor 1







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L3993	F3996	M4000	M4001	K4002	L4003	S4007	E4011	L4012	L4013	K4014	E4015	L4016	L4017	D4018	L4019	Q4020	K4021	D4022	E4032	G4033	M4034	G4038	A4041	D4046	M4047	L4048	V4049	E4050	M4054	V4055	E4056	M4057	L4058	L4059	K4060	F4061	F4062	D4063	M4064	F4065	L4066	K4067	L4068	K4069	D4070	G4073	S4074	E4075																																																																																							
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X2973	X2974	X2975	X2976	X2995	X2996	X2997	X2998	X2999	X3000	X3001	X3002	X3003	X3004	X3005	X3006	X3007	X3008	X3009	X3010	X3011	X3012	X3013	X3014	X3015	X3016	X3017	X3018	X3019	X3020	X3021	X3022	X3023	X3024	X3025	X3026	X3027	X3028	X3029	X3030	X3031	X3032	X3033	X3034	X3035	X3036	X3037	X3038	X3039	X3040	X3041	X3042	X3043	X3044	X3045	X3046	X3047	X3048	X3049	X3050																																																																												

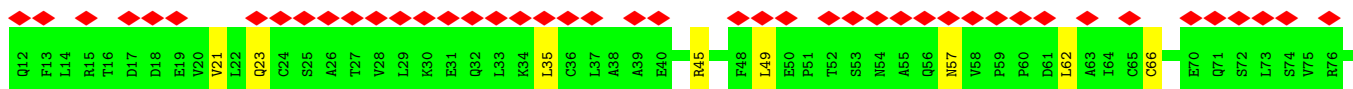
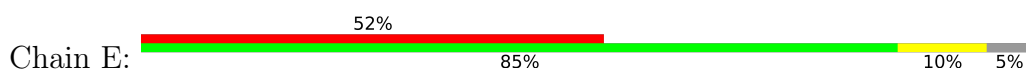




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X3551	X3442	X3380	X3189	X3053	X2975	A2913	GLU	P2793	X2703	X2643
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• Molecule 2: Ryanodine receptor 1

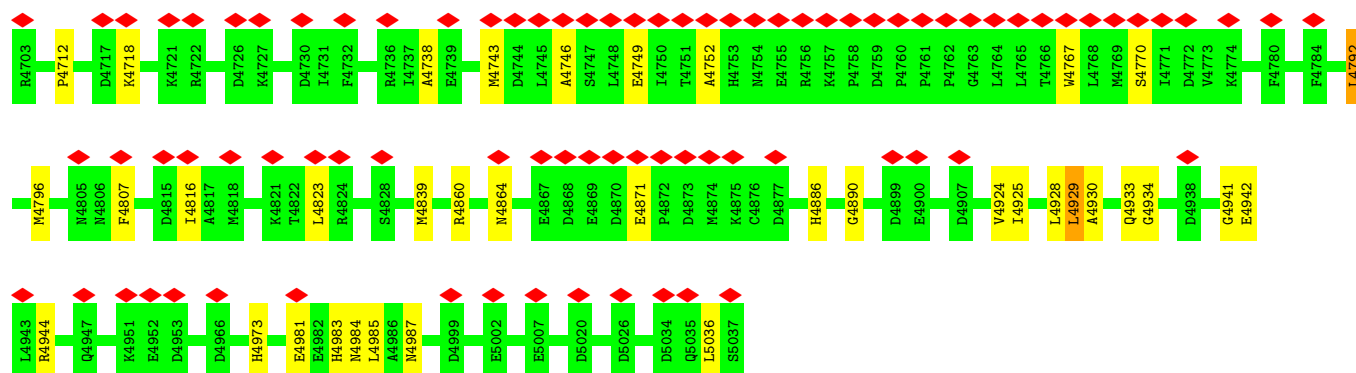




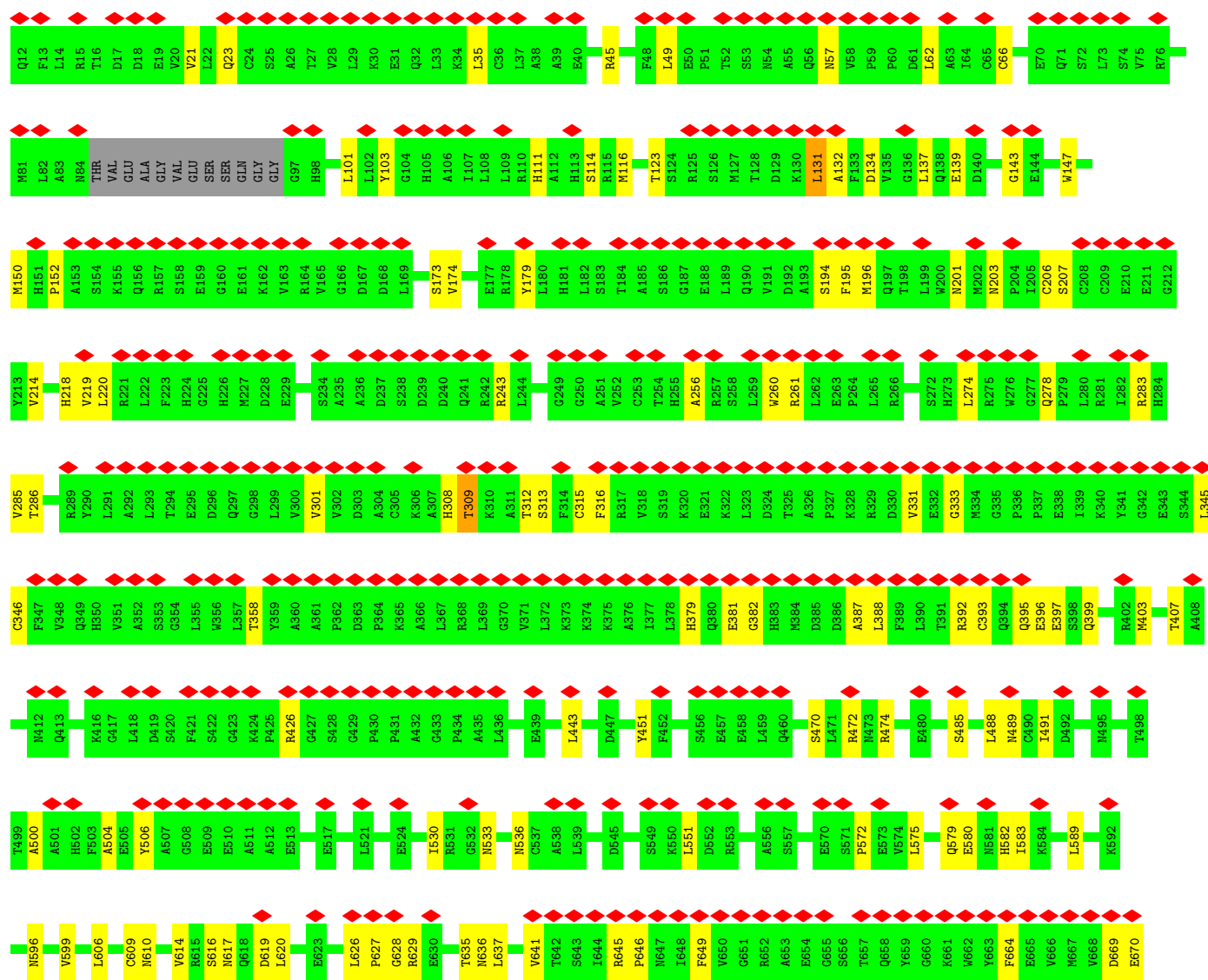
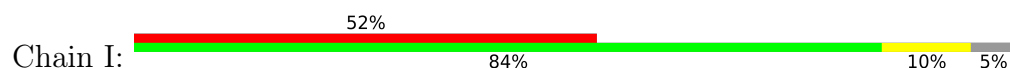


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GLY	N4654	X4368	E3766	D3885	E3766	N3884	X3682	X3682	X3582	X3477	X414	X3353	X3293
GLY	N4655	X4369	E3767	D3886	E3767	N3885	X3683	X3683	X3583	X3478	X415	X3354	X3294
GLY	N4656	X4370	E3768	D3887	E3768	N3886	X3684	X3684	X3584	X3479	X416	X3355	X3295
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GLY	N4658	X4372	E3770	D3889	E3770	N3888	X3686	X3686	X3586	X3481	X418	X3357	X3297
GLY	N4659	X4373	E3771	D3890	E3771	N3889	X3687	X3687	X3587	X3482	X419	X3358	X3298
GLY	N4660	X4374	E3772	D3891	E3772	N3890	X3688	X3688	X3588	X3483	X420	X3359	X3299
GLY	N4661	X4375	E3773	D3892	E3773	N3891	X3689	X3689	X3589	X3484	X421	X3360	X3300
GLY	N4662	X4376	E3774	D3893	E3774	N3892	X3690	X3690	X3590	X3485	X422	X3361	X3301
GLY	N4663	X4377	E3775	D3894	E3775	N3893	X3691	X3691	X3591	X3486	X423	X3362	X3302
GLY	N4664	X4378	E3776	D3895	E3776	N3894	X3692	X3692	X3592	X3487	X424	X3363	X3303
GLY	N4665	X4379	E3777	D3896	E3777	N3895	X3693	X3693	X3593	X3488	X425	X3364	X3304
GLY	N4666	X4380	E3778	D3897	E3778	N3896	X3694	X3694	X3594	X3489	X426	X3365	X3305
GLY	N4667	X4381	E3779	D3898	E3779	N3897	X3695	X3695	X3595	X3490	X427	X3366	X3306
GLY	N4668	X4382	E3780	D3899	E3780	N3898	X3696	X3696	X3596	X3491	X428	X3367	X3307
GLY	N4669	X4383	E3781	D3900	E3781	N3899	X3697	X3697	X3597	X3492	X429	X3368	X3308
GLY	N4670	X4384	E3782	D3901	E3782	N3900	X3698	X3698	X3598	X3493	X430	X3369	X3309
GLY	N4671	X4385	E3783	D3902	E3783	N3901	X3699	X3699	X3599	X3494	X431	X3370	X3310
GLY	N4672	X4386	E3784	D3903	E3784	N3902	X3700	X3700	X3600	X3495	X432	X3371	X3311
GLY	N4673	X4387	E3785	D3904	E3785	N3903	X3701	X3701	X3601	X3496	X433	X3372	X3312
GLY	N4674	X4388	E3786	D3905	E3786	N3904	X3702	X3702	X3602	X3497	X434	X3373	X3313
GLY	N4675	X4389	E3787	D3906	E3787	N3905	X3703	X3703	X3603	X3498	X435	X3374	X3314
GLY	N4676	X4390	E3788	D3907	E3788	N3906	X3704	X3704	X3604	X3499	X436	X3375	X3315
GLY	N4677	X4391	E3789	D3908	E3789	N3907	X3705	X3705	X3605	X3500	X440	X3376	X3316
GLY	N4678	X4392	E3790	D3909	E3790	N3908	X3706	X3706	X3606	X3501	X441	X3377	X3317
GLY	N4679	X4393	E3791	D3910	E3791	N3909	X3707	X3707	X3607	X3502	X442	X3378	X3318
GLY	N4680	X4394	E3792	D3911	E3792	N3910	X3708	X3708	X3608	X3503	X443	X3379	X3319
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GLY	N4682	X4396	E3794	D3913	E3794	N3912	X3710	X3710	X3610	X3505	X445	X3381	X3321
GLY	N4683	X4397	E3795	D3914	E3795	N3913	X3711	X3711	X3611	X3506	X446	X3382	X3322
GLY	N4684	X4398	E3796	D3915	E3796	N3914	X3712	X3712	X3612	X3507	X447	X3383	X3323
GLY	N4685	X4399	E3797	D3916	E3797	N3915	X3713	X3713	X3613	X3508	X448	X3384	X3324
GLY	N4686	X4400	E3798	D3917	E3798	N3916	X3714	X3714	X3614	X3509	X449	X3385	X3325
GLY	N4687	X4401	E3799	D3918	E3799	N3917	X3715	X3715	X3615	X3510	X450	X3386	X3326
GLY	N4688	X4402	E3800	D3919	E3800	N3918	X3716	X3716	X3616	X3511	X451	X3387	X3327
GLY	N4689	X4403	E3801	D3920	E3801	N3919	X3717	X3717	X3617	X3512	X452	X3388	X3328
GLY	N4690	X4404	E3802	D3921	E3802	N3920	X3718	X3718	X3618	X3513	X453	X3389	X3329
GLY	N4691	X4405	E3803	D3922	E3803	N3921	X3719	X3719	X3619	X3514	X454	X3390	X3330
GLY	N4692	X4406	E3804	D3923	E3804	N3922	X3720	X3720	X3620	X3515	X455	X3391	X3331
GLY	N4693	X4407	E3805	D3924	E3805	N3923	X3721	X3721	X3621	X3516	X456	X3392	X3332
GLY	N4694	X4408	E3806	D3925	E3806	N3924	X3722	X3722	X3622	X3517	X457	X3393	X3333
GLY	N4695	X4409	E3807	D3926	E3807	N3925	X3723	X3723	X3623	X3518	X458	X3394	X3334
GLY	N4696	X4410	E3808	D3927	E3808	N3926	X3724	X3724	X3624	X3519	X459	X3395	X3335
GLY	N4697	X4411	E3809	D3928	E3809	N3927	X3725	X3725	X3625	X3520	X460	X3396	X3336
GLY	N4698	X4412	E3810	D3929	E3810	N3928	X3726	X3726	X3626	X3521	X461	X3397	X3337
GLY	N4699	X4413	E3811	D3930	E3811	N3929	X3727	X3727	X3627	X3522	X462	X3398	X3338
GLY	N4700	X4414	E3812	D3931	E3812	N3930	X3728	X3728	X3628	X3523	X463	X3399	X3339
GLY	N4701	X4415	E3813	D3932	E3813	N3931	X3729	X3729	X3629	X3524	X464	X3400	X3280
GLY	N4702	X4416	E3814	D3933	E3814	N3932	X3730	X3730	X3630	X3525	X465	X3401	X3281
GLY	N4703	X4417	E3815	D3934	E3815	N3933	X3731	X3731	X3631	X3526	X466	X3402	X3282
GLY	N4704	X4418	E3816	D3935	E3816	N3934	X3732	X3732	X3632	X3527	X467	X3403	X3283
GLY	N4705	X4419	E3817	D3936	E3817	N3935	X3733	X3733	X3633	X3528	X468	X3404	X3284
GLY	N4706	X4420	E3818	D3937	E3818	N3936	X3734	X3734	X3634	X3529	X469	X3405	X3285
GLY	N4707	X4421	E3819	D3938	E3819	N3937	X3735	X3735	X3635	X3530	X470	X3406	X3286
GLY	N4708	X4422	E3820	D3939	E3820	N3938	X3736	X3736	X3636	X3531	X471	X3407	X3287
GLY	N4709	X4423	E3821	D3940	E3821	N3939	X3737	X3737	X3637	X3532	X472	X3408	X3288
GLY	N4710	X4424	E3822	D3941	E3822	N3940	X3738	X3738	X3638	X3533	X473	X3409	X3289
GLY	N4711	X4425	E3823	D3942	E3823	N3941	X3739	X3739	X3639	X3534	X474	X3410	X3290
GLY	N4712	X4426	E3824	D3943	E3824	N3942	X3740	X3740	X3640	X3535	X475	X3411	X3291
GLY	N4713	X4427	E3825	D3944	E3825	N3943	X3741	X3741	X3641	X3536	X476	X3412	X3292
GLY	N4714	X4428	E3826	D3945	E3826	N3944	X3742	X3742	X3642	X3537	X477	X3413	X3293
GLY	N4715	X4429	E3827	D3946	E3827	N3945	X3743	X3743	X3643	X3538	X478	X3414	X3294
GLY	N4716	X4430	E3828	D3947	E3828	N3946	X3744	X3744	X3644	X3539	X479	X3415	X3295
GLY	N4717	X4431	E3829	D3948	E3829	N3947	X3745	X3745	X3645	X3540	X480	X3416	X3296
GLY	N4718	X4432	E3830	D3949	E3830	N3948	X3746	X3746	X3646	X3541	X481	X3417	X3297
GLY	N4719	X4433	E3831	D3950	E3831	N3949	X3747	X3747	X3647	X3542	X482	X3418	X3298
GLY	N4720	X4434	E3832	D3951	E3832	N3950	X3748	X3748	X3648	X3543	X483	X3419	X3299
GLY	N4721	X4435	E3833	D3952	E3833	N3951	X3749	X3749	X3649	X3544	X484	X3420	X3300
GLY	N4722	X4436	E3834	D3953	E3834	N3952	X						



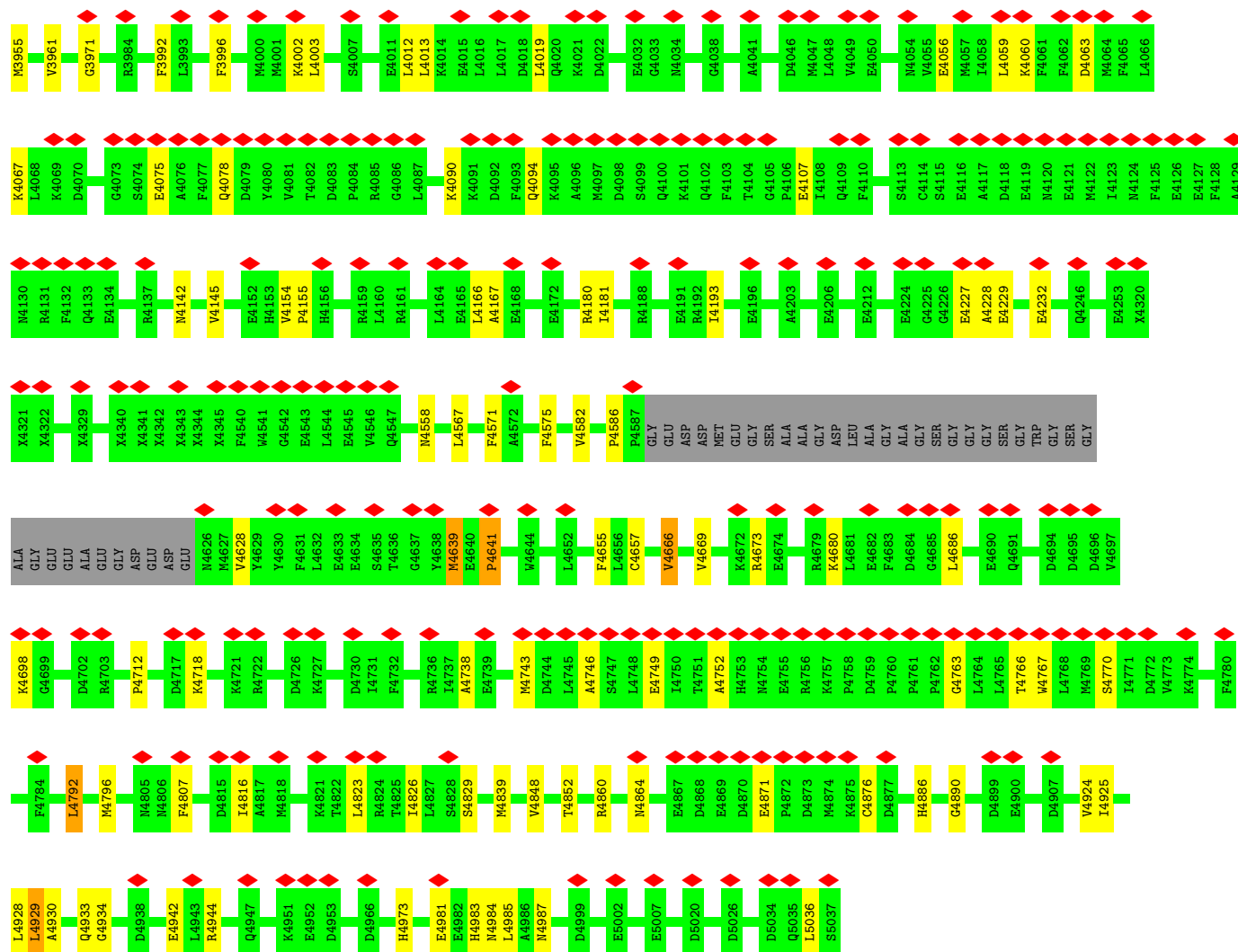
• Molecule 2: Ryanodine receptor 1



R1708	A1709	G1710	Y1711	Y1712	D1713	I1718	H1719	L1720	E1721	S1722	A1723	C1724	R1725	R1726	R1728	L1731	S1732	E1733	Y1734	I1735	E1741	T1742	R1743	F1748	P1749	P1750	G1751	K1752	G1753	G1754	N1756	A1757	R1758	R1759	H1760	G1766	V1767	L1771	H1775	V1783	A1784	A1785	L1786	P1787	A1788	ALA	GLY	VAL	ALA	E1793								
W1605	V1615	GLU	THR	ARG	ARG	ALA	GLY	E1622	R1623	L1624	G1625	V1626	A1627	V1628	Q1629	C1630	Q1631	D1632	M1636	M1637	A1638	L1639	E1644	N1645	R1646	D1649	E1655	L1656	R1661	H1665	R1668	R1671	L1676	N1679	R1680	D1690	Q1691	L1694	L1698	E1699	D1700	A1701	H1702	L1703														
X1520	X1521	X1522	X1523	X1524	X1525	X1526	X1527	X1528	X1529	X1530	X1531	X1532	X1533	X1534	X1535	X1536	X1537	X1538	X1542	X1543	X1544	X1545	X1546	X1547	X1548	X1549	X1550	X1551	X1552	X1553	X1554	X1555	X1556	X1557	X1562	M1573	P1574	L1575	S1576	A1577	A1578	M1579	F1580	E1583	P1587	A1588	P1589	Q1590	C1591	L1595	L1596							
G1126	H1127	R1128	G1129	Q1130	R1131	L1134	G1135	S1136	E1137	S1145	G1146	D1147	G1150	C1151	M1152	L1155	T1156	E1157	I1161	F1162	T1163	E1167	M1170	S1171	D1172	S1173	G1174	S1175	E1176	T1177	A1178	F1179	R1180	E1181	I1182	E1183	D1186	L1189	G1195	Q1198	V1199	G1200	H1201	L1202	N1203	L1204	G1205	Q1206	D1207									
S1210	L1211	R1212	F1213	F1214	A1215	I1216	C1217	Q1220	E1221	A1227	I1228	M1229	M1230	Q1231	M1237	Q1244	E1251	H1252	P1253	H1254	Y1255	E1256	R1259	M1260	D1261	G1262	T1263	V1264	D1265	T1266	P1267	F1268	C1269	L1270	R1271	L1272	A1273	X1276	X1277	X1278	X1279	X1280	X1281	X1282	X1283	X1284	X1285	X1292	X1430									
X1431	X1434	X1437	X1438	X1439	X1440	X1441	X1442	X1443	X1444	X1445	X1446	X1447	X1448	X1449	X1450	X1455	X1456	X1457	X1458	X1459	X1460	X1468	X1475	X1476	X1477	X1478	X1479	X1480	X1481	X1482	X1483	X1487	X1490	X1491	X1495	X1496	X1497	X1502	X1505	X1510	X1513	X1514	X1515	X1516	X1517	X1518	X1519											
X1520	X1521	X1522	X1523	X1524	X1525	X1526	X1527	X1528	X1529	X1530	X1531	X1532	X1533	X1534	X1535	X1536	X1537	X1538	X1542	X1543	X1544	X1545	X1546	X1547	X1548	X1549	X1550	X1551	X1552	X1553	X1554	X1555	X1556	X1557	X1562	M1573	P1574	L1575	S1576	A1577	A1578	M1579	F1580	E1583	P1587	A1588	P1589	Q1590	C1591	L1595	L1596							
W1605	V1615	GLU	THR	ARG	ARG	ALA	GLY	E1622	R1623	L1624	G1625	V1626	A1627	V1628	Q1629	C1630	Q1631	D1632	M1636	M1637	A1638	L1639	E1644	N1645	R1646	D1649	E1655	L1656	R1661	H1665	R1668	R1671	L1676	N1679	R1680	D1690	Q1691	L1694	L1698	E1699	D1700	A1701	H1702	L1703														
R1708	A1709	G1710	Y1711	Y1712	D1713	I1718	H1719	L1720	E1721	S1722	A1723	C1724	R1725	R1726	R1728	L1731	S1732	E1733	Y1734	I1735	E1741	T1742	R1743	F1748	P1749	P1750	G1751	K1752	G1753	G1754	N1756	A1757	R1758	R1759	H1760	G1766	V1767	L1771	H1775	V1783	A1784	A1785	L1786	P1787	A1788	ALA	GLY	VAL	ALA	E1793								
V671	T676	A677	Q678	A679	T680	H681	L682	R683	V684	G685	V686	A687	T688	T689	E690	G691	Y692	S693	P694	Y695	G698	G699	E700	G703	G704	N705	G706	V707	G708	D709	L710	L711	Y712	S713	Y714	G715	F716	D717	G718	L719	H720	L721	G724	H725	V726	A727	R728	P729	V730	T731	S732	P733	G734	Q735	H736			
L737	L738	A739	P740	E741	D742	S745	C746	C747	L748	D749	V750	S751	V752	P753	S754	F757	R758	I759	N760	G761	C762	P763	V764	Q765	F768	E769	A770	F771	N772	D773	D774	G775	L776	F777	F778	S779	V780	H781	S784	A785	C786	V787	K788	H789	R790	F791	L792	L793	R796	H797	K801	F802	L803					
P804	P805	P806	G807	Y808	A809	P810	C811	H812	E813	A814	V815	L816	P817	R818	E819	R820	L821	R822	L823	E824	R830	R831	E832	G833	P834	R835	G836	P837	H838	S843	R844	C845	L846	S847	H848	T849	D850	F851	V852	P853	C854	P855	V856	D857	THR	VAL	GLN	I861	V862	L863	P864	P865	H866	L867	E868	R869		
I870	R871	E872	K873	L874	A875	E876	N877	I878	H879	E880	L881	W882	L884	T885	R886	I887	E888	Q889	G890	W891	T892	Y893	G894	P895	V896	R897	D898	D899	N900	K901	R902	L903	H904	P905	C906	L907	V908	N909	F910	H911	S912	L913	P914	E915	P916	E917	R918	N919	Y920	N921	L922	Q923	N924	S925	G926	T928	L929	
K930	T931	L932	L933	A934	L935	G936	C937	H938	V939	G940	H941	A942	D943	E944	K945	A946	E947	D948	N949	L950	K951	K952	T953	K954	L955	P956	K957	T958	Y959	M960	H961	S962	N963	G964	Y965	K966	P967	A968	P969	L970	D971	L972	S973	H974	V975	R976	L977	T978	P979	A980	Q981	T982	T983	L984	V985	D986	L988	A989
E990	N991	G992	A997	R998	D999	R1000	V1001	A1002	Q1003	G1004	H1005	S1006	Y1007	S1008	A1009	VAL	GLN	ASP	ILE	PRO	ALA	ARG	ARG	ASN	PRO	R1020	L1021	V1022	P1023	Y1024	R1025	L1026	D1028	E1029	A1030	T1031	K1032	R1033	S1034	N1035	R1036	D1037	S1038	L1039	C1040	Q1041	A1042	V1043	R1044	T1045	L1046	L1047	G1048	Y1049	G1050	Y1051	N1052	
I1053	E1054	PRO	PRO	ASP	GLN	GLU	PRO	SER	GLN	VAL	ASN	GLN	SER	ARG	TRP	D1070	R1071	Y1072	R1073	R1076	A1077	E1078	K1079	S1085	G1086	R1087	E1093	A1094	V1095	T1096	T1097	G1098	E1099	M1100	R1101	V1102	G1103	P1107	E1108	L1109	R1110	P1111	D1112	L1115	G1116	A1117	D1118	E1119	L1120	V1123	F1124	N1125						
G1126	H1127	R1128	G1129	Q1130	R1131	L1134	G1135	S1136	E1137	S1145	G1146	D1147	G1150	C1151	M1152	L1155	T1156	E1157	I1161	F1162	T1163	E1167	M1170	S1171	D1172	S1173	G1174	S1175	E1176	T1177	A1178	F1179	R1180	E1181	I1182	E1183	D1186	L1189	G1195	Q1198	V1199	G1200	H1201	L1202	N1203	L1204	G1205	Q1206	D1207									
S1210	L1211	R1212	F1213	F1214	A1215	I1216	C1217	Q1220	E1221	A1227	I1228	M1229	M1230	Q1231	M1237	Q1244	E1251	H1252	P1253	H1254	Y1255	E1256	R1259	M1260	D1261	G1262	T1263	V1264	D1265	T1266	P1267	F1268	C1269	L1270	R1271	L1272	A1273	X1276	X1277	X1278	X1279	X1280	X1281	X1282	X1283	X1284	X1285	X1292	X1430									
X1431	X1434	X1437	X1438	X1439	X1440	X1441	X1442	X1443	X1444	X1445	X1446	X1447	X1448	X1449	X1450	X1455	X1456	X1457	X1458	X1459	X1460	X1468	X1475	X1476	X1477	X1478	X1479	X1480	X1481	X1482	X1483	X1487	X1490	X1491	X1495	X1496	X1497	X1502	X1505	X1510	X1513	X1514	X1515	X1516	X1517	X1518	X1519											
X1520	X1521	X1522	X1523	X1524	X1525	X1526	X1527	X1528	X1529	X1530	X1531	X1532	X1533	X1534	X1535	X1536	X1537	X1538	X1542	X1543	X1544	X1545	X1546	X1547	X1548	X1549	X1550	X1551	X1552	X1553	X1554	X1555	X1556	X1557	X1562	M1573	P1574	L1575	S1576	A1577	A1578	M1579	F1580	E1583	P1587	A1588	P1589	Q1590	C1591	L1595	L1596							
W1605	V1615	GLU	THR	ARG	ARG	ALA	GLY	E1622	R1623	L1624	G1625	V1626	A1627	V1628	Q1629	C1630	Q1631	D1632	M1636	M1637	A1638	L1639	E1644	N1645	R1646	D1649	E1655	L1656	R1661	H1665	R1668	R1671	L1676	N1679	R1680	D1690	Q1691	L1694	L1698	E1699	D1700	A1701	H1702	L1703														
R1708	A1709	G1710	Y1711	Y1712	D1713	I1718	H1719	L1720	E1721	S1722	A1723	C1724	R1725	R1726	R1728	L1731	S1732	E1733	Y1734	I1735	E1741	T1742	R1743	F1748	P1749	P1750	G1751	K1752	G1753	G1754	N1756	A1757	R1758	R1759	H1760	G1766	V1767	L1771	H1775	V1783	A1784	A1785	L1786	P1787	A1788	ALA	GLY	VAL	ALA	E1793								







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	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	0.081	Depositor
Minimum map value	-0.049	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	502.0, 502.0, 502.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.255, 1.255, 1.255	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.21	0/834	0.48	0/1123
1	F	0.21	0/834	0.48	0/1123
1	H	0.21	0/834	0.47	0/1123
1	J	0.21	0/834	0.47	0/1123
2	B	0.25	0/25428	0.55	3/34534 (0.0%)
2	E	0.25	0/25428	0.55	3/34534 (0.0%)
2	G	0.25	0/25428	0.55	3/34534 (0.0%)
2	I	0.25	0/25428	0.55	3/34534 (0.0%)
All	All	0.25	0/105048	0.55	12/142628 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	F	0	1
1	H	0	1
1	J	0	1
2	B	0	18
2	E	0	18
2	G	0	18
2	I	0	18
All	All	0	76

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	131	LEU	CA-CB-CG	5.46	135.39	116.30
2	B	131	LEU	CA-CB-CG	5.45	135.38	116.30
2	E	131	LEU	CA-CB-CG	5.45	135.36	116.30
2	I	131	LEU	CA-CB-CG	5.45	135.36	116.30
2	G	4639	MET	CA-C-N	5.16	134.38	121.80
2	G	4639	MET	C-N-CA	5.16	134.38	121.80
2	I	4639	MET	CA-C-N	5.15	134.37	121.80
2	I	4639	MET	C-N-CA	5.15	134.37	121.80
2	B	4639	MET	CA-C-N	5.14	134.34	121.80
2	B	4639	MET	C-N-CA	5.14	134.34	121.80
2	E	4639	MET	CA-C-N	5.14	134.34	121.80
2	E	4639	MET	C-N-CA	5.14	134.34	121.80

There are no chirality outliers.

All (76) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	SER	Peptide
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1690	ASP	Peptide
2	B	1712	TYR	Peptide
2	B	1720	LEU	Peptide
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide
2	B	1840	PRO	Peptide
2	B	2291	GLN	Peptide
2	B	2343	GLY	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	312	THR	Peptide
2	B	3971	GLY	Peptide
2	B	4641	PRO	Peptide
2	B	4666	VAL	Peptide
2	B	4807	PHE	Peptide
2	B	694	PRO	Peptide
2	E	139	GLU	Peptide
2	E	1676	LEU	Peptide
2	E	1690	ASP	Peptide
2	E	1712	TYR	Peptide
2	E	1720	LEU	Peptide
2	E	1795	PRO	Peptide
2	E	1828	ASP	Peptide

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Mol	Chain	Res	Type	Group
2	E	1840	PRO	Peptide
2	E	2291	GLN	Peptide
2	E	2343	GLY	Peptide
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	312	THR	Peptide
2	E	3971	GLY	Peptide
2	E	4641	PRO	Peptide
2	E	4666	VAL	Peptide
2	E	4807	PHE	Peptide
2	E	694	PRO	Peptide
1	F	8	SER	Peptide
2	G	139	GLU	Peptide
2	G	1676	LEU	Peptide
2	G	1690	ASP	Peptide
2	G	1712	TYR	Peptide
2	G	1720	LEU	Peptide
2	G	1795	PRO	Peptide
2	G	1828	ASP	Peptide
2	G	1840	PRO	Peptide
2	G	2291	GLN	Peptide
2	G	2343	GLY	Peptide
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	312	THR	Peptide
2	G	3971	GLY	Peptide
2	G	4641	PRO	Peptide
2	G	4666	VAL	Peptide
2	G	4807	PHE	Peptide
2	G	694	PRO	Peptide
1	H	8	SER	Peptide
2	I	139	GLU	Peptide
2	I	1676	LEU	Peptide
2	I	1690	ASP	Peptide
2	I	1712	TYR	Peptide
2	I	1720	LEU	Peptide
2	I	1795	PRO	Peptide
2	I	1828	ASP	Peptide
2	I	1840	PRO	Peptide
2	I	2291	GLN	Peptide
2	I	2343	GLY	Peptide
2	I	2472	LEU	Peptide

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Mol	Chain	Res	Type	Group
2	I	2807	TRP	Peptide
2	I	312	THR	Peptide
2	I	3971	GLY	Peptide
2	I	4641	PRO	Peptide
2	I	4666	VAL	Peptide
2	I	4807	PHE	Peptide
2	I	694	PRO	Peptide
1	J	8	SER	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	818	0	824	6	0
1	F	818	0	824	6	0
1	H	818	0	824	5	0
1	J	818	0	824	6	0
2	B	29499	0	24749	243	0
2	E	29499	0	24750	240	0
2	G	29499	0	24749	252	0
2	I	29499	0	24749	252	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
All	All	121272	0	102293	975	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 4.

All (975) 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)
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.55	0.72
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.55	0.71
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.55	0.71
2:B:1260:MET:HB2	2:B:1269:CYS:H	1.62	0.65
2:B:331:VAL:HG12	2:B:333:GLY:H	1.61	0.65
2:G:1260:MET:HB2	2:G:1269:CYS:H	1.62	0.65
2:E:1260:MET:HB2	2:E:1269:CYS:H	1.62	0.65
2:I:331:VAL:HG12	2:I:333:GLY:H	1.61	0.64
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.31	0.64
2:E:331:VAL:HG12	2:E:333:GLY:H	1.61	0.64
2:E:942:ALA:HB2	2:E:1052:ASN:HB2	1.80	0.64
2:I:1260:MET:HB2	2:I:1269:CYS:H	1.62	0.64
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.31	0.64
2:G:942:ALA:HB2	2:G:1052:ASN:HB2	1.80	0.64
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.31	0.63
2:I:942:ALA:HB2	2:I:1052:ASN:HB2	1.80	0.63
2:I:379:HIS:HD2	2:I:382:GLY:H	1.47	0.63
2:B:942:ALA:HB2	2:B:1052:ASN:HB2	1.80	0.63
2:G:331:VAL:HG12	2:G:333:GLY:H	1.61	0.63
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.64	0.63
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.31	0.62
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.64	0.62
2:B:379:HIS:HD2	2:B:382:GLY:H	1.47	0.62
2:E:2347:GLU:O	2:E:2351:ASN:N	2.32	0.62
2:G:4839:MET:HE2	2:I:4823:LEU:HD21	1.81	0.61
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.64	0.61
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.64	0.61
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.83	0.61
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.83	0.61
2:B:4973:HIS:NE2	2:I:4227:GLU:OE2	2.29	0.61
2:E:379:HIS:HD2	2:E:382:GLY:H	1.47	0.61
2:G:379:HIS:HD2	2:G:382:GLY:H	1.47	0.61
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.83	0.60
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.83	0.60
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.83	0.60
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.83	0.60
2:B:2347:GLU:O	2:B:2351:ASN:N	2.32	0.60
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.35	0.60
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.83	0.60
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.83	0.60
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.35	0.60
2:B:4984:ASN:OD1	2:B:4987:ASN:N	2.34	0.59
2:G:2347:GLU:O	2:G:2351:ASN:N	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.83	0.59
2:I:4180:ARG:NH1	2:I:4981:GLU:OE1	2.36	0.59
2:B:3675:ASP:OD1	2:B:3769:ARG:NH2	2.36	0.59
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.83	0.59
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.35	0.59
2:B:4227:GLU:OE2	2:E:4973:HIS:NE2	2.29	0.59
2:G:179:TYR:OH	2:I:2359:ARG:NH2	2.36	0.59
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.35	0.59
2:E:4180:ARG:NH1	2:E:4981:GLU:OE1	2.36	0.59
2:G:2359:ARG:NH2	2:E:179:TYR:OH	2.36	0.59
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.83	0.59
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.83	0.59
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.36	0.59
2:I:4984:ASN:OD1	2:I:4987:ASN:N	2.34	0.59
2:B:4180:ARG:NH1	2:B:4981:GLU:OE1	2.36	0.59
2:G:3675:ASP:OD1	2:G:3769:ARG:NH2	2.36	0.59
2:G:4180:ARG:NH1	2:G:4981:GLU:OE1	2.36	0.59
2:I:2347:GLU:O	2:I:2351:ASN:N	2.32	0.59
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.85	0.58
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	1.85	0.58
2:G:580:GLU:HG2	2:G:583:ILE:HD11	1.85	0.58
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.36	0.58
2:G:4227:GLU:OE2	2:I:4973:HIS:NE2	2.26	0.58
2:E:580:GLU:HG2	2:E:583:ILE:HD11	1.85	0.58
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	1.85	0.58
2:I:101:LEU:HB3	2:I:150:MET:HE1	1.86	0.58
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.85	0.58
2:B:101:LEU:HB3	2:B:150:MET:HE1	1.86	0.58
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.36	0.58
2:E:3675:ASP:OD1	2:E:3769:ARG:NH2	2.36	0.58
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.36	0.58
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	1.85	0.58
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.85	0.58
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.37	0.58
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	1.85	0.58
2:G:4984:ASN:OD1	2:G:4987:ASN:N	2.34	0.58
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.85	0.57
2:B:35:LEU:HD13	2:B:49:LEU:HD13	1.86	0.57
2:G:4582:VAL:HG11	2:E:4860:ARG:HD2	1.86	0.57
2:I:3675:ASP:OD1	2:I:3769:ARG:NH2	2.36	0.57
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4567:LEU:HA	2:I:4816:ILE:HD12	1.87	0.57
2:B:4567:LEU:HA	2:B:4816:ILE:HD12	1.87	0.57
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.87	0.57
2:G:393:CYS:SG	2:G:395:GLN:NE2	2.77	0.57
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.87	0.57
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.87	0.57
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.37	0.57
2:G:4567:LEU:HA	2:G:4816:ILE:HD12	1.87	0.57
2:B:580:GLU:HG2	2:B:583:ILE:HD11	1.85	0.57
2:B:2359:ARG:NH2	2:I:179:TYR:OH	2.37	0.57
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.86	0.57
2:G:35:LEU:HD13	2:G:49:LEU:HD13	1.86	0.57
2:G:4942:GLU:HA	2:I:4944:ARG:HH22	1.70	0.57
2:I:580:GLU:HG2	2:I:583:ILE:HD11	1.85	0.57
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.87	0.57
2:I:393:CYS:SG	2:I:395:GLN:NE2	2.77	0.57
2:B:393:CYS:SG	2:B:395:GLN:NE2	2.77	0.57
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.87	0.57
2:B:4839:MET:HE2	2:E:4823:LEU:HD21	1.87	0.57
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.37	0.56
2:G:4933:GLN:NE2	2:I:4933:GLN:OE1	2.38	0.56
2:E:393:CYS:SG	2:E:395:GLN:NE2	2.77	0.56
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.87	0.56
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.87	0.56
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.87	0.56
2:E:719:LEU:HD22	2:E:735:GLN:HG2	1.87	0.56
2:E:4984:ASN:OD1	2:E:4987:ASN:N	2.34	0.56
2:I:35:LEU:HD13	2:I:49:LEU:HD13	1.86	0.56
2:B:719:LEU:HD22	2:B:735:GLN:HG2	1.87	0.56
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.87	0.56
2:G:101:LEU:HB3	2:G:150:MET:HE1	1.86	0.56
2:E:35:LEU:HD13	2:E:49:LEU:HD13	1.86	0.56
2:E:101:LEU:HB3	2:E:150:MET:HE1	1.86	0.56
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.87	0.56
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.37	0.56
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.87	0.56
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.87	0.56
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.78	0.56
2:E:4567:LEU:HA	2:E:4816:ILE:HD12	1.87	0.56
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.87	0.56
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:23:GLN:OE1	2:I:203:ASN:ND2	2.34	0.56
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.87	0.56
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.87	0.56
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.87	0.56
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.78	0.56
2:B:23:GLN:OE1	2:B:203:ASN:ND2	2.34	0.56
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.87	0.56
2:G:2342:ASN:OD1	2:G:2342:ASN:N	2.39	0.56
2:E:4864:ASN:ND2	2:E:4871:GLU:OE1	2.39	0.56
2:I:719:LEU:HD22	2:I:735:GLN:HG2	1.87	0.56
2:B:179:TYR:OH	2:E:2359:ARG:NH2	2.38	0.56
2:G:4973:HIS:NE2	2:E:4227:GLU:OE2	2.32	0.56
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.39	0.56
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.88	0.55
2:B:4823:LEU:HD21	2:I:4839:MET:HE2	1.87	0.55
2:G:719:LEU:HD22	2:G:735:GLN:HG2	1.87	0.55
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.87	0.55
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.78	0.55
2:G:4864:ASN:ND2	2:G:4871:GLU:OE1	2.39	0.55
2:G:626:LEU:HG	2:G:628:GLY:H	1.72	0.55
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.88	0.55
2:E:485:SER:O	2:E:489:ASN:N	2.38	0.55
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.88	0.55
2:I:4864:ASN:ND2	2:I:4871:GLU:OE1	2.39	0.55
2:B:614:VAL:HG22	2:B:616:SER:H	1.72	0.55
2:E:614:VAL:HG22	2:E:616:SER:H	1.72	0.55
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.40	0.55
2:B:2342:ASN:OD1	2:B:2342:ASN:N	2.39	0.55
2:I:626:LEU:HG	2:I:628:GLY:H	1.72	0.55
2:B:4864:ASN:ND2	2:B:4871:GLU:OE1	2.39	0.55
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.39	0.55
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.40	0.55
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.89	0.55
2:I:315:CYS:SG	2:I:316:PHE:N	2.80	0.55
2:G:614:VAL:HG22	2:G:616:SER:H	1.72	0.55
2:I:619:ASP:OD1	2:I:1680:ARG:NH1	2.38	0.55
2:I:399:GLN:HG2	2:I:403:MET:HE3	1.89	0.55
2:E:23:GLN:OE1	2:E:203:ASN:ND2	2.34	0.55
2:E:399:GLN:HG2	2:E:403:MET:HE3	1.89	0.55
2:I:614:VAL:HG22	2:I:616:SER:H	1.72	0.55
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:315:CYS:SG	2:G:316:PHE:N	2.80	0.55
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.40	0.55
2:E:626:LEU:HG	2:E:628:GLY:H	1.72	0.55
2:B:399:GLN:HG2	2:B:403:MET:HE3	1.89	0.54
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.40	0.54
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.39	0.54
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.87	0.54
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.89	0.54
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.89	0.54
2:G:3809:ASN:HB3	2:G:3812:VAL:HG22	1.89	0.54
2:G:4823:LEU:HD21	2:E:4839:MET:HE2	1.88	0.54
2:E:3809:ASN:HB3	2:E:3812:VAL:HG22	1.89	0.54
2:B:626:LEU:HG	2:B:628:GLY:H	1.72	0.54
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.89	0.54
2:G:2346:VAL:HG22	2:G:2348:GLU:H	1.73	0.54
2:E:315:CYS:SG	2:E:316:PHE:N	2.80	0.54
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.87	0.54
2:G:399:GLN:HG2	2:G:403:MET:HE3	1.89	0.54
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.89	0.54
2:I:3809:ASN:HB3	2:I:3812:VAL:HG22	1.89	0.54
2:B:2346:VAL:HG22	2:B:2348:GLU:H	1.73	0.54
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.73	0.54
2:I:2342:ASN:OD1	2:I:2342:ASN:N	2.39	0.54
2:B:3809:ASN:HB3	2:B:3812:VAL:HG22	1.89	0.54
2:E:1679:ASN:ND2	2:E:1798:LEU:O	2.41	0.54
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.89	0.54
2:E:2342:ASN:N	2:E:2342:ASN:OD1	2.39	0.54
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.73	0.54
2:B:1679:ASN:ND2	2:B:1798:LEU:O	2.41	0.54
2:B:315:CYS:SG	2:B:316:PHE:N	2.80	0.54
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.73	0.54
2:B:358:THR:HG21	2:B:382:GLY:HA2	1.90	0.53
2:E:2003:GLN:O	2:E:2007:ASN:ND2	2.42	0.53
2:B:4738:ALA:HA	2:B:4743:MET:HE3	1.90	0.53
2:B:4930:ALA:O	2:B:4934:GLY:N	2.42	0.53
2:G:4738:ALA:HA	2:G:4743:MET:HE3	1.90	0.53
2:G:4930:ALA:O	2:G:4934:GLY:N	2.42	0.53
2:E:4738:ALA:HA	2:E:4743:MET:HE3	1.90	0.53
2:I:2346:VAL:HG22	2:I:2348:GLU:H	1.73	0.53
2:G:2003:GLN:O	2:G:2007:ASN:ND2	2.42	0.53
2:I:2003:GLN:O	2:I:2007:ASN:ND2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4738:ALA:HA	2:I:4743:MET:HE3	1.90	0.53
2:E:4090:LYS:O	2:E:4094:GLN:N	2.40	0.53
2:E:4075:GLU:HA	2:E:4078:GLN:HB2	1.91	0.53
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.89	0.53
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.89	0.53
2:I:1679:ASN:ND2	2:I:1798:LEU:O	2.41	0.53
2:I:1691:GLN:HE22	2:I:1802:ILE:HG12	1.74	0.53
2:I:4930:ALA:O	2:I:4934:GLY:N	2.42	0.53
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.74	0.53
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.89	0.53
2:G:1679:ASN:ND2	2:G:1798:LEU:O	2.41	0.53
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.73	0.53
2:E:2346:VAL:HG22	2:E:2348:GLU:H	1.73	0.53
2:E:4571:PHE:O	2:E:4575:PHE:N	2.42	0.53
2:E:4930:ALA:O	2:E:4934:GLY:N	2.41	0.53
2:B:2003:GLN:O	2:B:2007:ASN:ND2	2.42	0.53
2:B:4075:GLU:HA	2:B:4078:GLN:HB2	1.91	0.53
2:G:358:THR:HG21	2:G:382:GLY:HA2	1.90	0.53
2:E:358:THR:HG21	2:E:382:GLY:HA2	1.90	0.52
2:I:4571:PHE:O	2:I:4575:PHE:N	2.42	0.52
2:B:572:PRO:HA	2:B:575:LEU:HD13	1.92	0.52
2:B:4571:PHE:O	2:B:4575:PHE:N	2.42	0.52
2:G:4571:PHE:O	2:G:4575:PHE:N	2.42	0.52
2:G:619:ASP:OD1	2:G:1680:ARG:NH1	2.38	0.52
2:G:2199:ARG:NH2	2:G:2246:ASN:OD1	2.43	0.52
2:E:619:ASP:OD1	2:E:1680:ARG:NH1	2.39	0.52
2:I:358:THR:HG21	2:I:382:GLY:HA2	1.90	0.52
2:I:2199:ARG:NH2	2:I:2246:ASN:OD1	2.43	0.52
2:B:485:SER:O	2:B:489:ASN:N	2.38	0.52
2:E:1691:GLN:HE22	2:E:1802:ILE:HG12	1.74	0.52
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.92	0.52
2:I:4181:ILE:HG23	2:I:4193:ILE:HB	1.92	0.52
2:B:2199:ARG:NH2	2:B:2246:ASN:OD1	2.43	0.52
2:I:533:ASN:ND2	2:I:536:ASN:OD1	2.38	0.52
2:I:4075:GLU:HA	2:I:4078:GLN:HB2	1.91	0.52
2:G:669:ASP:OD2	2:G:790:ARG:NH2	2.43	0.52
2:G:1691:GLN:HE22	2:G:1802:ILE:HG12	1.74	0.52
2:I:173:SER:OG	2:I:174:VAL:N	2.43	0.52
2:I:572:PRO:HA	2:I:575:LEU:HD13	1.92	0.52
2:G:4181:ILE:HG23	2:G:4193:ILE:HB	1.92	0.52
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4181:ILE:HG23	2:E:4193:ILE:HB	1.92	0.52
2:B:173:SER:OG	2:B:174:VAL:N	2.43	0.51
2:G:4075:GLU:HA	2:G:4078:GLN:HB2	1.91	0.51
2:E:572:PRO:HA	2:E:575:LEU:HD13	1.92	0.51
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	1.92	0.51
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.92	0.51
2:I:1516:UNK:N	2:I:1529:UNK:O	2.44	0.51
2:I:4059:LEU:HD13	2:I:4167:ALA:HB2	1.92	0.51
2:I:4063:ASP:O	2:I:4067:LYS:NZ	2.36	0.51
2:B:619:ASP:OD1	2:B:1680:ARG:NH1	2.38	0.51
2:B:4181:ILE:HG23	2:B:4193:ILE:HB	1.92	0.51
2:I:4673:ARG:HH22	2:I:4698:LYS:HB2	1.75	0.51
2:B:4933:GLN:NE2	2:E:4933:GLN:OE1	2.43	0.51
2:G:572:PRO:HA	2:G:575:LEU:HD13	1.92	0.51
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.75	0.51
2:E:2199:ARG:NH2	2:E:2246:ASN:OD1	2.43	0.51
2:I:4003:LEU:HB2	2:I:4013:LEU:HD13	1.93	0.51
2:B:533:ASN:ND2	2:B:536:ASN:OD1	2.38	0.51
2:B:596:ASN:HB3	2:B:599:VAL:HG22	1.93	0.51
2:B:4063:ASP:O	2:B:4067:LYS:NZ	2.36	0.51
2:G:173:SER:OG	2:G:174:VAL:N	2.43	0.51
2:G:4003:LEU:HB2	2:G:4013:LEU:HD13	1.93	0.51
2:G:4860:ARG:HD2	2:I:4582:VAL:HG11	1.92	0.51
2:I:4090:LYS:O	2:I:4094:GLN:N	2.40	0.51
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.44	0.51
2:B:4003:LEU:HB2	2:B:4013:LEU:HD13	1.93	0.51
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.44	0.51
2:E:1516:UNK:N	2:E:1529:UNK:O	2.44	0.51
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.44	0.51
2:B:4942:GLU:HA	2:E:4944:ARG:HH22	1.76	0.51
2:E:4673:ARG:HH22	2:E:4698:LYS:HB2	1.75	0.51
2:I:596:ASN:HB3	2:I:599:VAL:HG22	1.93	0.51
2:B:4680:LYS:HD3	2:B:4686:LEU:HD22	1.93	0.51
2:B:4944:ARG:HH22	2:I:4942:GLU:HA	1.76	0.50
2:G:596:ASN:HB3	2:G:599:VAL:HG22	1.93	0.50
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.46	0.50
2:E:4003:LEU:HB2	2:E:4013:LEU:HD13	1.93	0.50
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	1.94	0.50
2:I:1694:LEU:O	2:I:1712:TYR:OH	2.26	0.50
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	1.93	0.50
2:B:4059:LEU:HD13	2:B:4167:ALA:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4059:LEU:HD13	2:E:4167:ALA:HB2	1.92	0.50
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.46	0.50
2:B:609:CYS:SG	2:B:610:ASN:N	2.85	0.50
2:G:609:CYS:SG	2:G:610:ASN:N	2.85	0.50
2:G:1516:UNK:N	2:G:1529:UNK:O	2.44	0.50
2:G:4059:LEU:HD13	2:G:4167:ALA:HB2	1.92	0.50
2:G:4090:LYS:O	2:G:4094:GLN:N	2.40	0.50
2:B:1516:UNK:N	2:B:1529:UNK:O	2.44	0.50
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.46	0.50
2:B:4933:GLN:OE1	2:I:4933:GLN:NE2	2.44	0.50
2:E:669:ASP:OD2	2:E:790:ARG:NH2	2.42	0.50
2:G:23:GLN:OE1	2:G:203:ASN:ND2	2.34	0.50
2:G:396:GLU:OE2	2:G:451:TYR:OH	2.28	0.50
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.94	0.50
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.44	0.50
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	1.94	0.50
2:B:4673:ARG:HH22	2:B:4698:LYS:HB2	1.75	0.50
2:G:4944:ARG:HH22	2:E:4942:GLU:HA	1.76	0.50
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.46	0.50
2:I:396:GLU:OE2	2:I:451:TYR:OH	2.28	0.50
2:I:609:CYS:SG	2:I:610:ASN:N	2.85	0.50
2:I:4680:LYS:HD3	2:I:4686:LEU:HD22	1.93	0.50
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.77	0.50
2:B:683:ARG:NH1	2:B:707:VAL:O	2.43	0.50
2:G:627:PRO:O	2:G:629:ARG:NH1	2.45	0.50
2:E:173:SER:OG	2:E:174:VAL:N	2.43	0.50
2:B:111:HIS:CD2	2:B:114:SER:H	2.30	0.50
2:B:669:ASP:OD2	2:B:790:ARG:NH2	2.43	0.50
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.94	0.50
2:I:627:PRO:O	2:I:629:ARG:NH1	2.45	0.50
2:I:864:PRO:HD2	2:I:867:LEU:HD12	1.94	0.50
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	1.94	0.50
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	1.93	0.50
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.45	0.50
2:E:111:HIS:CD2	2:E:114:SER:H	2.30	0.50
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.92	0.50
2:E:4680:LYS:HD3	2:E:4686:LEU:HD22	1.93	0.50
2:B:627:PRO:O	2:B:629:ARG:NH1	2.45	0.49
2:E:596:ASN:HB3	2:E:599:VAL:HG22	1.93	0.49
2:E:683:ARG:NH1	2:E:707:VAL:O	2.43	0.49
2:I:214:VAL:HG12	2:I:274:LEU:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.94	0.49
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.44	0.49
1:J:35:LYS:HD3	2:I:636:ASN:HD21	1.77	0.49
2:G:1244:GLN:OE1	2:G:1646:ARG:NH1	2.45	0.49
2:G:4239:GLU:OE2	2:G:5014:TYR:OH	2.27	0.49
2:E:396:GLU:OE2	2:E:451:TYR:OH	2.28	0.49
2:I:488:LEU:HD23	2:I:491:ILE:HD12	1.94	0.49
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.94	0.49
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.77	0.49
2:B:488:LEU:HD23	2:B:491:ILE:HD12	1.94	0.49
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.44	0.49
2:B:3753:PHE:HA	2:B:3756:LYS:HB3	1.93	0.49
2:G:214:VAL:HG12	2:G:274:LEU:HD12	1.94	0.49
2:G:533:ASN:ND2	2:G:536:ASN:OD1	2.38	0.49
2:E:609:CYS:SG	2:E:610:ASN:N	2.85	0.49
2:E:683:ARG:HG2	2:E:717:ASP:HB3	1.95	0.49
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.94	0.49
2:B:864:PRO:HD2	2:B:867:LEU:HD12	1.94	0.49
2:B:4090:LYS:O	2:B:4094:GLN:N	2.40	0.49
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.94	0.49
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	1.93	0.49
2:E:206:CYS:SG	2:E:207:SER:N	2.85	0.49
2:I:206:CYS:SG	2:I:207:SER:N	2.85	0.49
2:I:1244:GLN:OE1	2:I:1646:ARG:NH1	2.45	0.49
2:I:3753:PHE:HA	2:I:3756:LYS:HB3	1.93	0.49
2:B:2267:MET:HE3	2:B:2268:GLN:HG2	1.94	0.49
2:I:2332:LEU:HD13	2:I:2335:LEU:HD12	1.95	0.49
2:B:214:VAL:HG12	2:B:274:LEU:HD12	1.94	0.49
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.45	0.49
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.94	0.49
2:G:2894:LEU:HD11	2:G:2902:HIS:HB2	1.94	0.49
2:G:4680:LYS:HD3	2:G:4686:LEU:HD22	1.93	0.49
2:E:4924:VAL:HA	2:E:4928:LEU:HB2	1.94	0.49
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.93	0.49
2:I:3842:LEU:O	2:I:3929:SER:OG	2.31	0.49
2:B:1244:GLN:OE1	2:B:1646:ARG:NH1	2.45	0.49
2:B:1703:LEU:HD12	2:B:1708:ARG:HB2	1.95	0.49
2:G:111:HIS:CD2	2:G:114:SER:H	2.30	0.49
2:G:488:LEU:HD23	2:G:491:ILE:HD12	1.94	0.49
2:E:214:VAL:HG12	2:E:274:LEU:HD12	1.94	0.49
2:E:627:PRO:O	2:E:629:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1244:GLN:OE1	2:E:1646:ARG:NH1	2.45	0.49
2:E:3753:PHE:HA	2:E:3756:LYS:HB3	1.93	0.49
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.93	0.49
2:B:2332:LEU:HD13	2:B:2335:LEU:HD12	1.95	0.49
2:G:206:CYS:SG	2:G:207:SER:N	2.85	0.49
2:G:1694:LEU:O	2:G:1712:TYR:OH	2.26	0.49
2:G:2267:MET:HE3	2:G:2268:GLN:HG2	1.94	0.49
2:G:3842:LEU:O	2:G:3929:SER:OG	2.31	0.49
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	1.93	0.49
2:I:111:HIS:CD2	2:I:114:SER:H	2.30	0.49
2:I:1703:LEU:HD12	2:I:1708:ARG:HB2	1.95	0.49
1:A:87:HIS:HD2	1:A:90:VAL:HB	1.77	0.49
2:B:683:ARG:HG2	2:B:717:ASP:HB3	1.95	0.49
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.78	0.49
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.94	0.49
2:G:864:PRO:HD2	2:G:867:LEU:HD12	1.94	0.49
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.94	0.49
2:G:4933:GLN:OE1	2:E:4933:GLN:NE2	2.46	0.49
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.94	0.49
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.45	0.49
2:B:2894:LEU:HD11	2:B:2902:HIS:HB2	1.94	0.49
2:G:3753:PHE:HA	2:G:3756:LYS:HB3	1.93	0.49
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	1.94	0.49
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.94	0.49
2:I:2267:MET:HE3	2:I:2268:GLN:HG2	1.94	0.49
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	1.95	0.48
2:G:4063:ASP:O	2:G:4067:LYS:NZ	2.36	0.48
2:E:838:HIS:HA	2:E:1201:HIS:HB3	1.95	0.48
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.44	0.48
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.45	0.48
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.94	0.48
2:E:2420:HIS:ND1	2:E:2493:UNK:O	2.47	0.48
2:I:485:SER:O	2:I:489:ASN:N	2.38	0.48
2:I:669:ASP:OD2	2:I:790:ARG:NH2	2.43	0.48
2:I:683:ARG:NH1	2:I:707:VAL:O	2.43	0.48
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	1.96	0.48
2:I:3948:LYS:HG2	2:I:4012:LEU:HD22	1.95	0.48
2:B:838:HIS:HA	2:B:1201:HIS:HB3	1.95	0.48
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	1.93	0.48
2:G:683:ARG:HG2	2:G:717:ASP:HB3	1.95	0.48
2:E:2894:LEU:HD11	2:E:2902:HIS:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4924:VAL:HA	2:I:4928:LEU:HB2	1.94	0.48
2:B:206:CYS:SG	2:B:207:SER:N	2.85	0.48
2:B:395:GLN:NE2	2:B:397:GLU:OE1	2.47	0.48
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.46	0.48
2:B:3842:LEU:O	2:B:3929:SER:OG	2.31	0.48
2:G:2758:PHE:O	2:G:2762:THR:N	2.47	0.48
2:E:488:LEU:HD23	2:E:491:ILE:HD12	1.94	0.48
2:I:2894:LEU:HD11	2:I:2902:HIS:HB2	1.94	0.48
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.94	0.48
2:B:1100:MET:HE2	2:B:1198:GLN:HB3	1.96	0.48
2:B:3767:GLN:NE2	2:B:3804:ILE:O	2.47	0.48
2:G:1991:THR:O	2:G:1995:THR:OG1	2.32	0.48
2:G:4060:LYS:NZ	2:G:4107:GLU:OE2	2.47	0.48
2:G:4924:VAL:HA	2:G:4928:LEU:HB2	1.94	0.48
2:E:864:PRO:HD2	2:E:867:LEU:HD12	1.94	0.48
2:B:4239:GLU:OE2	2:B:5014:TYR:OH	2.27	0.48
2:E:1100:MET:HE2	2:E:1198:GLN:HB3	1.96	0.48
2:E:1991:THR:O	2:E:1995:THR:OG1	2.32	0.48
2:I:683:ARG:HG2	2:I:717:ASP:HB3	1.95	0.48
2:B:1991:THR:O	2:B:1995:THR:OG1	2.32	0.48
2:G:485:SER:O	2:G:489:ASN:N	2.38	0.48
2:G:3948:LYS:HG2	2:G:4012:LEU:HD22	1.96	0.48
2:E:395:GLN:NE2	2:E:397:GLU:OE1	2.47	0.48
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.46	0.48
2:E:2267:MET:HE3	2:E:2268:GLN:HG2	1.94	0.48
1:H:35:LYS:HD3	2:G:636:ASN:HD21	1.79	0.48
2:B:4924:VAL:HA	2:B:4928:LEU:HB2	1.94	0.48
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	1.96	0.48
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.94	0.48
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	1.96	0.48
2:E:4060:LYS:NZ	2:E:4107:GLU:OE2	2.47	0.48
2:I:681:HIS:HB3	2:I:784:SER:HB3	1.96	0.48
2:I:1991:THR:O	2:I:1995:THR:OG1	2.32	0.48
2:I:4666:VAL:HG23	2:I:4669:VAL:HB	1.96	0.48
2:G:838:HIS:HA	2:G:1201:HIS:HB3	1.95	0.48
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.96	0.48
2:G:2332:LEU:HD13	2:G:2335:LEU:HD12	1.95	0.48
2:E:3767:GLN:NE2	2:E:3804:ILE:O	2.47	0.48
2:G:1703:LEU:HD12	2:G:1708:ARG:HB2	1.95	0.47
2:G:3767:GLN:NE2	2:G:3804:ILE:O	2.47	0.47
2:E:1703:LEU:HD12	2:E:1708:ARG:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2332:LEU:HD13	2:E:2335:LEU:HD12	1.95	0.47
2:E:4666:VAL:HG23	2:E:4669:VAL:HB	1.96	0.47
1:A:35:LYS:HD3	2:B:636:ASN:HD21	1.79	0.47
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.77	0.47
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.47	0.47
2:G:2420:HIS:ND1	2:G:2493:UNK:O	2.47	0.47
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.49	0.47
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.47	0.47
2:G:681:HIS:HB3	2:G:784:SER:HB3	1.96	0.47
2:E:4063:ASP:O	2:E:4067:LYS:NZ	2.36	0.47
2:I:395:GLN:NE2	2:I:397:GLU:OE1	2.47	0.47
2:I:2758:PHE:O	2:I:2762:THR:N	2.47	0.47
2:B:2758:PHE:O	2:B:2762:THR:N	2.47	0.47
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.49	0.47
2:G:219:VAL:HG13	2:G:285:VAL:HG21	1.97	0.47
2:G:683:ARG:NH1	2:G:707:VAL:O	2.43	0.47
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.49	0.47
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.96	0.47
2:I:3767:GLN:NE2	2:I:3804:ILE:O	2.47	0.47
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	1.97	0.47
2:E:533:ASN:ND2	2:E:536:ASN:OD1	2.38	0.47
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.47	0.47
2:B:4155:PRO:HD2	2:B:5036:LEU:HD23	1.97	0.47
2:G:395:GLN:NE2	2:G:397:GLU:OE1	2.47	0.47
2:G:2159:LEU:HA	2:G:2162:ILE:HD12	1.97	0.47
2:I:395:GLN:HG3	2:I:397:GLU:H	1.80	0.47
2:I:838:HIS:HA	2:I:1201:HIS:HB3	1.95	0.47
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.47	0.47
2:I:4060:LYS:NZ	2:I:4107:GLU:OE2	2.47	0.47
2:B:395:GLN:HG3	2:B:397:GLU:H	1.80	0.47
2:B:396:GLU:OE2	2:B:451:TYR:OH	2.28	0.47
2:B:681:HIS:HB3	2:B:784:SER:HB3	1.96	0.47
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.48	0.47
2:B:1812:LEU:HD21	2:B:1861:GLN:HG2	1.97	0.47
2:B:2420:HIS:ND1	2:B:2493:UNK:O	2.47	0.47
2:B:3948:LYS:HG2	2:B:4012:LEU:HD22	1.96	0.47
2:B:4060:LYS:NZ	2:B:4107:GLU:OE2	2.47	0.47
2:G:395:GLN:HG3	2:G:397:GLU:H	1.80	0.47
2:E:1171:SER:OG	2:E:1175:SER:N	2.42	0.47
2:E:3842:LEU:O	2:E:3929:SER:OG	2.31	0.47
2:E:3948:LYS:HG2	2:E:4012:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4155:PRO:HD2	2:E:5036:LEU:HD23	1.97	0.47
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.96	0.47
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.46	0.47
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	1.97	0.47
2:G:4666:VAL:HG23	2:G:4669:VAL:HB	1.96	0.47
2:E:134:ASP:N	2:E:134:ASP:OD1	2.48	0.47
2:E:681:HIS:HB3	2:E:784:SER:HB3	1.96	0.47
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.96	0.47
2:E:3779:VAL:HG23	2:E:3780:LEU:HD12	1.97	0.47
2:I:4155:PRO:HD2	2:I:5036:LEU:HD23	1.97	0.47
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.44	0.47
2:G:1100:MET:HE2	2:G:1198:GLN:HB3	1.96	0.47
2:G:4155:PRO:HD2	2:G:5036:LEU:HD23	1.97	0.47
2:E:395:GLN:HG3	2:E:397:GLU:H	1.80	0.47
2:E:2159:LEU:HA	2:E:2162:ILE:HD12	1.97	0.47
2:I:219:VAL:HG13	2:I:285:VAL:HG21	1.97	0.47
2:I:1100:MET:HE2	2:I:1198:GLN:HB3	1.96	0.47
2:I:2420:HIS:ND1	2:I:2493:UNK:O	2.47	0.47
2:I:4767:TRP:HE3	2:I:4770:SER:HB2	1.80	0.47
2:B:3779:VAL:HG23	2:B:3780:LEU:HD12	1.97	0.47
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.96	0.46
2:E:1812:LEU:HD21	2:E:1861:GLN:HG2	1.97	0.46
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	1.97	0.46
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.97	0.46
2:B:2159:LEU:HA	2:B:2162:ILE:HD12	1.96	0.46
2:B:2277:ALA:HB1	2:B:2337:PHE:HD2	1.81	0.46
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.96	0.46
2:B:4666:VAL:HG23	2:B:4669:VAL:HB	1.96	0.46
2:B:4767:TRP:HE3	2:B:4770:SER:HB2	1.80	0.46
2:G:132:ALA:HA	2:G:194:SER:HB2	1.98	0.46
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.48	0.46
2:E:2236:LEU:HD23	2:E:2275:VAL:HG21	1.98	0.46
2:E:2758:PHE:O	2:E:2762:THR:N	2.47	0.46
2:I:2159:LEU:HA	2:I:2162:ILE:HD12	1.97	0.46
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.97	0.46
2:B:219:VAL:HG13	2:B:285:VAL:HG21	1.97	0.46
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	1.97	0.46
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.48	0.46
2:G:2236:LEU:HD23	2:G:2275:VAL:HG21	1.98	0.46
2:G:3779:VAL:HG23	2:G:3780:LEU:HD12	1.97	0.46
2:E:2277:ALA:HB1	2:E:2337:PHE:HD2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.48	0.46
2:G:1812:LEU:HD21	2:G:1861:GLN:HG2	1.97	0.46
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.49	0.46
2:E:3923:LEU:HD13	2:E:3961:VAL:HG11	1.98	0.46
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.96	0.46
2:I:3779:VAL:HG23	2:I:3780:LEU:HD12	1.97	0.46
2:B:1078:GLU:HG3	2:B:1237:TRP:HE1	1.81	0.46
2:B:2143:THR:O	2:B:3651:ASN:ND2	2.44	0.46
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	1.97	0.46
2:G:4749:GLU:HA	2:G:4752:ALA:HB3	1.97	0.46
2:G:765:GLN:NE2	2:G:1521:UNK:O	2.49	0.46
2:G:3923:LEU:HD13	2:G:3961:VAL:HG11	1.98	0.46
2:I:645:ARG:HH11	2:I:778:PHE:HE1	1.64	0.46
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.89	0.46
2:B:2236:LEU:HD23	2:B:2275:VAL:HG21	1.98	0.46
2:E:219:VAL:HG13	2:E:285:VAL:HG21	1.97	0.46
2:I:132:ALA:HA	2:I:194:SER:HB2	1.98	0.46
2:G:698:GLY:HA2	2:G:703:GLY:HA2	1.98	0.46
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.46	0.46
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.89	0.46
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.96	0.46
2:I:4749:GLU:HA	2:I:4752:ALA:HB3	1.97	0.46
2:G:1171:SER:OG	2:G:1175:SER:N	2.42	0.46
2:G:2277:ALA:HB1	2:G:2337:PHE:HD2	1.81	0.46
2:G:3365:UNK:O	2:G:3369:UNK:N	2.49	0.46
2:E:765:GLN:NE2	2:E:1521:UNK:O	2.49	0.46
2:I:134:ASP:OD1	2:I:134:ASP:N	2.48	0.46
2:I:698:GLY:HA2	2:I:703:GLY:HA2	1.98	0.46
2:I:3923:LEU:HD13	2:I:3961:VAL:HG11	1.98	0.46
2:G:134:ASP:OD1	2:G:134:ASP:N	2.48	0.45
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	1.97	0.45
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.89	0.45
2:I:2236:LEU:HD23	2:I:2275:VAL:HG21	1.98	0.45
2:B:4749:GLU:HA	2:B:4752:ALA:HB3	1.97	0.45
2:E:1078:GLU:HG3	2:E:1237:TRP:HE1	1.81	0.45
2:I:765:GLN:NE2	2:I:1521:UNK:O	2.49	0.45
2:I:2277:ALA:HB1	2:I:2337:PHE:HD2	1.81	0.45
2:E:4749:GLU:HA	2:E:4752:ALA:HB3	1.97	0.45
2:E:4767:TRP:HE3	2:E:4770:SER:HB2	1.80	0.45
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.97	0.45
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.89	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3923:LEU:HD13	2:B:3961:VAL:HG11	1.98	0.45
2:I:2004:GLU:HA	2:I:2007:ASN:HD22	1.82	0.45
2:B:403:MET:O	2:B:407:THR:N	2.50	0.45
2:B:765:GLN:NE2	2:B:1521:UNK:O	2.49	0.45
2:G:4767:TRP:HE3	2:G:4770:SER:HB2	1.80	0.45
2:E:551:LEU:HD21	2:E:589:LEU:HD13	1.98	0.45
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	1.97	0.45
2:E:4655:PHE:HA	2:E:4796:MET:HE1	1.99	0.45
2:I:4657:CYS:HB3	2:I:4792:LEU:HD11	1.99	0.45
2:B:551:LEU:HD21	2:B:589:LEU:HD13	1.98	0.45
2:B:645:ARG:HH11	2:B:778:PHE:HE1	1.64	0.45
2:B:2004:GLU:HA	2:B:2007:ASN:HD22	1.82	0.45
2:G:645:ARG:HH11	2:G:778:PHE:HE1	1.64	0.45
2:G:2004:GLU:HA	2:G:2007:ASN:HD22	1.82	0.45
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	1.97	0.45
2:E:2753:SER:O	2:E:2757:LYS:N	2.48	0.45
2:E:3365:UNK:O	2:E:3369:UNK:N	2.49	0.45
2:I:1078:GLU:HG3	2:I:1237:TRP:HE1	1.81	0.45
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.97	0.45
2:B:132:ALA:HA	2:B:194:SER:HB2	1.98	0.45
2:B:698:GLY:HA2	2:B:703:GLY:HA2	1.98	0.45
2:G:551:LEU:HD21	2:G:589:LEU:HD13	1.98	0.45
2:G:1078:GLU:HG3	2:G:1237:TRP:HE1	1.81	0.45
2:G:1457:UNK:N	2:G:1497:UNK:O	2.50	0.45
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	1.98	0.45
2:B:4657:CYS:HB3	2:B:4792:LEU:HD11	1.99	0.45
2:E:132:ALA:HA	2:E:194:SER:HB2	1.98	0.45
2:I:1812:LEU:HD21	2:I:1861:GLN:HG2	1.97	0.45
2:I:4925:ILE:HA	2:I:4929:LEU:HD23	1.99	0.45
2:B:3365:UNK:O	2:B:3369:UNK:N	2.49	0.45
2:G:3756:LYS:HA	2:G:3759:GLU:HG2	1.99	0.45
2:G:3992:PHE:O	2:G:3996:PHE:N	2.41	0.45
2:G:4655:PHE:HA	2:G:4796:MET:HE1	1.99	0.45
2:E:4558:ASN:OD1	2:E:4558:ASN:N	2.50	0.45
2:I:3365:UNK:O	2:I:3369:UNK:N	2.49	0.45
1:F:35:LYS:HD3	2:E:636:ASN:HD21	1.82	0.45
2:B:379:HIS:CD2	2:B:381:GLU:H	2.35	0.45
2:G:4848:VAL:O	2:G:4852:THR:OG1	2.32	0.45
2:E:4142:ASN:HA	2:E:4145:VAL:HG12	1.99	0.45
2:B:886:ARG:HB3	2:B:891:TRP:HB2	2.00	0.44
2:B:2753:SER:O	2:B:2757:LYS:N	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2004:GLU:HA	2:E:2007:ASN:HD22	1.82	0.44
2:E:4925:ILE:HA	2:E:4929:LEU:HD23	1.99	0.44
2:I:45:ARG:HG2	2:I:443:LEU:HD21	1.99	0.44
2:I:1171:SER:OG	2:I:1175:SER:N	2.42	0.44
2:I:4142:ASN:HA	2:I:4145:VAL:HG12	1.99	0.44
2:B:4142:ASN:HA	2:B:4145:VAL:HG12	1.99	0.44
2:G:978:THR:HB	2:G:980:ALA:H	1.82	0.44
2:G:4142:ASN:HA	2:G:4145:VAL:HG12	1.99	0.44
2:E:346:CYS:N	2:E:388:LEU:O	2.50	0.44
2:E:4229:GLU:HA	2:E:4232:GLU:HB3	2.00	0.44
2:I:143:GLY:HA3	2:I:147:TRP:HE1	1.82	0.44
2:B:346:CYS:N	2:B:388:LEU:O	2.50	0.44
2:G:2880:GLU:O	2:G:2884:ASN:N	2.46	0.44
2:E:379:HIS:CD2	2:E:381:GLU:H	2.35	0.44
2:E:698:GLY:HA2	2:E:703:GLY:HA2	1.98	0.44
2:E:886:ARG:HB3	2:E:891:TRP:HB2	2.00	0.44
2:E:1457:UNK:N	2:E:1497:UNK:O	2.50	0.44
2:I:1457:UNK:N	2:I:1497:UNK:O	2.50	0.44
2:I:3676:ASP:OD1	2:I:3676:ASP:N	2.50	0.44
2:B:1973:GLN:HA	2:B:1976:ARG:HB3	2.00	0.44
2:B:4227:GLU:HG3	2:B:4228:ALA:H	1.82	0.44
2:B:4655:PHE:HA	2:B:4796:MET:HE1	1.99	0.44
2:G:4657:CYS:HB3	2:G:4792:LEU:HD11	1.99	0.44
2:E:978:THR:HB	2:E:980:ALA:H	1.82	0.44
2:I:403:MET:O	2:I:407:THR:N	2.50	0.44
2:I:579:GLN:H	2:I:582:HIS:HD2	1.66	0.44
2:B:1457:UNK:N	2:B:1497:UNK:O	2.50	0.44
2:B:3676:ASP:OD1	2:B:3676:ASP:N	2.50	0.44
2:B:4229:GLU:HA	2:B:4232:GLU:HB3	2.00	0.44
2:E:220:LEU:O	2:E:260:TRP:N	2.50	0.44
2:E:645:ARG:HH11	2:E:778:PHE:HE1	1.64	0.44
2:I:218:HIS:HB3	2:I:392:ARG:HD3	2.00	0.44
2:I:379:HIS:CD2	2:I:381:GLU:H	2.35	0.44
2:I:470:SER:O	2:I:474:ARG:NE	2.43	0.44
2:I:2226:PRO:HA	2:I:2229:VAL:HG12	2.00	0.44
2:I:4227:GLU:HG3	2:I:4228:ALA:H	1.82	0.44
2:B:1972:ASN:O	2:B:1976:ARG:N	2.49	0.44
2:B:4925:ILE:HA	2:B:4929:LEU:HD23	1.99	0.44
2:I:551:LEU:HD21	2:I:589:LEU:HD13	1.98	0.44
2:I:2880:GLU:O	2:I:2884:ASN:N	2.47	0.44
2:I:4826:ILE:O	2:I:4829:SER:OG	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4886:HIS:O	2:I:4890:GLY:N	2.46	0.44
1:A:77:THR:OG1	1:A:79:ASP:OD1	2.35	0.44
2:B:978:THR:HB	2:B:980:ALA:H	1.82	0.44
2:B:2208:MET:HE1	2:B:2253:HIS:HB3	2.00	0.44
2:G:143:GLY:HA3	2:G:147:TRP:HE1	1.82	0.44
2:G:2226:PRO:HA	2:G:2229:VAL:HG12	2.00	0.44
2:G:3676:ASP:OD1	2:G:3676:ASP:N	2.50	0.44
2:G:4925:ILE:HA	2:G:4929:LEU:HD23	1.99	0.44
2:E:3729:MET:O	2:E:3732:SER:OG	2.34	0.44
2:I:606:LEU:HG	2:I:617:ASN:HD22	1.82	0.44
2:I:1760:HIS:CE1	2:I:2041:HIS:HA	2.53	0.44
2:I:3756:LYS:HA	2:I:3759:GLU:HG2	1.99	0.44
2:B:143:GLY:HA3	2:B:147:TRP:HE1	1.82	0.44
2:G:379:HIS:CD2	2:G:381:GLU:H	2.35	0.44
2:G:886:ARG:HB3	2:G:891:TRP:HB2	2.00	0.44
2:G:3729:MET:O	2:G:3732:SER:OG	2.34	0.44
2:E:1171:SER:HG	2:E:1175:SER:H	1.65	0.44
2:I:4763:GLY:O	2:I:4766:THR:OG1	2.34	0.44
2:B:3850:GLN:HA	2:B:3853:ALA:HB3	2.00	0.44
2:B:4558:ASN:OD1	2:B:4558:ASN:N	2.50	0.44
2:B:4886:HIS:O	2:B:4890:GLY:N	2.46	0.44
2:G:346:CYS:N	2:G:388:LEU:O	2.50	0.44
2:G:606:LEU:HG	2:G:617:ASN:HD22	1.82	0.44
2:G:4227:GLU:HG3	2:G:4228:ALA:H	1.82	0.44
2:E:143:GLY:HA3	2:E:147:TRP:HE1	1.82	0.44
2:I:1973:GLN:HA	2:I:1976:ARG:HB3	2.00	0.44
2:I:4229:GLU:HA	2:I:4232:GLU:HB3	2.00	0.44
2:G:218:HIS:HB3	2:G:392:ARG:HD3	2.00	0.43
2:G:220:LEU:O	2:G:260:TRP:N	2.50	0.43
2:E:243:ARG:NH1	2:E:301:VAL:O	2.46	0.43
2:E:403:MET:O	2:E:407:THR:N	2.50	0.43
2:E:3756:LYS:HA	2:E:3759:GLU:HG2	1.99	0.43
2:I:886:ARG:HB3	2:I:891:TRP:HB2	2.00	0.43
2:B:278:GLN:N	2:B:315:CYS:SG	2.91	0.43
2:B:1760:HIS:CE1	2:B:2041:HIS:HA	2.53	0.43
2:G:451:TYR:O	2:G:474:ARG:NH1	2.45	0.43
2:G:579:GLN:H	2:G:582:HIS:HD2	1.66	0.43
2:G:718:GLY:HA3	2:G:737:LEU:HA	2.01	0.43
2:E:606:LEU:HG	2:E:617:ASN:HD22	1.82	0.43
2:E:4227:GLU:HG3	2:E:4228:ALA:H	1.82	0.43
2:E:4657:CYS:HB3	2:E:4792:LEU:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:346:CYS:N	2:I:388:LEU:O	2.50	0.43
2:B:218:HIS:HB3	2:B:392:ARG:HD3	2.00	0.43
2:B:718:GLY:HA3	2:B:737:LEU:HA	2.01	0.43
2:B:3756:LYS:HA	2:B:3759:GLU:HG2	1.99	0.43
2:G:243:ARG:NH1	2:G:301:VAL:O	2.46	0.43
2:G:915:GLU:O	2:G:919:ASN:ND2	2.51	0.43
2:G:2208:MET:HE1	2:G:2253:HIS:HB3	2.00	0.43
2:G:3362:UNK:O	2:G:3366:UNK:N	2.52	0.43
2:G:4229:GLU:HA	2:G:4232:GLU:HB3	2.00	0.43
2:E:530:ILE:HD13	2:E:536:ASN:HB3	2.01	0.43
2:E:3362:UNK:O	2:E:3366:UNK:N	2.52	0.43
2:I:4655:PHE:HA	2:I:4796:MET:HE1	1.99	0.43
2:B:4586:PRO:HB3	2:B:4628:VAL:HG21	2.01	0.43
2:G:1972:ASN:O	2:G:1976:ARG:N	2.49	0.43
2:G:4941:GLY:C	2:I:4944:ARG:HH12	2.26	0.43
2:E:959:TYR:HB3	2:E:967:PRO:HD2	2.01	0.43
2:I:907:LEU:O	2:I:963:ASN:ND2	2.39	0.43
2:G:530:ILE:HD13	2:G:536:ASN:HB3	2.01	0.43
2:E:2208:MET:HE1	2:E:2253:HIS:HB3	2.00	0.43
2:E:3850:GLN:HA	2:E:3853:ALA:HB3	2.00	0.43
2:I:2095:GLN:NE2	2:I:2127:GLN:O	2.50	0.43
2:I:4586:PRO:HB3	2:I:4628:VAL:HG21	2.01	0.43
2:B:579:GLN:H	2:B:582:HIS:HD2	1.66	0.43
2:G:1973:GLN:HA	2:G:1976:ARG:HB3	2.00	0.43
2:G:4586:PRO:HB3	2:G:4628:VAL:HG21	2.01	0.43
2:G:4944:ARG:HH12	2:E:4941:GLY:C	2.27	0.43
2:E:345:LEU:HD22	2:E:387:ALA:HB1	2.01	0.43
2:E:915:GLU:O	2:E:919:ASN:ND2	2.51	0.43
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	2.01	0.43
2:E:4886:HIS:O	2:E:4890:GLY:N	2.46	0.43
2:I:978:THR:HB	2:I:980:ALA:H	1.82	0.43
2:B:309:THR:O	2:B:313:SER:OG	2.37	0.43
2:B:2226:PRO:HA	2:B:2229:VAL:HG12	2.00	0.43
2:B:4712:PRO:HG2	2:B:4718:LYS:HG2	2.01	0.43
2:G:3850:GLN:HA	2:G:3853:ALA:HB3	2.00	0.43
2:E:718:GLY:HA3	2:E:737:LEU:HA	2.01	0.43
2:E:1760:HIS:CE1	2:E:2041:HIS:HA	2.53	0.43
2:I:580:GLU:HG3	2:I:620:LEU:HD22	2.01	0.43
2:I:2208:MET:HE1	2:I:2253:HIS:HB3	2.00	0.43
2:I:2271:THR:HG22	2:I:2273:LEU:H	1.83	0.43
2:I:3362:UNK:O	2:I:3366:UNK:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:45:ARG:HG2	2:B:443:LEU:HD21	1.99	0.43
2:B:134:ASP:OD1	2:B:134:ASP:N	2.48	0.43
2:B:915:GLU:O	2:B:919:ASN:ND2	2.51	0.43
2:G:45:ARG:HG2	2:G:443:LEU:HD21	1.99	0.43
2:E:45:ARG:HG2	2:E:443:LEU:HD21	2.00	0.43
2:E:62:LEU:O	2:E:261:ARG:NH2	2.52	0.43
2:E:218:HIS:HB3	2:E:392:ARG:HD3	2.00	0.43
2:E:470:SER:O	2:E:474:ARG:NE	2.43	0.43
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.83	0.43
2:I:111:HIS:HD2	2:I:114:SER:H	1.66	0.43
2:I:195:PHE:HB3	2:I:196:MET:HG2	2.01	0.43
2:I:530:ILE:HD13	2:I:536:ASN:HB3	2.01	0.43
2:I:718:GLY:HA3	2:I:737:LEU:HA	2.01	0.43
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	2.01	0.43
2:B:21:VAL:HG12	2:B:66:CYS:HA	2.00	0.43
2:B:345:LEU:HD22	2:B:387:ALA:HB1	2.01	0.43
2:B:530:ILE:HD13	2:B:536:ASN:HB3	2.01	0.43
2:B:898:ASP:HB3	2:B:901:LYS:HB2	2.01	0.43
2:B:2102:VAL:HB	2:B:2124:LEU:HD12	2.00	0.43
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.83	0.43
2:B:2880:GLU:O	2:B:2884:ASN:N	2.46	0.43
2:G:309:THR:O	2:G:313:SER:OG	2.37	0.43
2:G:403:MET:O	2:G:407:THR:N	2.50	0.43
2:G:1760:HIS:CE1	2:G:2041:HIS:HA	2.53	0.43
2:G:2095:GLN:NE2	2:G:2127:GLN:O	2.50	0.43
2:E:195:PHE:HB3	2:E:196:MET:HG2	2.01	0.43
2:E:2226:PRO:HA	2:E:2229:VAL:HG12	2.00	0.43
2:I:1972:ASN:O	2:I:1976:ARG:N	2.49	0.43
2:G:345:LEU:HD22	2:G:387:ALA:HB1	2.01	0.43
2:I:932:LEU:HA	2:I:935:LEU:HD12	2.01	0.43
2:I:4712:PRO:HG2	2:I:4718:LYS:HG2	2.01	0.43
2:B:111:HIS:HD2	2:B:114:SER:H	1.66	0.42
2:B:734:GLY:O	2:B:736:HIS:ND1	2.52	0.42
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	2.01	0.42
2:B:4763:GLY:O	2:B:4766:THR:OG1	2.34	0.42
2:G:4712:PRO:HG2	2:G:4718:LYS:HG2	2.01	0.42
2:G:4826:ILE:O	2:G:4829:SER:OG	2.32	0.42
2:E:309:THR:O	2:E:313:SER:OG	2.37	0.42
2:E:579:GLN:H	2:E:582:HIS:HD2	1.66	0.42
2:I:793:LEU:HD22	2:I:821:LEU:HD13	2.01	0.42
2:I:915:GLU:O	2:I:919:ASN:ND2	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:195:PHE:HB3	2:G:196:MET:HG2	2.01	0.42
2:G:959:TYR:HB3	2:G:967:PRO:HD2	2.01	0.42
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	2.01	0.42
2:E:103:TYR:HB3	2:E:152:PRO:HD3	2.01	0.42
2:E:111:HIS:HD2	2:E:114:SER:H	1.66	0.42
2:E:1931:LEU:HB3	2:E:1935:VAL:HB	2.02	0.42
2:E:2143:THR:O	2:E:3651:ASN:ND2	2.44	0.42
2:E:4586:PRO:HB3	2:E:4628:VAL:HG21	2.01	0.42
2:I:3850:GLN:HA	2:I:3853:ALA:HB3	2.00	0.42
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	2.01	0.42
2:G:940:GLY:O	2:G:1052:ASN:N	2.50	0.42
2:G:1931:LEU:HB3	2:G:1935:VAL:HB	2.02	0.42
2:E:580:GLU:HG3	2:E:620:LEU:HD22	2.01	0.42
2:I:309:THR:O	2:I:313:SER:OG	2.37	0.42
2:I:898:ASP:HB3	2:I:901:LYS:HB2	2.01	0.42
2:B:959:TYR:HB3	2:B:967:PRO:HD2	2.01	0.42
2:G:62:LEU:O	2:G:261:ARG:NH2	2.52	0.42
2:G:2102:VAL:HB	2:G:2124:LEU:HD12	2.00	0.42
2:E:793:LEU:HD12	2:E:797:HIS:HB2	2.02	0.42
2:B:62:LEU:O	2:B:261:ARG:NH2	2.52	0.42
2:B:220:LEU:O	2:B:260:TRP:N	2.50	0.42
2:B:580:GLU:HG3	2:B:620:LEU:HD22	2.01	0.42
2:B:606:LEU:HG	2:B:617:ASN:HD22	1.82	0.42
2:B:1171:SER:OG	2:B:1175:SER:N	2.42	0.42
2:E:21:VAL:HG12	2:E:66:CYS:HA	2.00	0.42
2:E:932:LEU:HA	2:E:935:LEU:HD12	2.01	0.42
2:E:4712:PRO:HG2	2:E:4718:LYS:HG2	2.01	0.42
2:I:21:VAL:HG12	2:I:66:CYS:HA	2.00	0.42
2:I:123:THR:OG1	2:I:134:ASP:OD1	2.38	0.42
2:I:3992:PHE:O	2:I:3996:PHE:N	2.41	0.42
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	2.01	0.42
2:G:4558:ASN:OD1	2:G:4558:ASN:N	2.50	0.42
2:E:451:TYR:O	2:E:474:ARG:NH1	2.45	0.42
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	2.01	0.42
1:F:34:LYS:HD3	2:E:629:ARG:HD2	2.01	0.42
2:B:195:PHE:HB3	2:B:196:MET:HG2	2.01	0.42
2:B:793:LEU:HD22	2:B:821:LEU:HD13	2.01	0.42
2:B:3362:UNK:O	2:B:3366:UNK:N	2.52	0.42
2:G:103:TYR:HB3	2:G:152:PRO:HD3	2.01	0.42
2:E:1973:GLN:HA	2:E:1976:ARG:HB3	2.00	0.42
2:I:261:ARG:HB3	2:I:283:ARG:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2102:VAL:HB	2:I:2124:LEU:HD12	2.00	0.42
2:B:932:LEU:HA	2:B:935:LEU:HD12	2.01	0.42
2:G:2753:SER:O	2:G:2757:LYS:N	2.48	0.42
2:G:4101:LYS:HD3	2:G:4101:LYS:HA	1.86	0.42
2:E:898:ASP:HB3	2:E:901:LYS:HB2	2.01	0.42
2:E:3676:ASP:N	2:E:3676:ASP:OD1	2.50	0.42
2:I:2753:SER:O	2:I:2757:LYS:N	2.48	0.42
2:B:649:PHE:HB3	2:B:776:LEU:HB3	2.02	0.42
2:B:1665:HIS:HA	2:B:1668:ARG:HG2	2.02	0.42
2:G:580:GLU:HG3	2:G:620:LEU:HD22	2.01	0.42
2:G:870:ILE:HD12	2:G:870:ILE:HA	1.95	0.42
2:E:123:THR:OG1	2:E:134:ASP:OD1	2.38	0.42
2:E:793:LEU:HD22	2:E:821:LEU:HD13	2.01	0.42
2:I:62:LEU:O	2:I:261:ARG:NH2	2.52	0.42
2:I:220:LEU:O	2:I:260:TRP:N	2.50	0.42
2:I:940:GLY:O	2:I:1052:ASN:N	2.50	0.42
2:B:23:GLN:HB3	2:B:201:ASN:HB2	2.02	0.42
2:B:1723:ALA:HB1	2:B:1775:HIS:HD2	1.85	0.42
2:G:21:VAL:HG12	2:G:66:CYS:HA	2.00	0.42
2:G:472:ARG:NH2	2:G:3712:GLU:OE2	2.53	0.42
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.83	0.42
2:E:23:GLN:HB3	2:E:201:ASN:HB2	2.02	0.42
2:I:345:LEU:HD22	2:I:387:ALA:HB1	2.01	0.42
2:I:1665:HIS:HA	2:I:1668:ARG:HG2	2.02	0.42
2:I:4056:GLU:HG2	2:I:4166:LEU:HD23	2.02	0.42
2:I:4558:ASN:OD1	2:I:4558:ASN:N	2.50	0.42
2:B:583:ILE:H	2:B:583:ILE:HG13	1.70	0.41
2:B:880:GLU:OE1	2:B:968:ALA:N	2.43	0.41
2:B:4056:GLU:HG2	2:B:4166:LEU:HD23	2.02	0.41
2:G:470:SER:O	2:G:474:ARG:NE	2.43	0.41
2:E:2102:VAL:HB	2:E:2124:LEU:HD12	2.00	0.41
2:I:670:GLU:HG3	2:I:787:VAL:HG13	2.03	0.41
2:B:793:LEU:HD12	2:B:797:HIS:HB2	2.01	0.41
2:B:914:PRO:HD2	2:B:917:GLU:HB2	2.02	0.41
2:B:940:GLY:O	2:B:1052:ASN:N	2.50	0.41
2:G:23:GLN:HB3	2:G:201:ASN:HB2	2.02	0.41
2:G:123:THR:OG1	2:G:134:ASP:OD1	2.38	0.41
2:E:472:ARG:NH2	2:E:3712:GLU:OE2	2.53	0.41
2:E:914:PRO:HD2	2:E:917:GLU:HB2	2.02	0.41
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	2.01	0.41
2:E:1723:ALA:HB1	2:E:1775:HIS:HD2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:243:ARG:NH1	2:I:301:VAL:O	2.46	0.41
2:I:959:TYR:HB3	2:I:967:PRO:HD2	2.01	0.41
2:I:4639:MET:HE2	2:I:4639:MET:HB3	1.96	0.41
2:G:793:LEU:HD12	2:G:797:HIS:HB2	2.01	0.41
2:G:898:ASP:HB3	2:G:901:LYS:HB2	2.01	0.41
2:E:649:PHE:HB3	2:E:776:LEU:HB3	2.02	0.41
2:E:983:THR:O	2:E:987:ARG:N	2.52	0.41
2:I:793:LEU:HD12	2:I:797:HIS:HB2	2.01	0.41
2:I:1931:LEU:HB3	2:I:1935:VAL:HB	2.02	0.41
2:B:103:TYR:HB3	2:B:152:PRO:HD3	2.01	0.41
2:B:1931:LEU:HB3	2:B:1935:VAL:HB	2.02	0.41
2:G:793:LEU:HD22	2:G:821:LEU:HD13	2.01	0.41
2:G:2155:LEU:HD21	2:G:2198:MET:HE1	2.03	0.41
2:E:2868:SER:O	2:E:2872:GLN:N	2.39	0.41
2:I:1676:LEU:HD23	2:I:2167:ILE:HG23	2.03	0.41
2:I:1735:ILE:HG23	2:I:1771:LEU:HB2	2.02	0.41
2:B:261:ARG:HB3	2:B:283:ARG:HB3	2.02	0.41
2:B:1676:LEU:HD23	2:B:2167:ILE:HG23	2.03	0.41
2:G:1665:HIS:HA	2:G:1668:ARG:HG2	2.02	0.41
2:G:1723:ALA:HB1	2:G:1775:HIS:HD2	1.85	0.41
2:G:2874:MET:O	2:G:2878:LEU:N	2.43	0.41
2:G:4056:GLU:HG2	2:G:4166:LEU:HD23	2.02	0.41
2:E:1665:HIS:HA	2:E:1668:ARG:HG2	2.02	0.41
2:E:1972:ASN:O	2:E:1976:ARG:N	2.49	0.41
2:E:4056:GLU:HG2	2:E:4166:LEU:HD23	2.02	0.41
1:J:87:HIS:HA	1:J:88:PRO:HD3	1.90	0.41
2:G:111:HIS:HD2	2:G:114:SER:H	1.66	0.41
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.53	0.41
2:I:1723:ALA:HB1	2:I:1775:HIS:HD2	1.85	0.41
2:I:3816:MET:HE3	2:I:3816:MET:HB2	2.00	0.41
2:B:2862:LEU:HB3	2:B:2928:LYS:HB3	2.03	0.41
2:G:261:ARG:HB3	2:G:283:ARG:HB3	2.02	0.41
2:G:670:GLU:HG3	2:G:787:VAL:HG13	2.03	0.41
2:G:4639:MET:HE2	2:G:4639:MET:HB3	1.96	0.41
2:E:734:GLY:O	2:E:736:HIS:ND1	2.52	0.41
2:G:932:LEU:HA	2:G:935:LEU:HD12	2.01	0.41
2:G:1735:ILE:HG23	2:G:1771:LEU:HB2	2.02	0.41
2:G:1865:MET:N	2:G:1865:MET:SD	2.94	0.41
2:G:2022:PRO:HB2	2:G:2024:PRO:HD2	2.03	0.41
2:G:4860:ARG:HG3	2:G:4876:CYS:HB3	2.03	0.41
2:E:1676:LEU:HD23	2:E:2167:ILE:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1735:ILE:HG23	2:E:1771:LEU:HB2	2.02	0.41
2:I:103:TYR:HB3	2:I:152:PRO:HD3	2.01	0.41
2:I:451:TYR:O	2:I:474:ARG:NH1	2.45	0.41
2:I:914:PRO:HD2	2:I:917:GLU:HB2	2.02	0.41
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.53	0.41
2:B:2095:GLN:NE2	2:B:2127:GLN:O	2.50	0.41
2:G:939:VAL:HG22	2:G:1053:ILE:HG12	2.03	0.41
2:G:2674:UNK:O	2:G:2676:UNK:N	2.54	0.41
2:E:2862:LEU:HB3	2:E:2928:LYS:HB3	2.03	0.41
2:E:3889:GLN:HG3	2:E:3967:GLU:HG3	2.03	0.41
2:E:4005:GLN:HE21	2:E:4110:PHE:HE1	1.69	0.41
2:I:734:GLY:O	2:I:736:HIS:ND1	2.52	0.41
2:I:2155:LEU:HD21	2:I:2198:MET:HE1	2.03	0.41
2:I:2674:UNK:O	2:I:2676:UNK:N	2.54	0.41
2:I:2868:SER:O	2:I:2872:GLN:N	2.39	0.41
2:B:123:THR:OG1	2:B:134:ASP:OD1	2.38	0.41
2:G:256:ALA:HB1	2:G:286:THR:HG21	2.03	0.41
2:G:2868:SER:O	2:G:2872:GLN:N	2.39	0.41
2:G:3733:CYS:HB2	2:G:3803:SER:HB3	2.03	0.41
2:E:2022:PRO:HB2	2:E:2024:PRO:HD2	2.03	0.41
2:E:3722:TYR:CZ	2:E:3782:MET:HE3	2.56	0.41
2:I:278:GLN:N	2:I:315:CYS:SG	2.91	0.41
2:I:1865:MET:SD	2:I:1865:MET:N	2.94	0.41
2:I:2022:PRO:HB2	2:I:2024:PRO:HD2	2.03	0.41
2:I:4848:VAL:O	2:I:4852:THR:OG1	2.32	0.41
2:I:4860:ARG:HG3	2:I:4876:CYS:HB3	2.03	0.41
2:B:2022:PRO:HB2	2:B:2024:PRO:HD2	2.03	0.40
2:B:4860:ARG:HG3	2:B:4876:CYS:HB3	2.03	0.40
2:G:649:PHE:HB3	2:G:776:LEU:HB3	2.02	0.40
2:G:914:PRO:HD2	2:G:917:GLU:HB2	2.02	0.40
2:G:2143:THR:O	2:G:3651:ASN:ND2	2.44	0.40
2:I:23:GLN:HB3	2:I:201:ASN:HB2	2.02	0.40
2:I:500:ALA:HB1	2:I:504:ALA:HB2	2.03	0.40
2:B:57:ASN:HD22	2:B:308:HIS:HB2	1.87	0.40
2:B:359:TYR:HA	2:B:376:ALA:HA	2.03	0.40
2:B:1865:MET:SD	2:B:1865:MET:N	2.94	0.40
2:B:2674:UNK:O	2:B:2676:UNK:N	2.54	0.40
2:B:3889:GLN:HG3	2:B:3967:GLU:HG3	2.03	0.40
2:G:1671:ARG:NH2	2:G:1713:ASP:HB3	2.36	0.40
2:G:1676:LEU:HD23	2:G:2167:ILE:HG23	2.03	0.40
2:G:4886:HIS:O	2:G:4890:GLY:N	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:57:ASN:HD22	2:E:308:HIS:HB2	1.87	0.40
2:E:670:GLU:HG3	2:E:787:VAL:HG13	2.03	0.40
2:E:1671:ARG:NH2	2:E:1713:ASP:HB3	2.36	0.40
2:E:2155:LEU:HD21	2:E:2198:MET:HE1	2.02	0.40
2:E:2880:GLU:O	2:E:2884:ASN:N	2.47	0.40
2:I:1671:ARG:NH2	2:I:1713:ASP:HB3	2.36	0.40
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.54	0.40
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.86	0.40
2:B:1671:ARG:NH2	2:B:1713:ASP:HB3	2.36	0.40
2:B:4848:VAL:O	2:B:4852:THR:OG1	2.32	0.40
2:G:57:ASN:HD22	2:G:308:HIS:HB2	1.87	0.40
2:I:256:ALA:HB1	2:I:286:THR:HG21	2.03	0.40
2:I:983:THR:O	2:I:987:ARG:N	2.52	0.40
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.86	0.40
2:I:3729:MET:O	2:I:3732:SER:OG	2.34	0.40
2:B:256:ALA:HB1	2:B:286:THR:HG21	2.03	0.40
2:G:1641:ILE:HA	2:G:1642:PRO:HD3	1.90	0.40
2:G:4929:LEU:HD13	2:G:4929:LEU:HA	1.95	0.40
2:E:870:ILE:HD12	2:E:873:LYS:HB2	2.04	0.40
2:B:451:TYR:O	2:B:474:ARG:NH1	2.45	0.40
2:B:939:VAL:HG22	2:B:1053:ILE:HG12	2.03	0.40
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.54	0.40
2:B:2318:TYR:HA	2:B:2319:PRO:HD3	1.94	0.40
2:G:734:GLY:O	2:G:736:HIS:ND1	2.52	0.40
2:E:261:ARG:HB3	2:E:283:ARG:HB3	2.02	0.40
2:I:57:ASN:HD22	2:I:308:HIS:HB2	1.87	0.40
2:I:116:MET:HB2	2:I:137:LEU:HD12	2.04	0.40
2:I:649:PHE:HB3	2:I:776:LEU:HB3	2.02	0.40
2:I:3733:CYS:HB2	2:I:3803:SER:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
1	F	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
1	H	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
1	J	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
2	B	3235/4416 (73%)	2874 (89%)	357 (11%)	4 (0%)	48	83
2	E	3235/4416 (73%)	2873 (89%)	358 (11%)	4 (0%)	48	83
2	G	3235/4416 (73%)	2875 (89%)	356 (11%)	4 (0%)	48	83
2	I	3235/4416 (73%)	2873 (89%)	358 (11%)	4 (0%)	48	83
All	All	13360/18096 (74%)	11875 (89%)	1469 (11%)	16 (0%)	49	83

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	G	1708	ARG
2	E	1708	ARG
2	I	1708	ARG
2	B	1932	PRO
2	G	1932	PRO
2	E	1932	PRO
2	I	1932	PRO
2	B	1840	PRO
2	B	4641	PRO
2	G	1840	PRO
2	G	4641	PRO
2	E	1840	PRO
2	E	4641	PRO
2	I	1840	PRO
2	I	4641	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	88/89 (99%)	88 (100%)	0	100	100
1	F	88/89 (99%)	88 (100%)	0	100	100
1	H	88/89 (99%)	88 (100%)	0	100	100
1	J	88/89 (99%)	88 (100%)	0	100	100
2	B	2493/3022 (82%)	2480 (100%)	13 (0%)	81	81
2	E	2493/3022 (82%)	2480 (100%)	13 (0%)	81	81
2	G	2493/3022 (82%)	2480 (100%)	13 (0%)	81	81
2	I	2493/3022 (82%)	2480 (100%)	13 (0%)	81	81
All	All	10324/12444 (83%)	10272 (100%)	52 (0%)	78	81

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	131	LEU
2	B	309	THR
2	B	719	LEU
2	B	1600	LEU
2	B	1676	LEU
2	B	2010	LEU
2	B	2339	VAL
2	B	3805	LEU
2	B	4154	VAL
2	B	4792	LEU
2	B	4929	LEU
2	B	4983	HIS
2	B	4985	LEU
2	G	131	LEU
2	G	309	THR
2	G	719	LEU
2	G	1600	LEU
2	G	1676	LEU
2	G	2010	LEU
2	G	2339	VAL
2	G	3805	LEU
2	G	4154	VAL
2	G	4792	LEU
2	G	4929	LEU
2	G	4983	HIS
2	G	4985	LEU
2	E	131	LEU

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Mol	Chain	Res	Type
2	E	309	THR
2	E	719	LEU
2	E	1600	LEU
2	E	1676	LEU
2	E	2010	LEU
2	E	2339	VAL
2	E	3805	LEU
2	E	4154	VAL
2	E	4792	LEU
2	E	4929	LEU
2	E	4983	HIS
2	E	4985	LEU
2	I	131	LEU
2	I	309	THR
2	I	719	LEU
2	I	1600	LEU
2	I	1676	LEU
2	I	2010	LEU
2	I	2339	VAL
2	I	3805	LEU
2	I	4154	VAL
2	I	4792	LEU
2	I	4929	LEU
2	I	4983	HIS
2	I	4985	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (207) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	32	ASN
1	F	87	HIS
1	A	32	ASN
1	A	87	HIS
1	H	32	ASN
1	H	87	HIS
1	J	32	ASN
1	J	87	HIS
2	B	57	ASN
2	B	111	HIS
2	B	151	HIS
2	B	201	ASN
2	B	273	HIS

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Mol	Chain	Res	Type
2	B	284	HIS
2	B	379	HIS
2	B	479	GLN
2	B	489	ASN
2	B	582	HIS
2	B	725	HIS
2	B	838	HIS
2	B	919	ASN
2	B	1220	GLN
2	B	1229	ASN
2	B	1598	GLN
2	B	1611	HIS
2	B	1679	ASN
2	B	1688	HIS
2	B	1691	GLN
2	B	1693	GLN
2	B	1719	HIS
2	B	1775	HIS
2	B	1861	GLN
2	B	1973	GLN
2	B	2100	HIS
2	B	2127	GLN
2	B	2194	HIS
2	B	2260	ASN
2	B	2772	GLN
2	B	2788	HIS
2	B	2856	ASN
2	B	3767	GLN
2	B	3809	ASN
2	B	3814	GLN
2	B	3896	ASN
2	B	3960	GLN
2	B	3976	ASN
2	B	3994	HIS
2	B	3998	HIS
2	B	4005	GLN
2	B	4034	ASN
2	B	4054	ASN
2	B	4120	ASN
2	B	4130	ASN
2	B	4553	ASN
2	B	4707	ASN

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Mol	Chain	Res	Type
2	B	4806	ASN
2	B	4949	GLN
2	G	57	ASN
2	G	111	HIS
2	G	151	HIS
2	G	201	ASN
2	G	273	HIS
2	G	284	HIS
2	G	379	HIS
2	G	395	GLN
2	G	479	GLN
2	G	489	ASN
2	G	582	HIS
2	G	725	HIS
2	G	765	GLN
2	G	838	HIS
2	G	919	ASN
2	G	1220	GLN
2	G	1598	GLN
2	G	1679	ASN
2	G	1688	HIS
2	G	1691	GLN
2	G	1693	GLN
2	G	1719	HIS
2	G	1775	HIS
2	G	1861	GLN
2	G	1973	GLN
2	G	2100	HIS
2	G	2127	GLN
2	G	2194	HIS
2	G	2260	ASN
2	G	2772	GLN
2	G	2773	ASN
2	G	2788	HIS
2	G	2856	ASN
2	G	3767	GLN
2	G	3809	ASN
2	G	3814	GLN
2	G	3889	GLN
2	G	3896	ASN
2	G	3960	GLN
2	G	3976	ASN

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Mol	Chain	Res	Type
2	G	3994	HIS
2	G	3998	HIS
2	G	4034	ASN
2	G	4054	ASN
2	G	4120	ASN
2	G	4130	ASN
2	G	4553	ASN
2	G	4707	ASN
2	G	4806	ASN
2	G	4946	GLN
2	G	4949	GLN
2	E	57	ASN
2	E	111	HIS
2	E	151	HIS
2	E	201	ASN
2	E	273	HIS
2	E	284	HIS
2	E	379	HIS
2	E	395	GLN
2	E	461	HIS
2	E	479	GLN
2	E	489	ASN
2	E	582	HIS
2	E	725	HIS
2	E	765	GLN
2	E	838	HIS
2	E	919	ASN
2	E	1158	ASN
2	E	1220	GLN
2	E	1598	GLN
2	E	1679	ASN
2	E	1688	HIS
2	E	1691	GLN
2	E	1693	GLN
2	E	1719	HIS
2	E	1775	HIS
2	E	1861	GLN
2	E	1973	GLN
2	E	2100	HIS
2	E	2127	GLN
2	E	2194	HIS
2	E	2260	ASN

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Mol	Chain	Res	Type
2	E	2788	HIS
2	E	2856	ASN
2	E	3767	GLN
2	E	3809	ASN
2	E	3814	GLN
2	E	3889	GLN
2	E	3896	ASN
2	E	3960	GLN
2	E	3976	ASN
2	E	3994	HIS
2	E	3998	HIS
2	E	4005	GLN
2	E	4034	ASN
2	E	4054	ASN
2	E	4120	ASN
2	E	4553	ASN
2	E	4707	ASN
2	E	4806	ASN
2	E	4946	GLN
2	E	4949	GLN
2	I	57	ASN
2	I	111	HIS
2	I	151	HIS
2	I	201	ASN
2	I	273	HIS
2	I	379	HIS
2	I	395	GLN
2	I	479	GLN
2	I	489	ASN
2	I	582	HIS
2	I	725	HIS
2	I	765	GLN
2	I	838	HIS
2	I	919	ASN
2	I	1220	GLN
2	I	1598	GLN
2	I	1611	HIS
2	I	1679	ASN
2	I	1688	HIS
2	I	1691	GLN
2	I	1693	GLN
2	I	1719	HIS

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Mol	Chain	Res	Type
2	I	1775	HIS
2	I	1861	GLN
2	I	1973	GLN
2	I	2100	HIS
2	I	2127	GLN
2	I	2194	HIS
2	I	2260	ASN
2	I	2772	GLN
2	I	2773	ASN
2	I	2788	HIS
2	I	2856	ASN
2	I	3767	GLN
2	I	3809	ASN
2	I	3814	GLN
2	I	3896	ASN
2	I	3960	GLN
2	I	3976	ASN
2	I	3994	HIS
2	I	3998	HIS
2	I	4034	ASN
2	I	4054	ASN
2	I	4120	ASN
2	I	4553	ASN
2	I	4707	ASN
2	I	4806	ASN
2	I	4949	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	14
2	G	14
2	E	14
2	I	14

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4345:UNK	C	4540:PHE	N	73.03
1	G	4345:UNK	C	4540:PHE	N	73.03
1	E	4345:UNK	C	4540:PHE	N	73.03
1	I	4345:UNK	C	4540:PHE	N	73.03
1	B	3613:UNK	C	3639:THR	N	46.34
1	G	3613:UNK	C	3639:THR	N	46.34
1	E	3613:UNK	C	3639:THR	N	46.34
1	I	3613:UNK	C	3639:THR	N	46.34
1	B	4253:GLU	C	4320:UNK	N	27.01
1	G	4253:GLU	C	4320:UNK	N	27.01
1	E	4253:GLU	C	4320:UNK	N	27.01
1	I	4253:GLU	C	4320:UNK	N	27.01
1	B	3163:UNK	C	3170:UNK	N	16.37

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	3163:UNK	C	3170:UNK	N	16.37
1	E	3163:UNK	C	3170:UNK	N	16.37
1	I	3163:UNK	C	3170:UNK	N	16.37
1	B	3063:UNK	C	3134:UNK	N	15.02
1	E	3063:UNK	C	3134:UNK	N	15.02
1	G	3063:UNK	C	3134:UNK	N	15.01
1	I	3063:UNK	C	3134:UNK	N	15.01
1	B	3468:UNK	C	3511:UNK	N	14.70
1	G	3468:UNK	C	3511:UNK	N	14.70
1	E	3468:UNK	C	3511:UNK	N	14.70
1	I	3468:UNK	C	3511:UNK	N	14.70
1	B	2703:UNK	C	2734:ASN	N	14.05
1	G	2703:UNK	C	2734:ASN	N	14.05
1	E	2703:UNK	C	2734:ASN	N	14.05
1	I	2703:UNK	C	2734:ASN	N	14.05
1	B	3236:UNK	C	3241:UNK	N	13.51
1	G	3236:UNK	C	3241:UNK	N	13.51
1	E	3236:UNK	C	3241:UNK	N	13.51
1	I	3236:UNK	C	3241:UNK	N	13.50
1	B	2976:UNK	C	2995:UNK	N	12.41
1	G	2976:UNK	C	2995:UNK	N	12.41
1	E	2976:UNK	C	2995:UNK	N	12.41
1	I	2976:UNK	C	2995:UNK	N	12.41
1	B	1564:UNK	C	1573:MET	N	12.19
1	G	1564:UNK	C	1573:MET	N	12.19
1	E	1564:UNK	C	1573:MET	N	12.19
1	I	1564:UNK	C	1573:MET	N	12.19
1	B	3254:UNK	C	3261:UNK	N	8.04
1	G	3254:UNK	C	3261:UNK	N	8.04
1	E	3254:UNK	C	3261:UNK	N	8.04
1	I	3254:UNK	C	3261:UNK	N	8.04
1	B	1297:UNK	C	1430:UNK	N	5.71
1	G	1297:UNK	C	1430:UNK	N	5.71
1	E	1297:UNK	C	1430:UNK	N	5.71
1	I	1297:UNK	C	1430:UNK	N	5.71
1	B	2479:LEU	C	2487:UNK	N	3.30
1	G	2479:LEU	C	2487:UNK	N	3.30
1	E	2479:LEU	C	2487:UNK	N	3.30
1	I	2479:LEU	C	2487:UNK	N	3.30
1	B	2939:ARG	C	2942:UNK	N	3.28
1	G	2939:ARG	C	2942:UNK	N	3.28
1	E	2939:ARG	C	2942:UNK	N	3.28

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	2939:ARG	C	2942:UNK	N	3.28

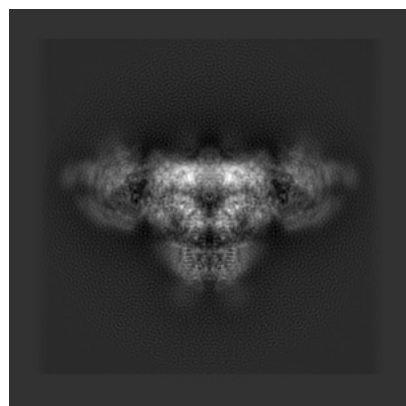
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8391. These allow visual inspection of the internal detail of the map and identification of artifacts.

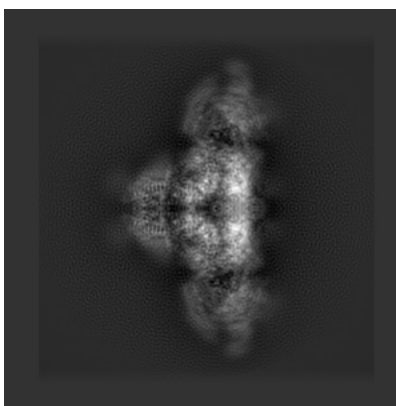
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

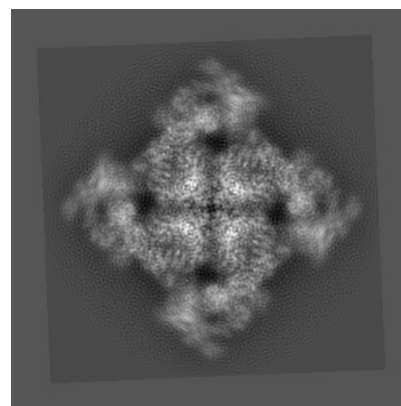
6.1.1 Primary map



X

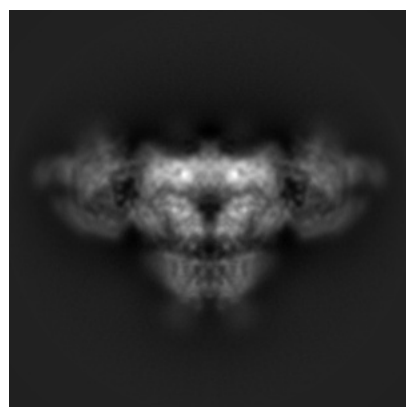


Y

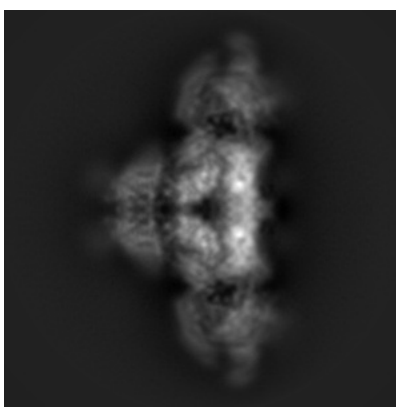


Z

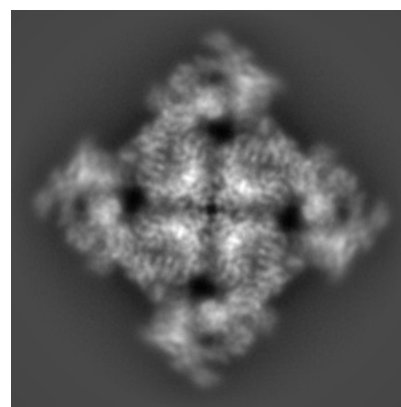
6.1.2 Raw map



X



Y



Z

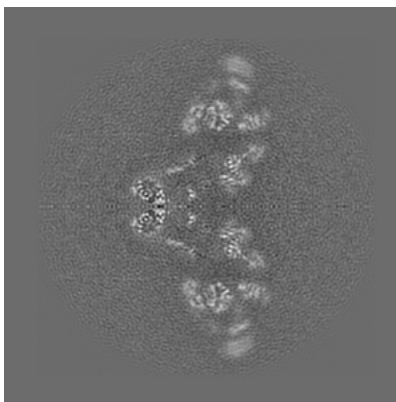
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

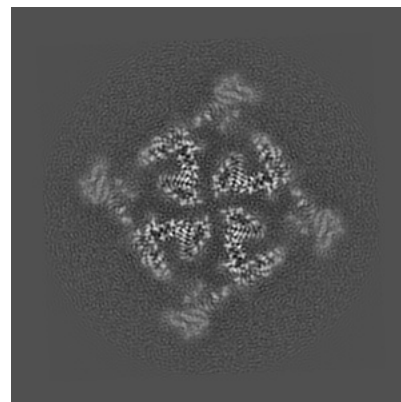
6.2.1 Primary map



X Index: 200

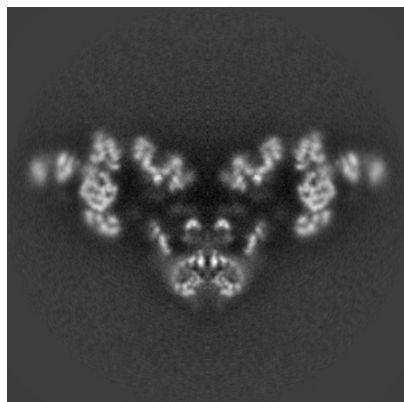


Y Index: 200

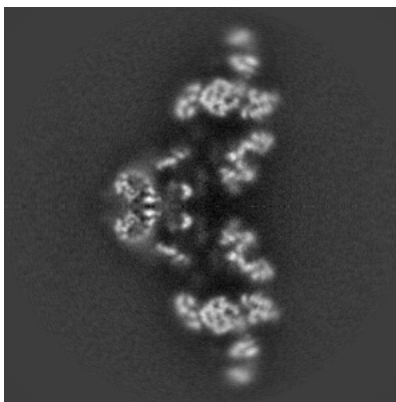


Z Index: 200

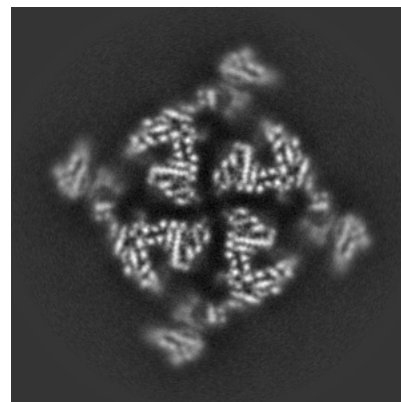
6.2.2 Raw map



X Index: 168



Y Index: 168

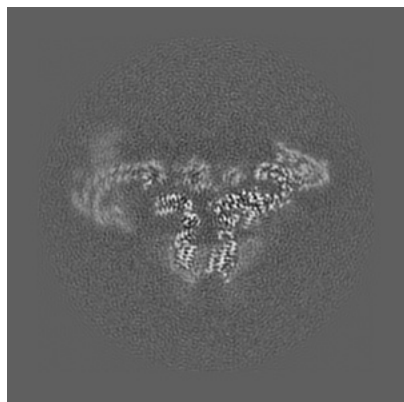


Z Index: 168

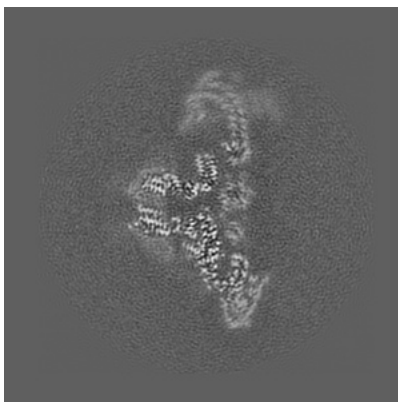
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

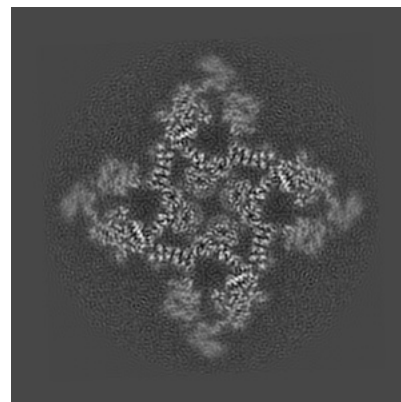
6.3.1 Primary map



X Index: 176

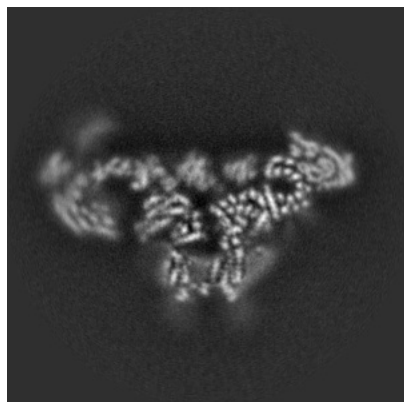


Y Index: 176

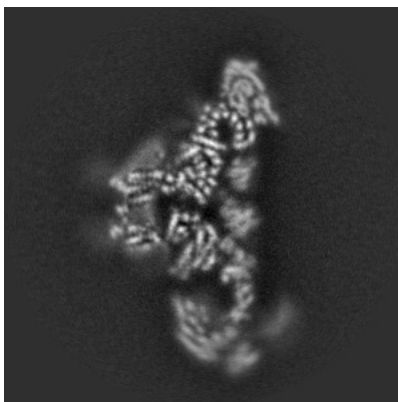


Z Index: 228

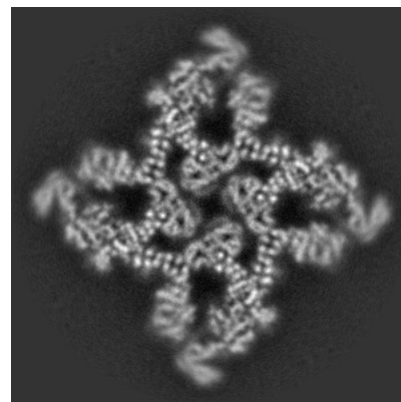
6.3.2 Raw map



X Index: 147



Y Index: 189

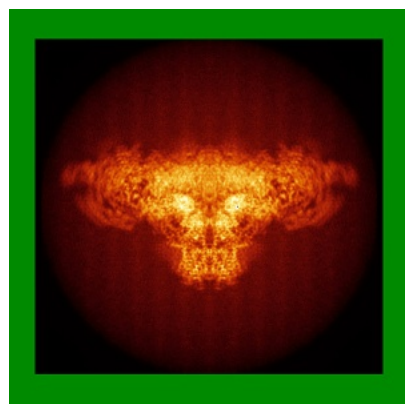


Z Index: 196

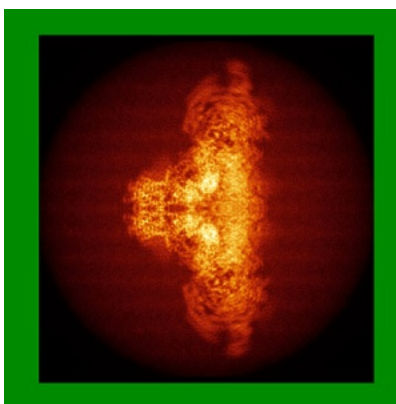
The images above show the largest variance slices of the map in three orthogonal directions.

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

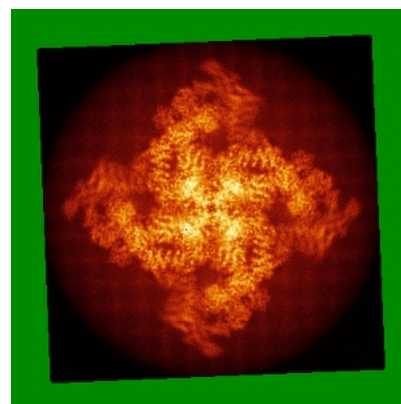
6.4.1 Primary map



X



Y

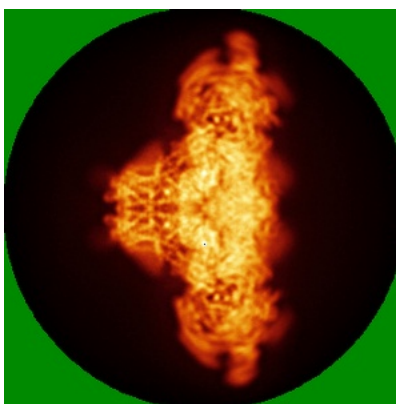


Z

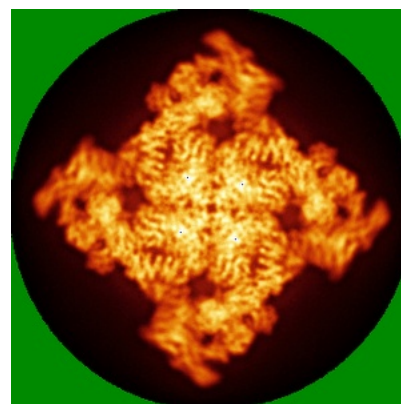
6.4.2 Raw map



X



Y

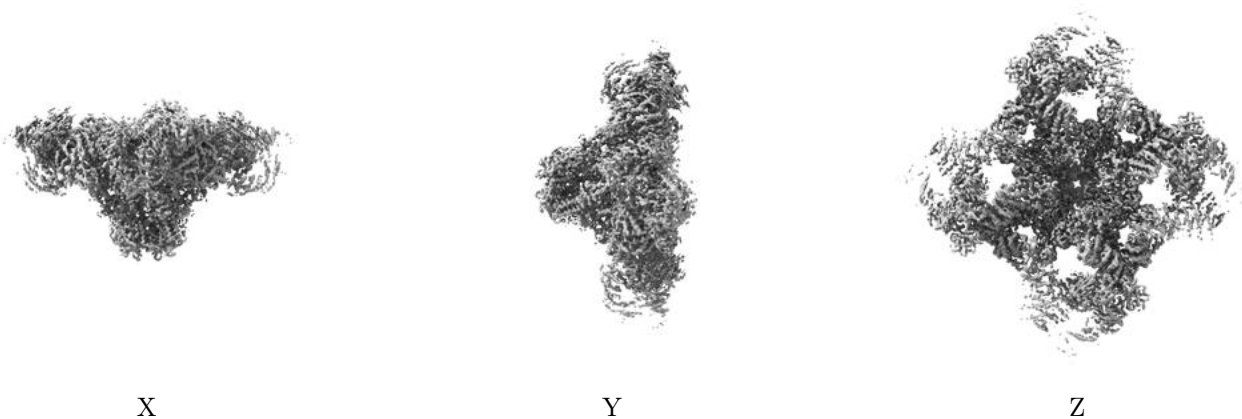


Z

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

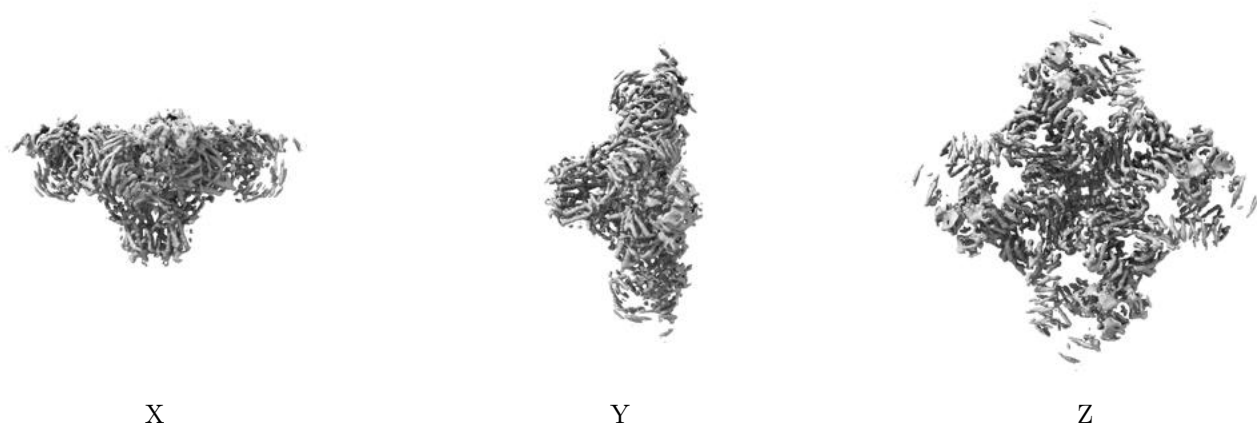
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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.

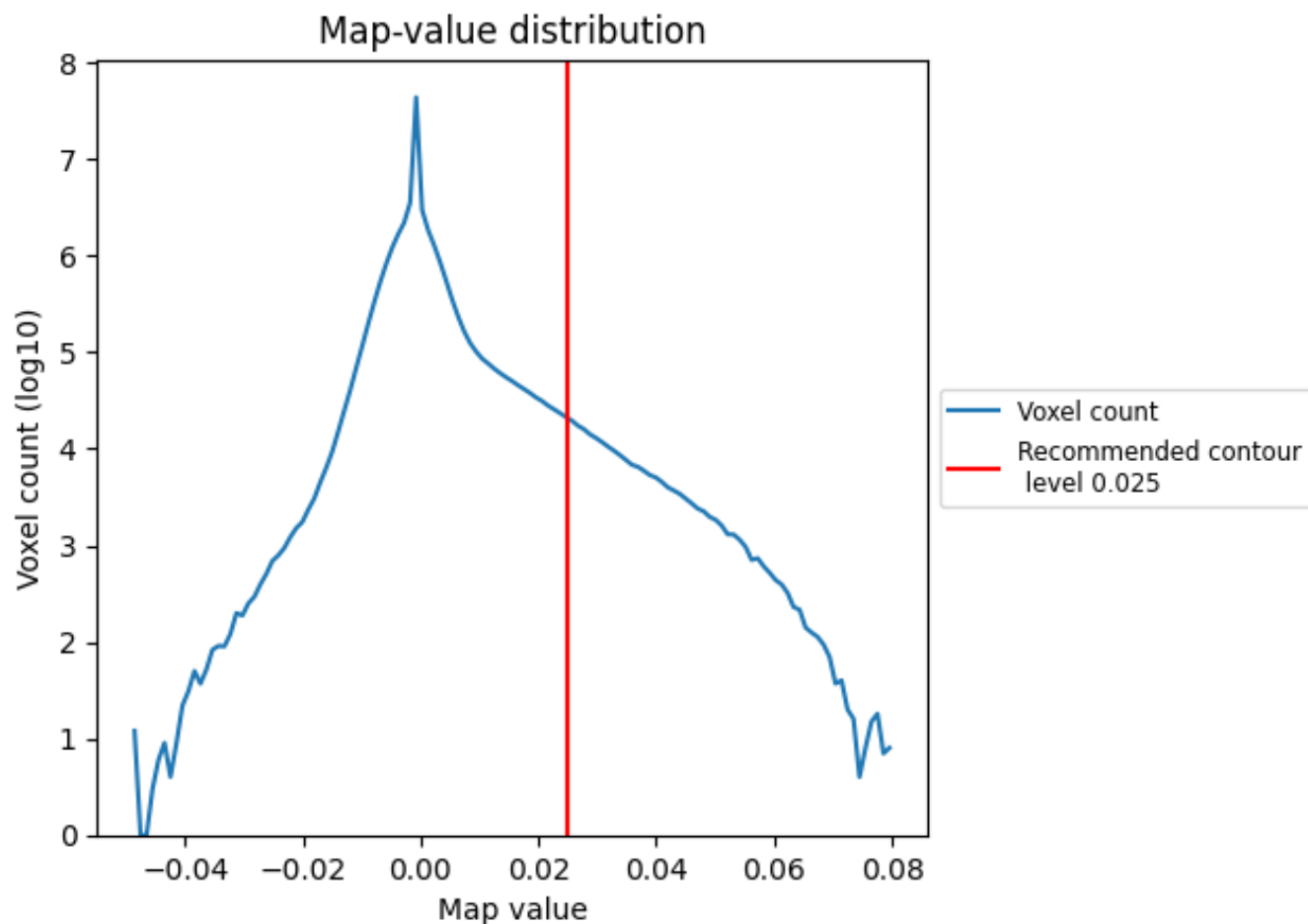
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

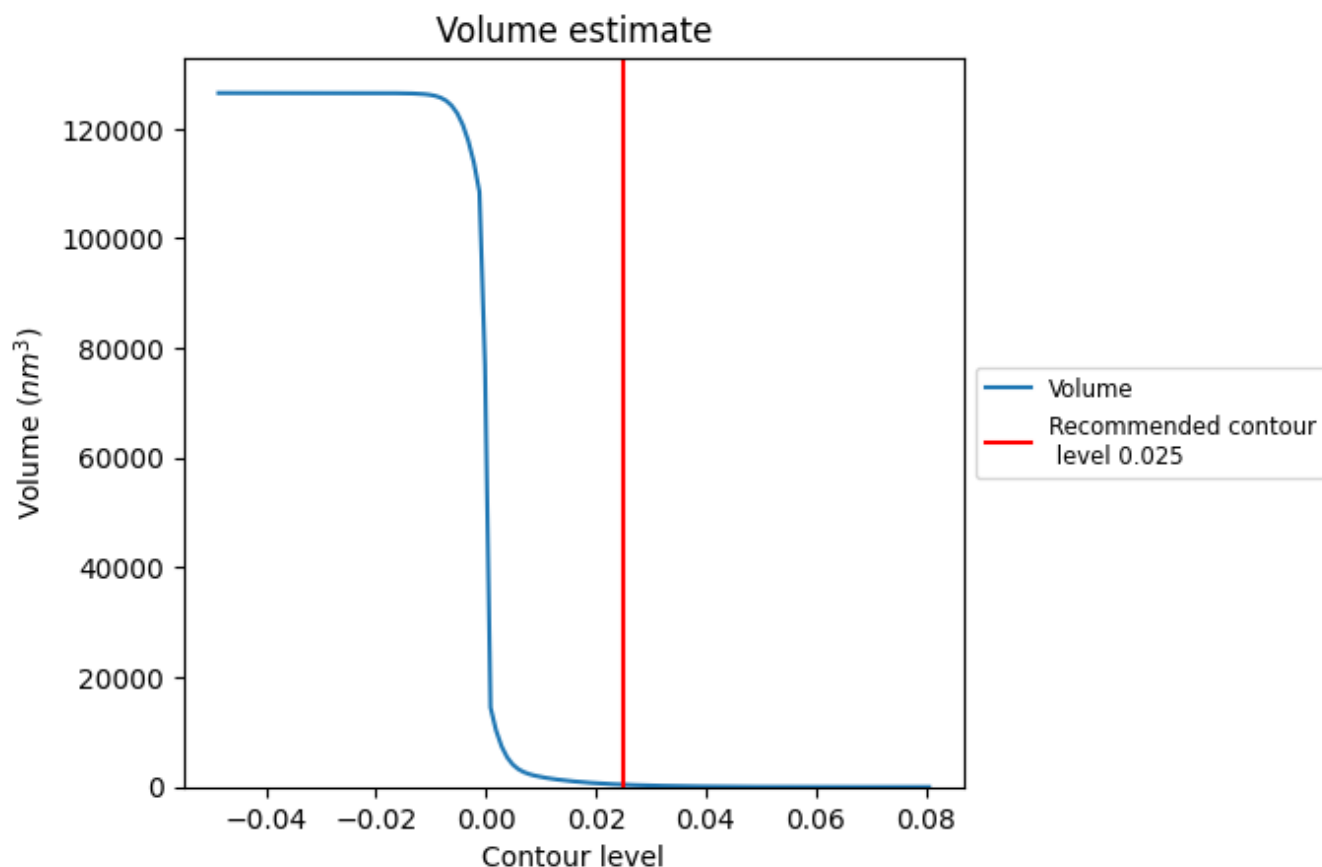
This section contains the results of statistical analysis of the map.

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.

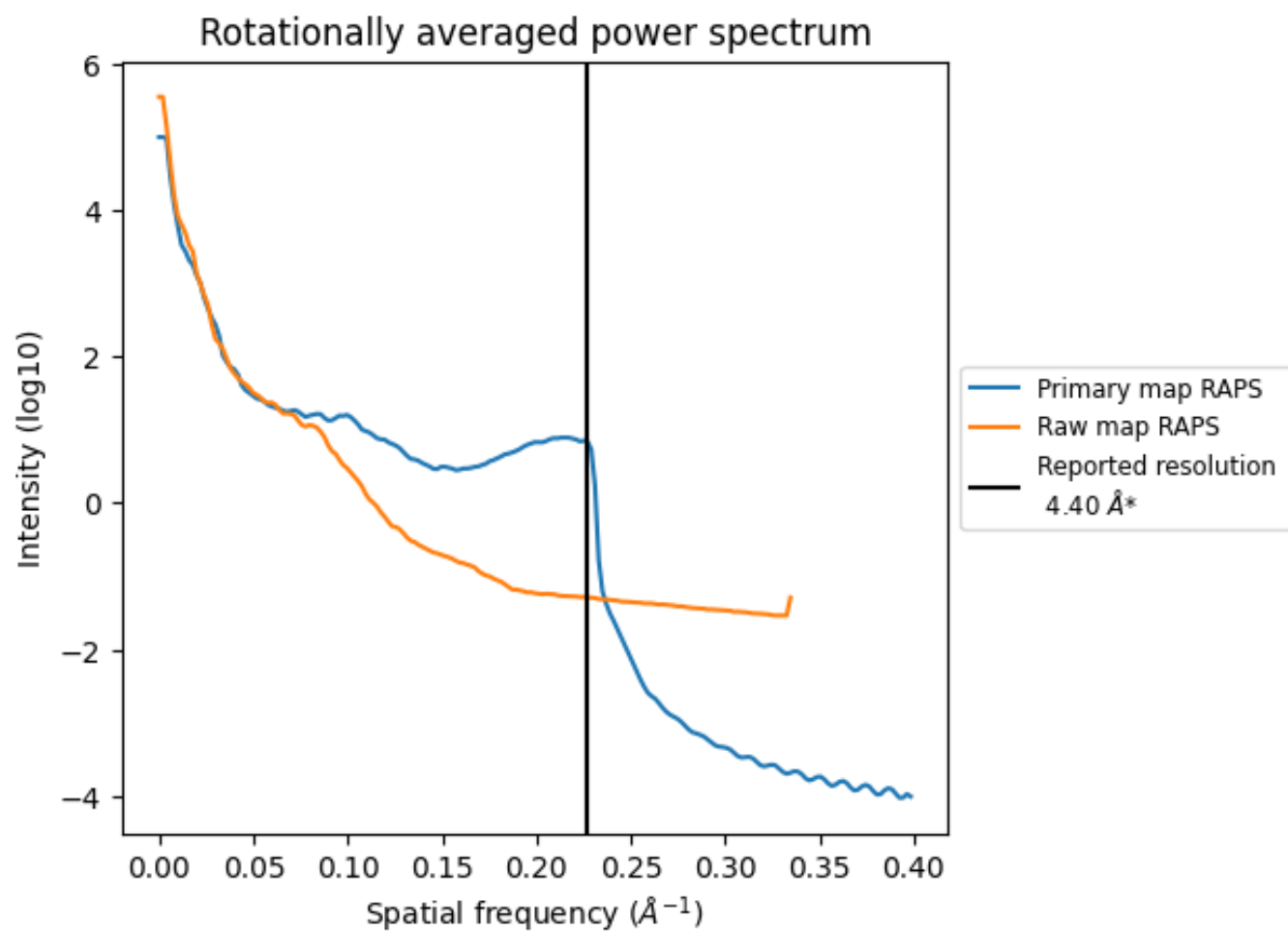
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 422 nm³; this corresponds to an approximate mass of 381 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](#)

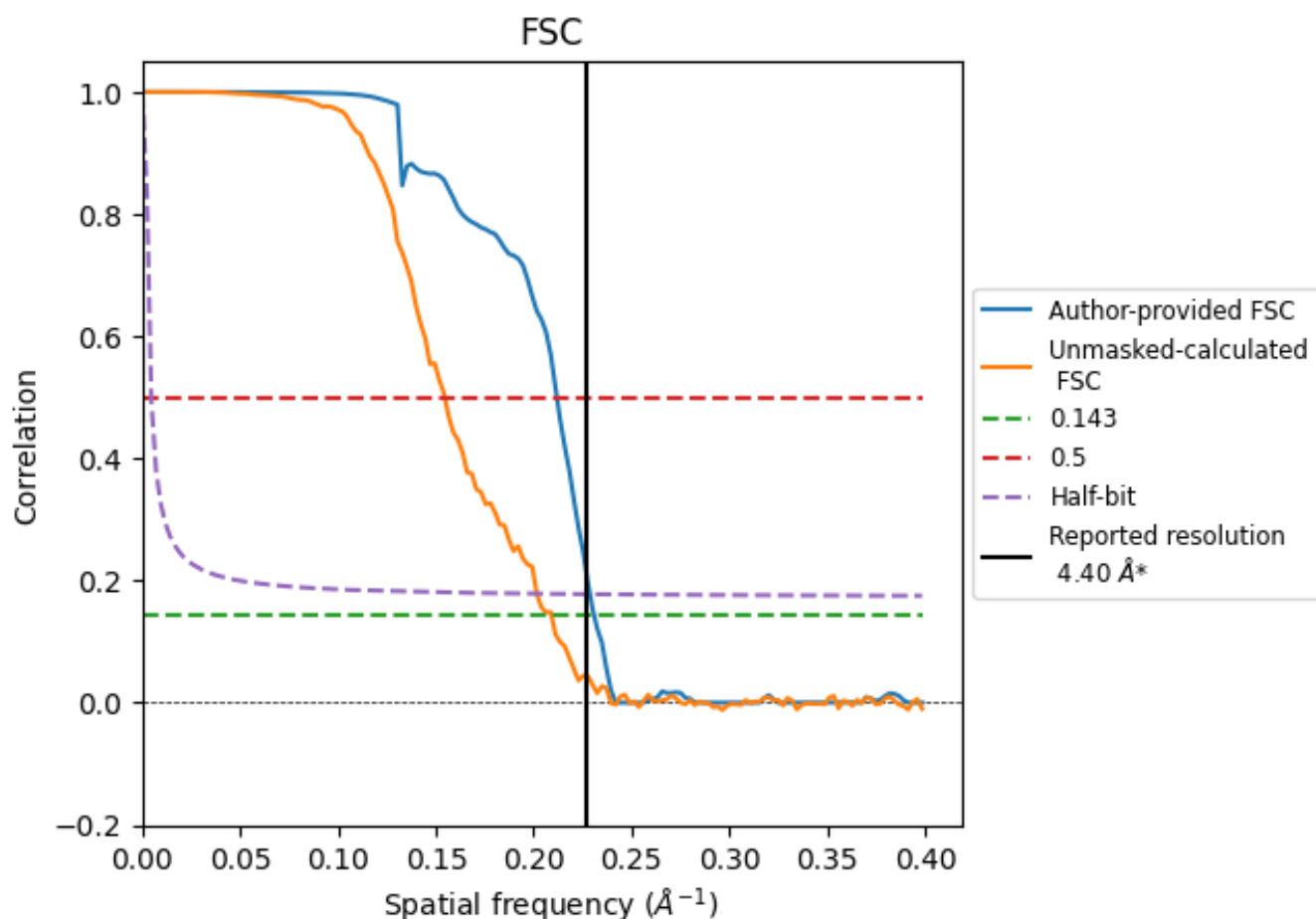


*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.227 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

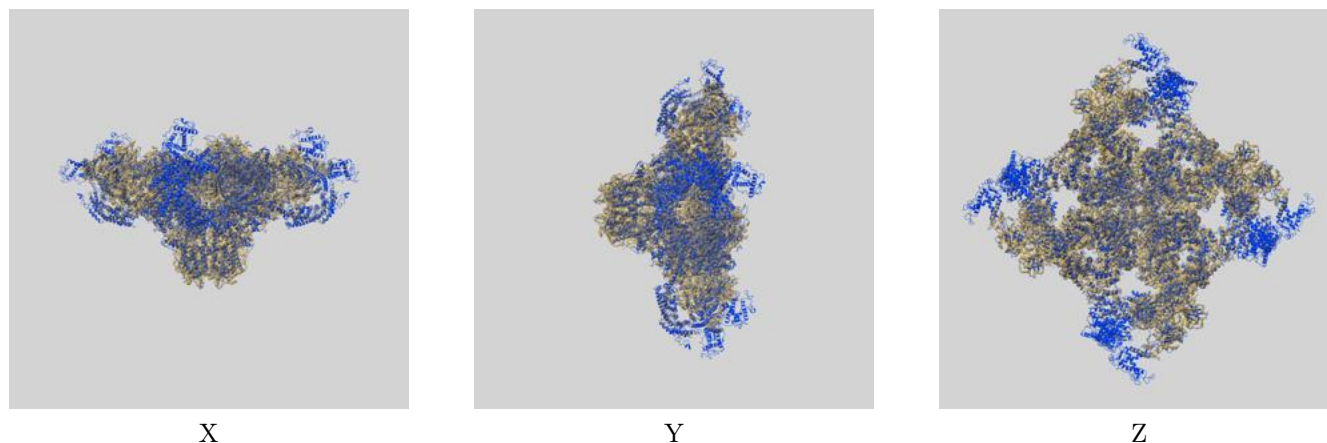
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.33	4.72	4.37
Unmasked-calculated*	4.78	6.47	4.96

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

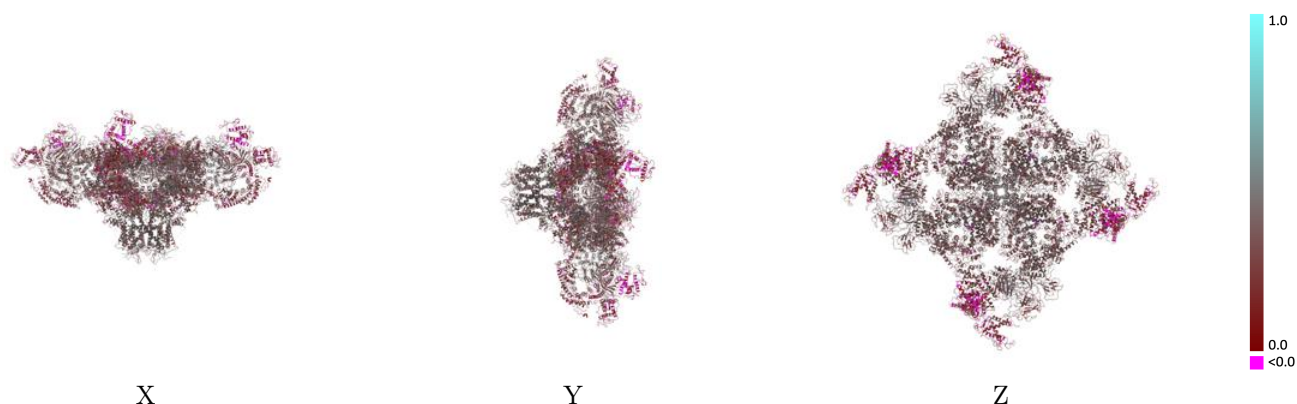
This section contains information regarding the fit between EMDB map EMD-8391 and PDB model 5TB0. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



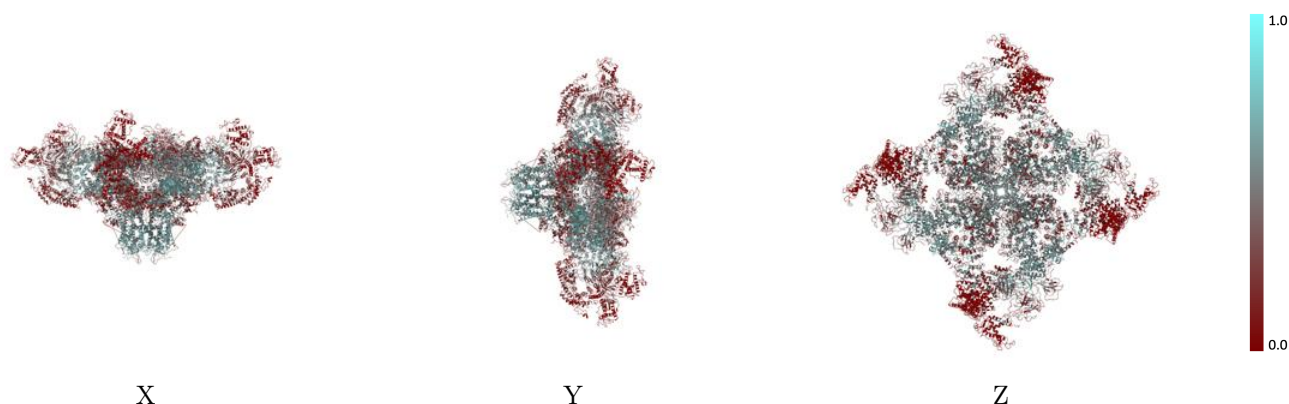
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



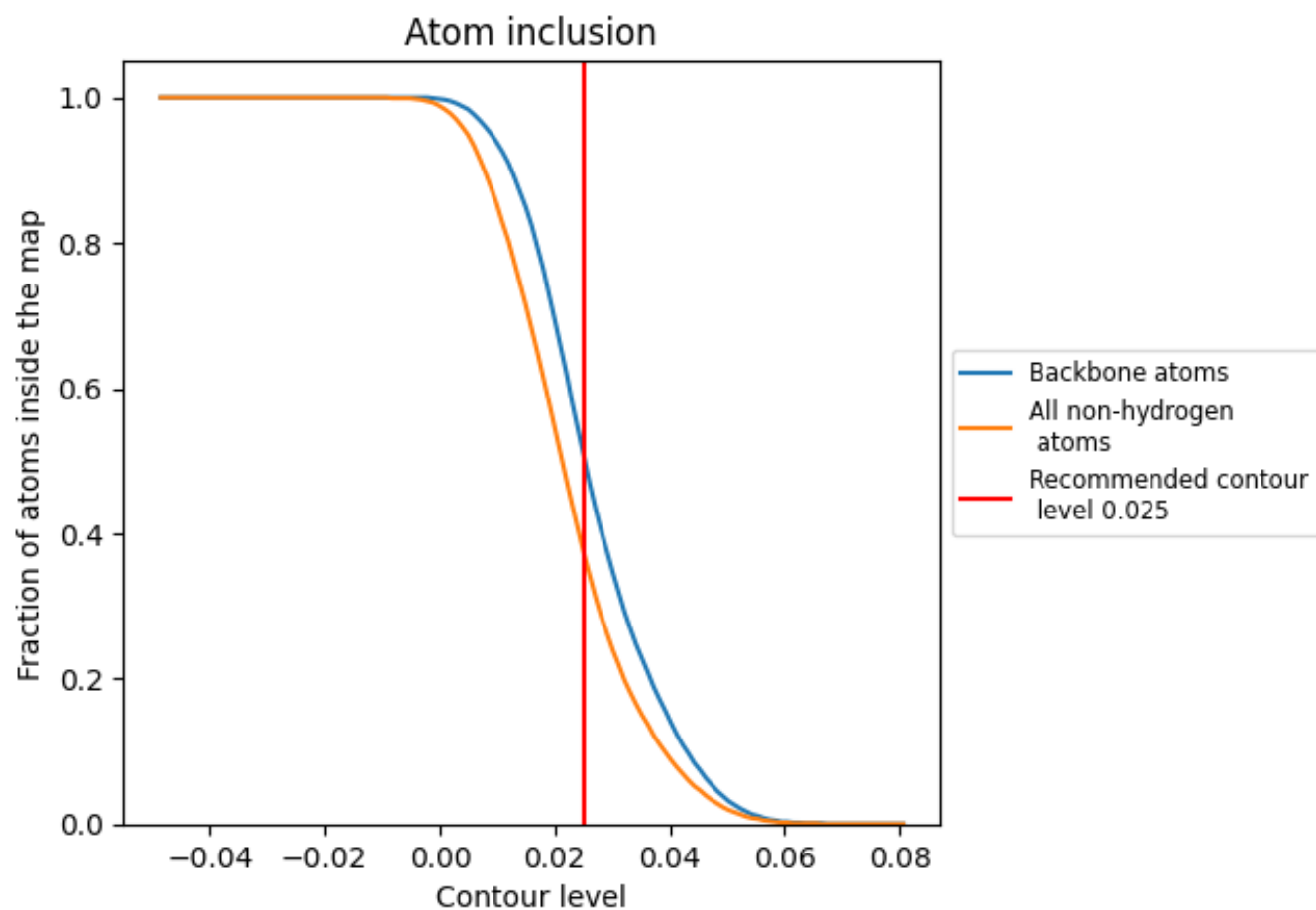
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 51% of all backbone atoms, 37% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3740	0.3120
A	0.3810	0.3450
B	0.3750	0.3110
E	0.3730	0.3110
F	0.3780	0.3490
G	0.3740	0.3110
H	0.3810	0.3480
I	0.3740	0.3110
J	0.3800	0.3450

