



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:39 AM UTC

PDB ID : 6DBW / pdb_00006dbw
EMDB ID : EMD-7852
Title : Cryo-EM structure of RAG in complex with 12-RSS substrate DNA
Authors : Wu, H.; Liao, M.; Ru, H.; Mi, W.
Deposited on : 2018-05-03
Resolution : 4.70 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

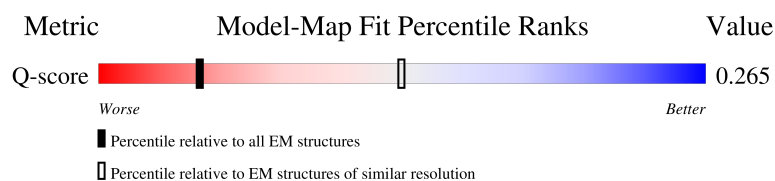
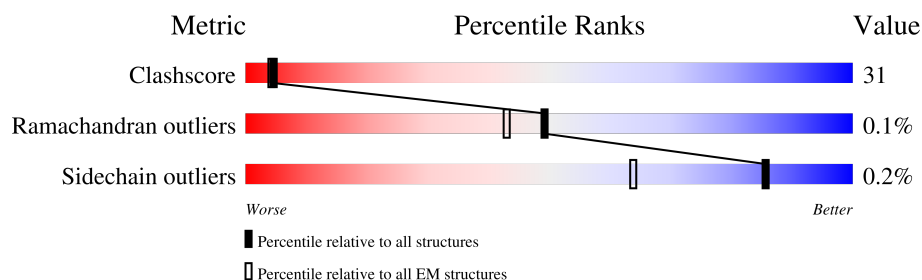
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.70 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.



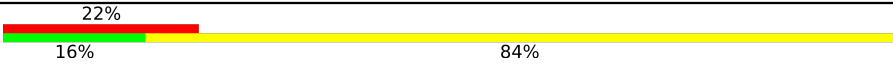
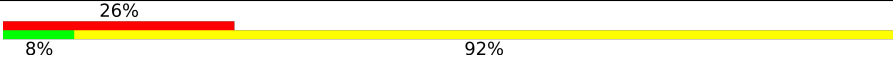
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1989 (4.20 - 5.20)

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	1159	 26% 26% 47%
1	C	1159	 6% 27% 25% 47%
2	B	533	 28% 38% 34%
2	D	533	 32% 33% 34%

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Mol	Chain	Length	Quality of chain
3	E	50	
4	F	50	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17418 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 Recombination activating gene 1 - MBP chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	614	Total	C	N	O	S	0	0
			4954	3102	890	925	37		
1	C	615	Total	C	N	O	S	2	0
			4980	3116	898	929	37		

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-127	MET	-	initiating methionine	UNP P0AEX9
A	-126	GLY	-	expression tag	UNP P0AEX9
A	-125	SER	-	expression tag	UNP P0AEX9
A	-124	SER	-	expression tag	UNP P0AEX9
A	-123	HIS	-	expression tag	UNP P0AEX9
A	-122	HIS	-	expression tag	UNP P0AEX9
A	-121	HIS	-	expression tag	UNP P0AEX9
A	-120	HIS	-	expression tag	UNP P0AEX9
A	-119	HIS	-	expression tag	UNP P0AEX9
A	-118	HIS	-	expression tag	UNP P0AEX9
A	-117	GLY	-	expression tag	UNP P0AEX9
A	-116	THR	-	expression tag	UNP P0AEX9
A	-115	LYS	-	expression tag	UNP P0AEX9
A	-114	THR	-	expression tag	UNP P0AEX9
A	251	GLY	-	linker	UNP P0AEX9
A	252	THR	-	linker	UNP P0AEX9
A	253	ASP	-	linker	UNP P0AEX9
A	254	TYR	-	linker	UNP P0AEX9
A	255	ASP	-	linker	UNP P0AEX9
A	256	ILE	-	linker	UNP P0AEX9
A	257	PRO	-	linker	UNP P0AEX9
A	258	THR	-	linker	UNP P0AEX9
A	259	THR	-	linker	UNP P0AEX9
A	260	LEU	-	linker	UNP P0AEX9
A	261	GLU	-	linker	UNP P0AEX9
A	262	VAL	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	263	LEU	-	linker	UNP P0AEX9
A	264	PHE	-	linker	UNP P0AEX9
A	265	GLN	-	linker	UNP P0AEX9
A	266	GLY	-	linker	UNP P0AEX9
A	267	PRO	-	linker	UNP P0AEX9
A	268	LEU	-	linker	UNP P0AEX9
A	269	GLY	-	linker	UNP P0AEX9
A	270	SER	-	linker	UNP P0AEX9
C	-127	MET	-	initiating methionine	UNP P0AEX9
C	-126	GLY	-	expression tag	UNP P0AEX9
C	-125	SER	-	expression tag	UNP P0AEX9
C	-124	SER	-	expression tag	UNP P0AEX9
C	-123	HIS	-	expression tag	UNP P0AEX9
C	-122	HIS	-	expression tag	UNP P0AEX9
C	-121	HIS	-	expression tag	UNP P0AEX9
C	-120	HIS	-	expression tag	UNP P0AEX9
C	-119	HIS	-	expression tag	UNP P0AEX9
C	-118	HIS	-	expression tag	UNP P0AEX9
C	-117	GLY	-	expression tag	UNP P0AEX9
C	-116	THR	-	expression tag	UNP P0AEX9
C	-115	LYS	-	expression tag	UNP P0AEX9
C	-114	THR	-	expression tag	UNP P0AEX9
C	251	GLY	-	linker	UNP P0AEX9
C	252	THR	-	linker	UNP P0AEX9
C	253	ASP	-	linker	UNP P0AEX9
C	254	TYR	-	linker	UNP P0AEX9
C	255	ASP	-	linker	UNP P0AEX9
C	256	ILE	-	linker	UNP P0AEX9
C	257	PRO	-	linker	UNP P0AEX9
C	258	THR	-	linker	UNP P0AEX9
C	259	THR	-	linker	UNP P0AEX9
C	260	LEU	-	linker	UNP P0AEX9
C	261	GLU	-	linker	UNP P0AEX9
C	262	VAL	-	linker	UNP P0AEX9
C	263	LEU	-	linker	UNP P0AEX9
C	264	PHE	-	linker	UNP P0AEX9
C	265	GLN	-	linker	UNP P0AEX9
C	266	GLY	-	linker	UNP P0AEX9
C	267	PRO	-	linker	UNP P0AEX9
C	268	LEU	-	linker	UNP P0AEX9
C	269	GLY	-	linker	UNP P0AEX9
C	270	SER	-	linker	UNP P0AEX9

- Molecule 2 is a protein called Recombination activating gene 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	351	Total	C	N	O	S	0	0
			2714	1716	470	509	19		
2	D	351	Total	C	N	O	S	0	0
			2714	1716	470	509	19		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP Q1RLW7
B	-1	GLY	-	expression tag	UNP Q1RLW7
B	0	SER	-	expression tag	UNP Q1RLW7
D	-2	GLY	-	expression tag	UNP Q1RLW7
D	-1	GLY	-	expression tag	UNP Q1RLW7
D	0	SER	-	expression tag	UNP Q1RLW7

- Molecule 3 is a DNA chain called Forward strand of 12-RSS substrate DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	50	Total	C	N	O	P	0	0
			1023	486	192	295	50		

- Molecule 4 is a DNA chain called Reverse strand of 12-RSS substrate DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	50	Total	C	N	O	P	0	0
			1027	489	183	305	50		

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Zn	0
			1	1	
5	C	1	Total	Zn	0
			1	1	

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
6	A	2	Total	Ca	0
			2	2	

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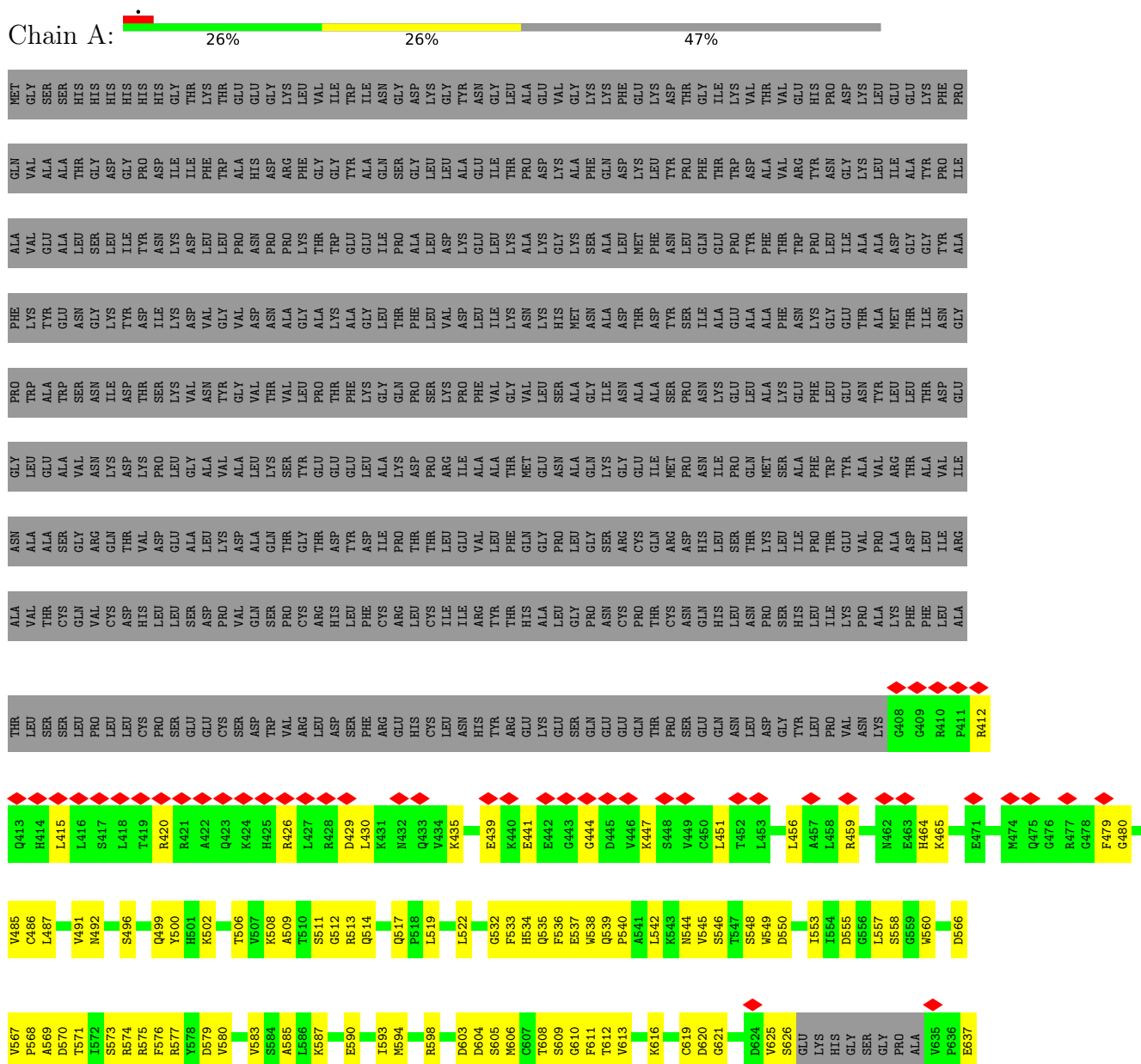
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Mol	Chain	Residues	Atoms		AltConf
6	C	2	Total	Ca	0
			2	2	

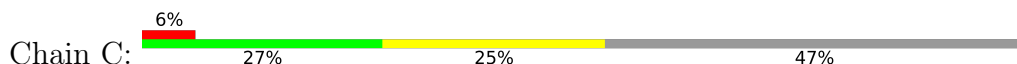
3 Residue-property plots

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.

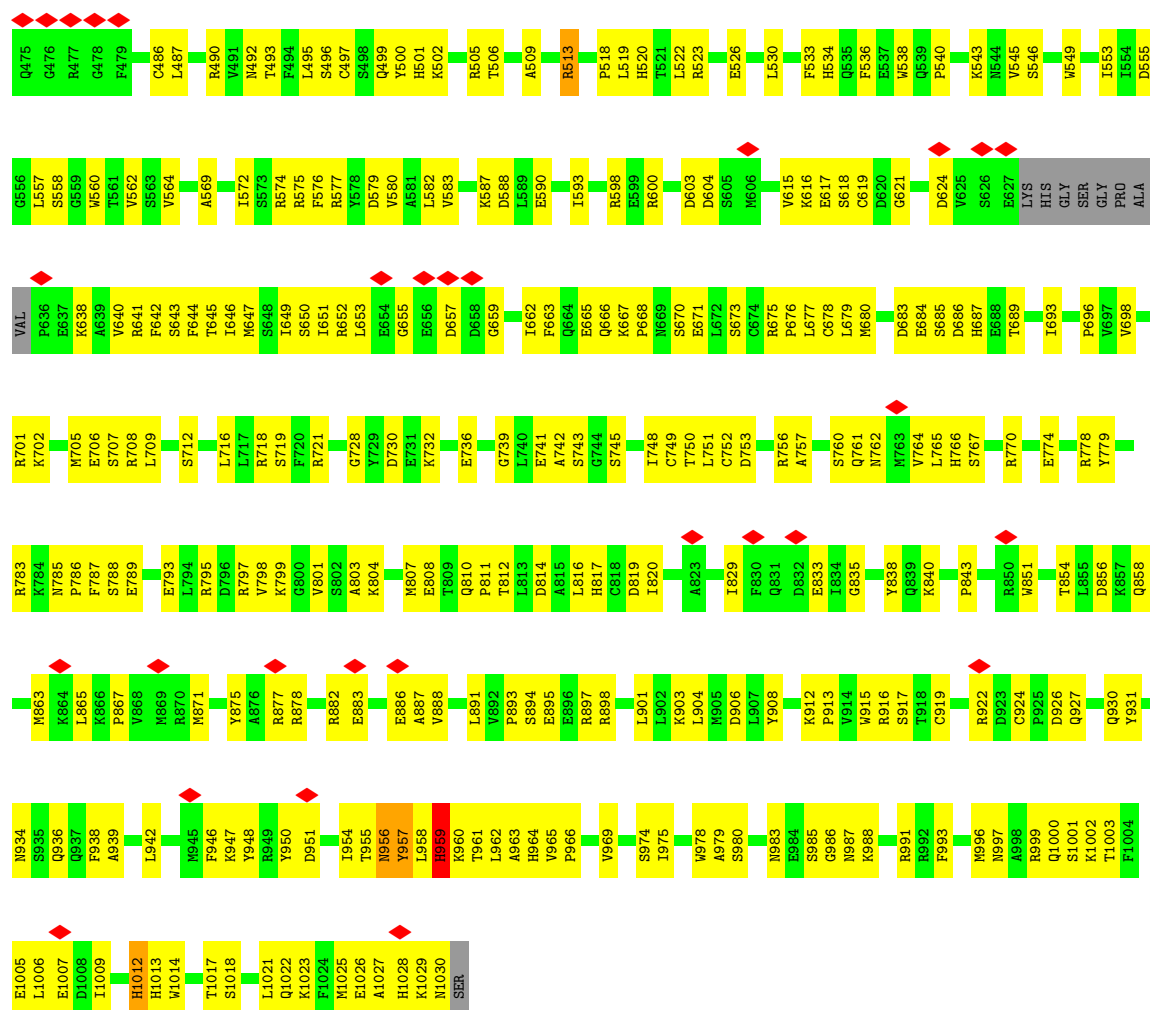
- Molecule 1: Recombination activating gene 1 - MBP chimera



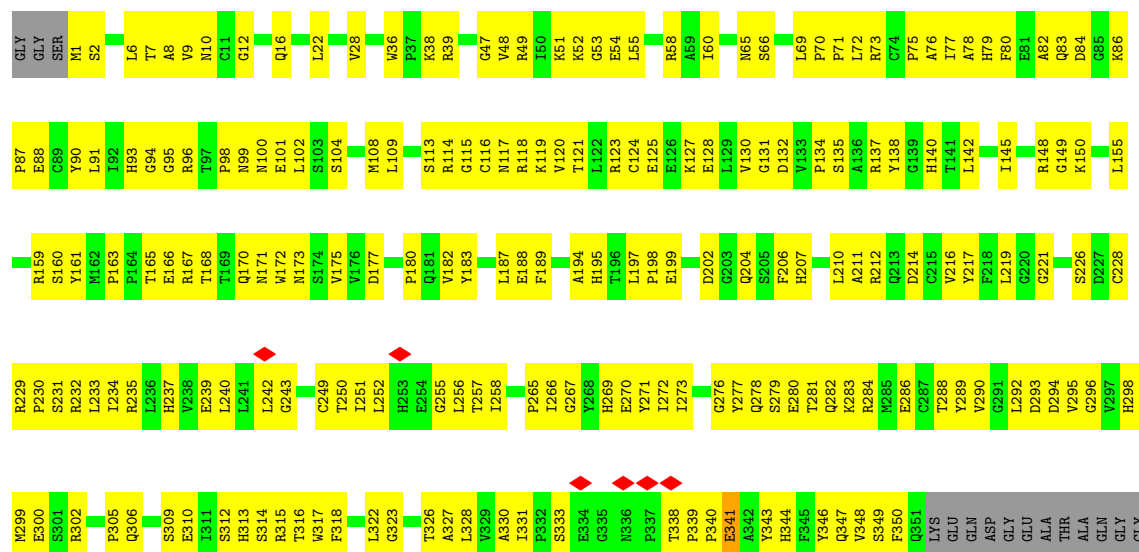
- Molecule 1: Recombination activating gene 1 - MBP chimera



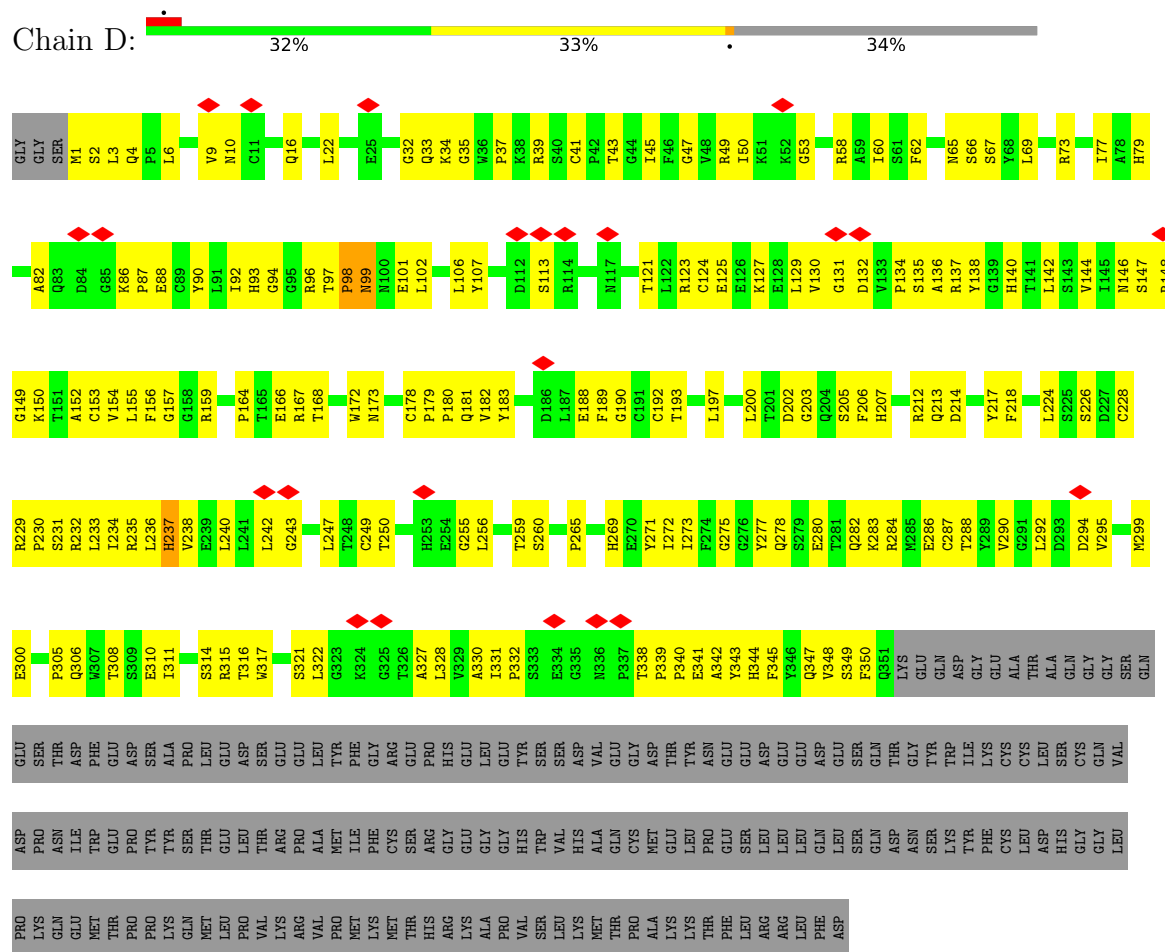
Q413	Q414	Q415	Q416	Q417	Q418	Q419	Q420	Q421	Q422	Q423	Q424	Q425	Q426	Q427	Q428	Q429	Q430	Q431	Q432	Q433	Q434	Q435	Q436	Q437	Q438	Q439	Q440	Q441	Q442	Q443	Q444	Q445	Q446	Q447	Q448	Q449	Q450	Q451	Q452	Q453	Q454	Q455	Q456	Q457	Q458	Q459	Q460	Q461	Q462	Q463	Q464	Q465	Q466	Q467	Q468	Q469	Q470	Q471	Q472	Q473	Q474	Q475	Q476	Q477	Q478	Q479	Q480	Q481	Q482	Q483	Q484	Q485	Q486	Q487	Q488	Q489	Q490	Q491	Q492	Q493	Q494	Q495	Q496	Q497	Q498	Q499	Q500	Q501	Q502	Q503	Q504	Q505	Q506	Q507	Q508	Q509	Q510	Q511	Q512	Q513	Q514	Q515	Q516	Q517	Q518	Q519	Q520	Q521	Q522	Q523	Q524	Q525	Q526	Q527	Q528	Q529	Q530	Q531	Q532	Q533	Q534	Q535	Q536	Q537	Q538	Q539	Q540	Q541	Q542	Q543	Q544	Q545	Q546	Q547	Q548	Q549	Q550	Q551	Q552	Q553	Q554	Q555	Q556	Q557	Q558	Q559	Q560	Q561	Q562	Q563	Q564	Q565	Q566	Q567	Q568	Q569	Q570	Q571	Q572	Q573	Q574	Q575	Q576	Q577	Q578	Q579	Q580	Q581	Q582	Q583	Q584	Q585	Q586	Q587	Q588	Q589	Q590	Q591	Q592	Q593	Q594	Q595	Q596	Q597	Q598	Q599	Q600	Q601	Q602	Q603	Q604	Q605	Q606	Q607	Q608	Q609	Q610	Q611	Q612	Q613	Q614	Q615	Q616	Q617	Q618	Q619	Q620	Q621	Q622	Q623	Q624	Q625	Q626	Q627	Q628	Q629	Q630	Q631	Q632	Q633	Q634	Q635	Q636	Q637	Q638	Q639	Q640	Q641	Q642	Q643	Q644	Q645	Q646	Q647	Q648	Q649	Q650	Q651	Q652	Q653	Q654	Q655	Q656	Q657	Q658	Q659	Q660	Q661	Q662	Q663	Q664	Q665	Q666	Q667	Q668	Q669	Q670	Q671	Q672	Q673	Q674	Q675	Q676	Q677	Q678	Q679	Q680	Q681	Q682	Q683	Q684	Q685	Q686	Q687	Q688	Q689	Q690	Q691	Q692	Q693	Q694	Q695	Q696	Q697	Q698	Q699	Q700	Q701	Q702	Q703	Q704	Q705	Q706	Q707	Q708	Q709	Q710	Q711	Q712	Q713	Q714	Q715	Q716	Q717	Q718	Q719	Q720	Q721	Q722	Q723	Q724	Q725	Q726	Q727	Q728	Q729	Q730	Q731	Q732	Q733	Q734	Q735	Q736	Q737	Q738	Q739	Q740	Q741	Q742	Q743	Q744	Q745	Q746	Q747	Q748	Q749	Q750	Q751	Q752	Q753	Q754	Q755	Q756	Q757	Q758	Q759	Q760	Q761	Q762	Q763	Q764	Q765	Q766	Q767	Q768	Q769	Q770	Q771	Q772	Q773	Q774	Q775	Q776	Q777	Q778	Q779	Q780	Q781	Q782	Q783	Q784	Q785	Q786	Q787	Q788	Q789	Q790	Q791	Q792	Q793	Q794	Q795	Q796	Q797	Q798	Q799	Q800	Q801	Q802	Q803	Q804	Q805	Q806	Q807	Q808	Q809	Q810	Q811	Q812	Q813	Q814	Q815	Q816	Q817	Q818	Q819	Q820	Q821	Q822	Q823	Q824	Q825	Q826	Q827	Q828	Q829	Q830	Q831	Q832	Q833	Q834	Q835	Q836	Q837	Q838	Q839	Q840	Q841	Q842	Q843	Q844	Q845	Q846	Q847	Q848	Q849	Q850	Q851	Q852	Q853	Q854	Q855	Q856	Q857	Q858	Q859	Q860	Q861	Q862	Q863	Q864	Q865	Q866	Q867	Q868	Q869	Q870	Q871	Q872	Q873	Q874	Q875	Q876	Q877	Q878	Q879	Q880	Q881	Q882	Q883	Q884	Q885	Q886	Q887	Q888	Q889	Q890	Q891	Q892	Q893	Q894	Q895	Q896	Q897	Q898	Q899	Q900	Q901	Q902	Q903	Q904	Q905	Q906	Q907	Q908	Q909	Q910	Q911	Q912	Q913	Q914	Q915	Q916	Q917	Q918	Q919	Q920	Q921	Q922	Q923	Q924	Q925	Q926	Q927	Q928	Q929	Q930	Q931	Q932	Q933	Q934	Q935	Q936	Q937	Q938	Q939	Q940	Q941	Q942	Q943	Q944	Q945	Q946	Q947	Q948	Q949	Q950	Q951	Q952	Q953	Q954	Q955	Q956	Q957	Q958	Q959	Q960	Q961	Q962	Q963	Q964	Q965	Q966	Q967	Q968	Q969	Q970	Q971	Q972	Q973	Q974	Q975	Q976	Q977	Q978	Q979	Q980	Q981	Q982	Q983	Q984	Q985	Q986	Q987	Q988	Q989	Q990	Q991	Q992	Q993	Q994	Q995	Q996	Q997	Q998	Q999	Q1000



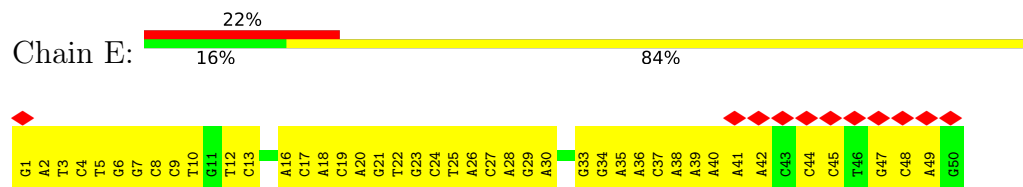
• Molecule 2: Recombination activating gene 2



- Molecule 2: Recombination activating gene 2

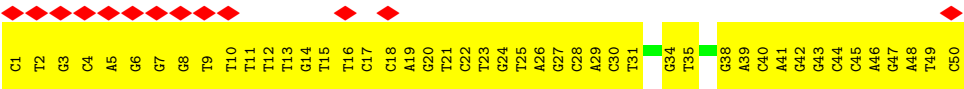


- Molecule 3: Forward strand of 12-RSS substrate DNA



- Molecule 4: Reverse strand of 12-RSS substrate DNA





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	48851	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 ($e^-/\text{\AA}^2$)	47	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	0.152	Depositor
Minimum map value	-0.053	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	271.36, 271.36, 271.36	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	0.36	3/5049 (0.1%)	0.90	12/6789 (0.2%)
1	C	0.38	4/5081 (0.1%)	1.07	31/6829 (0.5%)
2	B	0.22	0/2784	0.48	0/3784
2	D	0.24	0/2784	0.91	11/3784 (0.3%)
3	E	0.25	0/1148	0.41	0/1768
4	F	0.27	0/1150	0.48	0/1774
All	All	0.32	7/17996 (0.0%)	0.85	54/24728 (0.2%)

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	2
1	C	0	4
2	D	0	1
All	All	0	7

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	517	GLN	CD-NE2	12.21	1.58	1.33
1	A	517	GLN	CD-OE1	-11.00	1.02	1.23
1	C	414	HIS	CG-ND1	-8.43	1.28	1.38
1	C	1012	HIS	CG-CD2	8.16	1.44	1.35
1	C	1012	HIS	CA-C	-7.36	1.43	1.52
1	A	517	GLN	CB-CG	-6.40	1.33	1.52
1	C	1012	HIS	CE1-NE2	-5.89	1.26	1.32

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1012	HIS	CB-CG-CD2	-31.32	90.48	131.20
1	C	1012	HIS	CB-CG-ND1	30.68	168.72	122.70
2	D	237	HIS	CB-CG-CD2	-30.34	91.75	131.20
1	C	959	HIS	CB-CG-CD2	-29.59	92.73	131.20
1	A	517	GLN	CG-CD-OE1	29.40	179.59	120.80
1	A	1028	HIS	CB-CG-CD2	-28.42	94.25	131.20
2	D	237	HIS	CB-CG-ND1	26.09	161.84	122.70
1	A	517	GLN	OE1-CD-NE2	-26.01	96.59	122.60
1	A	1028	HIS	CB-CG-ND1	22.24	156.05	122.70
1	A	517	GLN	CG-CD-NE2	-22.11	83.23	116.40
1	C	1012	HIS	ND1-CG-CD2	-19.88	86.22	106.10
1	C	959	HIS	CB-CG-ND1	19.75	152.32	122.70
1	C	414	HIS	CB-CA-C	19.43	139.41	110.26
1	C	959	HIS	CB-CA-C	-16.54	84.77	110.90
1	C	1012	HIS	CA-CB-CG	-14.55	99.25	113.80
2	D	237	HIS	ND1-CG-CD2	-14.54	91.56	106.10
1	C	414	HIS	ND1-CG-CD2	-14.42	91.68	106.10
1	A	1028	HIS	ND1-CG-CD2	-13.90	92.20	106.10
1	A	517	GLN	CA-CB-CG	13.55	141.21	114.10
1	C	959	HIS	N-CA-C	-13.43	96.64	111.14
1	C	1012	HIS	N-CA-CB	13.15	129.79	110.20
1	C	959	HIS	ND1-CG-CD2	-12.38	93.72	106.10
1	C	414	HIS	ND1-CE1-NE2	-10.60	97.80	108.40
1	C	1012	HIS	N-CA-C	-9.43	100.09	111.69
1	C	414	HIS	N-CA-CB	-8.93	95.96	109.71
1	C	1012	HIS	ND1-CE1-NE2	-8.21	100.19	108.40
1	C	1012	HIS	CG-ND1-CE1	7.84	122.63	109.30
1	C	1012	HIS	CG-CD2-NE2	7.81	115.01	107.20
1	A	1028	HIS	CB-CA-C	7.76	125.85	112.27
2	D	99	ASN	N-CA-C	-7.73	98.37	109.96
1	A	1028	HIS	ND1-CE1-NE2	-7.63	100.77	108.40
2	D	237	HIS	N-CA-CB	7.58	122.08	109.94
1	C	413	GLN	CA-C-N	7.38	131.87	121.24
1	C	413	GLN	C-N-CA	7.38	131.87	121.24
1	C	414	HIS	CB-CG-CD2	-7.30	121.71	131.20
1	C	959	HIS	N-CA-CB	7.24	120.56	110.07
2	D	237	HIS	CG-CD2-NE2	7.05	114.25	107.20
2	D	237	HIS	ND1-CE1-NE2	-6.99	101.41	108.40
1	C	414	HIS	CE1-NE2-CD2	-6.80	102.19	109.00
1	C	414	HIS	CA-CB-CG	6.78	120.58	113.80
2	D	237	HIS	CA-C-O	6.59	128.05	120.60
1	C	414	HIS	O-C-N	-6.40	114.89	122.96
1	C	1012	HIS	CE1-NE2-CD2	-6.10	102.90	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1028	HIS	CG-CD2-NE2	6.02	113.22	107.20
1	A	1027	ALA	CA-C-N	-5.94	113.96	122.93
1	A	1027	ALA	C-N-CA	-5.94	113.96	122.93
1	C	959	HIS	ND1-CE1-NE2	-5.90	102.50	108.40
1	C	959	HIS	CE1-NE2-CD2	-5.82	103.19	109.00
2	D	237	HIS	CG-ND1-CE1	5.65	118.91	109.30
1	C	959	HIS	CG-CD2-NE2	5.52	112.72	107.20
1	C	959	HIS	CA-CB-CG	-5.42	108.38	113.80
2	D	98	PRO	N-CA-C	-5.27	105.93	113.47
1	C	519	LEU	N-CA-C	5.09	116.83	111.28
2	D	237	HIS	N-CA-C	5.06	116.52	108.67

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1028	HIS	Sidechain,Mainchain
1	C	1012	HIS	Sidechain
1	C	414	HIS	Sidechain,Mainchain
1	C	959	HIS	Sidechain
2	D	237	HIS	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4954	0	4918	308	0
1	C	4980	0	4948	292	0
2	B	2714	0	2665	208	0
2	D	2714	0	2665	150	0
3	E	1023	0	561	73	0
4	F	1027	0	566	81	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	2	0	0	0	0
6	C	2	0	0	0	0
All	All	17418	0	16323	1023	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 31.

All (1023) 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:D:86:LYS:NZ	2:D:125:GLU:OE2	1.79	1.13
1:C:435:LYS:NZ	1:C:439:GLU:OE2	1.81	1.12
1:A:638:LYS:NZ	1:A:683:ASP:OD2	1.85	1.10
2:B:76:ALA:HB3	2:B:93:HIS:O	1.53	1.07
2:D:159:ARG:NH1	2:D:205:SER:OG	1.87	1.07
1:C:1023:LYS:O	1:C:1027:ALA:N	1.88	1.05
1:A:641:ARG:NH1	1:A:983:ASN:O	1.91	1.04
1:C:410:ARG:NH1	3:E:41:DA:N3	2.07	1.02
2:D:338:THR:HG22	2:D:340:PRO:HA	1.43	1.01
1:A:860:ARG:O	1:A:860:ARG:NH1	1.95	0.99
2:B:310:GLU:OE2	2:B:344:HIS:ND1	1.97	0.97
2:B:86:LYS:NZ	2:B:87:PRO:O	1.96	0.97
1:C:641:ARG:NH1	1:C:987:ASN:OD1	1.97	0.97
1:C:778:ARG:NH1	1:C:798:VAL:O	1.98	0.97
2:B:1:MET:HA	2:B:349:SER:O	1.63	0.96
2:D:1:MET:HA	2:D:349:SER:O	1.65	0.96
1:A:412:ARG:NH1	1:C:441:GLU:O	1.99	0.95
1:C:675:ARG:NH1	1:C:1014:TRP:O	1.99	0.94
2:D:167:ARG:NH1	2:D:172:TRP:O	1.99	0.94
1:C:745:SER:O	1:C:756:ARG:NH1	2.00	0.94
1:C:575:ARG:NH1	1:C:576:PHE:O	2.01	0.93
1:A:435:LYS:NZ	1:A:439:GLU:OE2	2.02	0.93
1:A:573:SER:O	1:A:574:ARG:NH1	2.01	0.92
1:A:846:GLU:OE2	1:A:850:ARG:NH2	2.03	0.92
1:A:840:LYS:NZ	1:A:842:ASN:O	2.03	0.92
1:A:575:ARG:NH1	1:A:576:PHE:O	2.03	0.92
3:E:9:DC:N3	4:F:42:DG:N1	2.20	0.90
1:C:814:ASP:OD2	1:C:817:HIS:ND1	2.04	0.90
1:C:882:ARG:NH1	1:C:886:GLU:OE2	2.03	0.90
1:C:665:GLU:OE2	1:C:667:LYS:N	2.07	0.88
1:A:626:SER:O	1:A:994:ARG:NH1	2.07	0.88
1:A:789:GLU:OE2	1:A:797:ARG:NH2	2.06	0.87
1:A:756:ARG:NH1	1:A:954:ILE:O	2.07	0.87
1:C:778:ARG:NH1	1:C:799:LYS:HB2	1.89	0.87
1:A:577:ARG:NH1	2:B:170:GLN:OE1	2.06	0.87
1:A:882:ARG:HH12	1:A:906:ASP:CG	1.83	0.87
1:C:424:LYS:NZ	3:E:33:DG:OP1	2.07	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:PHE:HA	1:A:513:ARG:HH11	1.40	0.86
1:A:738:GLU:OE2	1:A:775:ASN:ND2	2.09	0.86
2:B:39:ARG:NH1	4:F:40:DC:OP2	2.09	0.86
2:B:339:PRO:HB2	2:B:341:GLU:OE1	1.76	0.86
3:E:37:DC:O2	4:F:14:DG:N2	2.09	0.86
2:B:128:GLU:OE2	2:B:130:VAL:HG23	1.76	0.85
1:C:877:ARG:HE	1:C:916:ARG:HH12	1.20	0.85
1:A:566:ASP:OD2	2:B:138:TYR:OH	1.96	0.83
1:C:774:GLU:OE2	1:C:778:ARG:NE	2.09	0.83
1:C:671:GLU:OE2	1:C:985:SER:OG	1.95	0.83
2:B:123:ARG:NH2	2:B:125:GLU:OE2	2.12	0.83
1:C:783:ARG:O	2:D:67:SER:OG	1.96	0.83
1:A:727:THR:HG21	1:A:978:TRP:HB3	1.61	0.83
2:B:38:LYS:NZ	4:F:38:DG:OP1	2.12	0.82
1:A:713:VAL:HG13	1:A:718:ARG:HD2	1.61	0.82
1:C:598:ARG:NH2	1:C:604:ASP:OD2	2.12	0.82
1:C:956:ASN:O	1:C:960:LYS:HG2	1.79	0.81
2:B:284:ARG:NE	2:B:286:GLU:OE2	2.12	0.81
1:C:520:HIS:NE2	4:F:23:DT:OP2	2.14	0.81
1:C:778:ARG:HH12	1:C:799:LYS:HB2	1.41	0.80
1:C:789:GLU:OE2	1:C:797:ARG:NH2	2.13	0.80
3:E:9:DC:O2	4:F:42:DG:N2	2.13	0.80
2:B:165:THR:OG1	2:B:166:GLU:OE2	1.98	0.80
1:C:575:ARG:HH12	1:C:577:ARG:HA	1.44	0.80
2:B:277:TYR:OH	2:B:317:TRP:N	2.15	0.79
1:C:931:TYR:OH	1:C:961:THR:O	2.00	0.79
1:C:770:ARG:NH2	1:C:799:LYS:O	2.15	0.79
2:B:258:ILE:HD13	2:B:284:ARG:HH11	1.45	0.79
1:C:1006:LEU:HA	1:C:1009:ILE:HG22	1.64	0.78
2:D:167:ARG:HE	2:D:172:TRP:HA	1.48	0.78
1:A:996:MET:HE3	1:C:996:MET:HG2	1.66	0.77
2:B:277:TYR:HH	2:B:317:TRP:H	1.31	0.77
1:C:1026:GLU:HA	1:C:1029:LYS:HE3	1.66	0.77
2:D:218:PHE:HB2	2:D:234:ILE:HB	1.67	0.77
1:C:701:ARG:HH21	1:C:705:MET:HE1	1.49	0.76
3:E:9:DC:N4	4:F:42:DG:O6	2.17	0.76
1:A:486:CYS:SG	1:A:500:TYR:OH	2.44	0.76
2:D:152:ALA:HB2	2:D:240:LEU:HD21	1.67	0.76
1:A:903:LYS:HZ3	1:A:907:LEU:HD11	1.51	0.75
2:D:86:LYS:HZ1	2:D:123:ARG:HD3	1.50	0.75
1:A:447:LYS:NZ	1:C:463:GLU:OE2	2.12	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:877:ARG:NE	1:C:916:ARG:HH12	1.85	0.74
2:B:65:ASN:O	2:B:123:ARG:NH1	2.21	0.74
2:B:235:ARG:HB3	2:B:250:THR:HG23	1.69	0.74
1:A:590:GLU:OE2	1:A:714:GLY:N	2.15	0.74
1:A:735:ARG:HH11	1:A:735:ARG:HB3	1.52	0.74
2:B:58:ARG:NH1	2:B:118:ARG:O	2.20	0.74
2:D:331:ILE:O	2:D:343:TYR:HA	1.87	0.74
1:A:897:ARG:HH12	1:A:948:TYR:HE2	1.34	0.73
2:D:43:THR:HG22	2:D:45:ILE:H	1.54	0.73
1:C:1023:LYS:O	1:C:1027:ALA:CB	2.37	0.73
2:B:167:ARG:NH2	2:B:172:TRP:O	2.22	0.73
2:D:50:ILE:HD12	2:D:322:LEU:HD11	1.71	0.73
2:B:6:LEU:HD21	2:B:347:GLN:HB2	1.69	0.72
3:E:29:DG:N2	4:F:23:DT:O2	2.22	0.72
2:B:281:THR:HG22	2:B:315:ARG:HH12	1.55	0.72
1:A:903:LYS:NZ	1:A:907:LEU:HD11	2.03	0.72
2:B:114:ARG:HB2	2:B:120:VAL:HG13	1.72	0.72
1:C:501:HIS:CE1	1:C:505:ARG:HH11	2.07	0.72
1:A:553:ILE:HG13	1:A:576:PHE:HE1	1.55	0.72
1:C:523:ARG:HH12	3:E:25:DT:H71	1.53	0.72
1:A:485:VAL:HG12	1:A:1024:PHE:HB3	1.71	0.72
2:B:281:THR:HG22	2:B:315:ARG:NH1	2.04	0.72
2:D:341:GLU:OE2	2:D:343:TYR:N	2.23	0.71
1:C:486:CYS:SG	1:C:500:TYR:OH	2.48	0.71
2:B:283:LYS:NZ	2:B:314:SER:O	2.23	0.71
1:A:892:VAL:O	1:A:898:ARG:NH2	2.23	0.71
1:C:760:SER:HB2	1:C:954:ILE:HD11	1.72	0.71
1:C:518:PRO:CG	1:C:520:HIS:CE1	2.73	0.71
1:C:616:LYS:NZ	1:C:979:ALA:O	2.24	0.71
2:D:99:ASN:O	2:D:101:GLU:N	2.23	0.71
2:B:72:LEU:HB3	2:B:95:GLY:HA3	1.72	0.70
3:E:34:DG:O6	4:F:17:DC:N4	2.25	0.70
2:B:188:GLU:OE2	2:B:189:PHE:HD1	1.73	0.70
1:C:749:CYS:SG	1:C:752:CYS:N	2.59	0.70
2:D:339:PRO:HB2	2:D:341:GLU:H	1.57	0.70
2:B:219:LEU:HD21	2:B:256:LEU:HB3	1.73	0.70
2:D:22:LEU:HD11	2:D:92:ILE:HD11	1.74	0.70
1:A:585:ALA:HB2	1:A:675:ARG:HH12	1.57	0.70
3:E:8:DC:OP2	3:E:8:DC:H6	1.74	0.69
2:B:51:LYS:HB3	2:B:52:LYS:HE2	1.74	0.69
1:C:518:PRO:HG2	1:C:520:HIS:CE1	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:LYS:NZ	4:F:23:DT:OP1	2.19	0.69
2:B:142:LEU:HD12	2:B:155:LEU:HB2	1.74	0.69
2:B:96:ARG:NH2	2:B:100:ASN:OD1	2.25	0.69
2:B:226:SER:OG	2:B:228:CYS:SG	2.48	0.69
4:F:42:DG:H2''	4:F:43:DG:OP2	1.92	0.69
1:A:548:SER:OG	1:A:550:ASP:OD1	2.10	0.69
1:A:885:VAL:HG21	1:A:905:MET:HG2	1.75	0.69
1:A:908:TYR:O	1:A:912:LYS:HB3	1.93	0.69
1:A:756:ARG:HD2	1:A:954:ILE:H	1.58	0.68
1:C:647:MET:HE1	1:C:668:PRO:HB3	1.76	0.68
1:A:651:ILE:HD11	1:A:653:LEU:HB2	1.75	0.68
1:A:849:ARG:O	1:A:849:ARG:NH2	2.27	0.68
1:C:687:HIS:NE2	1:C:736:GLU:O	2.25	0.68
4:F:21:DT:H2'	4:F:21:DT:OP2	1.93	0.68
1:A:683:ASP:OD1	1:A:684:GLU:N	2.27	0.68
1:A:590:GLU:CG	1:A:713:VAL:HG23	2.23	0.68
3:E:28:DA:OP2	3:E:28:DA:H8	1.77	0.68
2:B:281:THR:HA	2:B:315:ARG:HH22	1.59	0.68
1:C:858:GLN:NE2	1:C:887:ALA:O	2.26	0.68
2:B:66:SER:HA	2:B:123:ARG:HH11	1.59	0.67
1:C:762:ASN:ND2	1:C:765:LEU:HB3	2.09	0.67
2:D:212:ARG:HH11	2:D:269:HIS:CE1	2.12	0.67
1:A:590:GLU:HG3	1:A:713:VAL:HG23	1.77	0.67
1:A:737:MET:HB3	1:A:807:MET:HB3	1.76	0.67
2:B:272:ILE:HG22	2:B:289:TYR:HB2	1.77	0.67
1:C:523:ARG:HH22	3:E:24:DC:H6	1.43	0.67
1:C:730:ASP:OD2	1:C:732:LYS:HB3	1.95	0.67
1:C:958:LEU:O	1:C:962:LEU:HG	1.93	0.67
2:D:308:THR:HG22	2:D:310:GLU:H	1.59	0.67
1:A:961:THR:HA	1:A:965:VAL:HG23	1.77	0.67
4:F:10:DT:H2''	4:F:11:DT:OP2	1.95	0.67
1:A:913:PRO:HA	1:A:916:ARG:HB3	1.78	0.66
1:C:954:ILE:HG22	1:C:955:THR:H	1.60	0.66
2:D:314:SER:OG	2:D:316:THR:O	2.11	0.66
1:C:749:CYS:HA	1:C:960:LYS:NZ	2.10	0.66
1:C:624:ASP:OD1	1:C:991:ARG:NH1	2.28	0.66
1:A:555:ASP:HB2	1:A:557:LEU:HD12	1.78	0.66
1:A:762:ASN:HD21	1:A:765:LEU:HB3	1.59	0.66
1:A:836:GLU:OE1	1:A:839:GLN:N	2.26	0.66
1:C:762:ASN:HD21	1:C:765:LEU:HB3	1.60	0.66
1:C:901:LEU:HA	1:C:904:LEU:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:309:SER:O	2:B:313:HIS:ND1	2.29	0.66
1:C:490:ARG:NH1	1:C:497:CYS:SG	2.69	0.66
4:F:43:DG:OP2	4:F:43:DG:H8	1.78	0.66
1:A:748:ILE:HD12	1:A:749:CYS:H	1.60	0.66
1:A:641:ARG:NH1	1:A:987:ASN:OD1	2.16	0.66
1:A:778:ARG:HH21	1:A:799:LYS:HB2	1.61	0.65
1:C:706:GLU:N	1:C:706:GLU:OE1	2.29	0.65
2:D:273:ILE:HG22	2:D:275:GLY:H	1.61	0.65
1:A:441:GLU:O	1:C:412:ARG:NH1	2.29	0.65
1:A:997:ASN:OD1	1:A:1012:HIS:NE2	2.29	0.65
2:B:76:ALA:CB	2:B:93:HIS:O	2.40	0.65
2:B:267:GLY:H	2:B:270:GLU:HB2	1.62	0.65
1:C:748:ILE:O	1:C:960:LYS:NZ	2.30	0.65
1:A:609:SER:H	1:A:653:LEU:HD12	1.62	0.65
2:B:150:LYS:HG3	2:B:240:LEU:HD23	1.79	0.65
1:C:641:ARG:NH1	1:C:983:ASN:O	2.28	0.64
4:F:24:DG:OP2	4:F:24:DG:H8	1.79	0.64
1:A:882:ARG:HH21	1:A:902:LEU:HB3	1.62	0.64
2:D:183:TYR:HA	2:D:193:THR:O	1.97	0.64
2:B:279:SER:OG	2:B:282:GLN:N	2.31	0.64
1:C:865:LEU:HG	1:C:878:ARG:NH1	2.13	0.64
1:C:745:SER:C	1:C:756:ARG:HH11	2.06	0.64
1:A:479:PHE:HA	1:A:513:ARG:NH1	2.12	0.64
2:B:2:SER:HA	2:B:305:PRO:HB3	1.79	0.64
1:C:496:SER:OG	3:E:23:DG:OP2	2.09	0.64
2:D:99:ASN:HB3	2:D:101:GLU:OE2	1.97	0.64
2:D:290:VAL:HG22	2:D:299:MET:HB2	1.80	0.64
1:C:741:GLU:CD	1:C:795:ARG:HH11	2.04	0.64
2:D:97:THR:OG1	2:D:99:ASN:O	2.12	0.64
2:B:160:SER:C	2:B:175:VAL:HG23	2.23	0.63
1:C:1022:GLN:HA	1:C:1025:MET:HG2	1.78	0.63
4:F:18:DC:H2'	4:F:19:DA:C8	2.33	0.63
1:A:1020:TYR:HD1	1:A:1021:LEU:HD12	1.62	0.63
2:B:323:GLY:O	2:B:326:THR:OG1	2.14	0.63
1:A:833:GLU:OE2	1:A:897:ARG:NH1	2.32	0.63
1:A:860:ARG:NH1	1:A:864:LYS:HA	2.13	0.63
1:A:465:LYS:HZ3	4:F:23:DT:P	2.21	0.63
1:C:877:ARG:HH21	1:C:916:ARG:NH1	1.97	0.63
2:B:278:GLN:HB3	2:B:284:ARG:NH1	2.14	0.63
2:D:238:VAL:HG12	2:D:247:LEU:HG	1.80	0.63
2:B:322:LEU:H	2:B:327:ALA:HA	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:789:GLU:HB3	1:C:793:GLU:HG3	1.81	0.63
2:D:102:LEU:HB2	2:D:136:ALA:HB1	1.80	0.63
2:D:256:LEU:HD21	2:D:284:ARG:HH12	1.64	0.63
2:D:284:ARG:NE	2:D:286:GLU:O	2.30	0.63
2:B:310:GLU:OE1	2:B:346:TYR:OH	2.17	0.62
1:A:590:GLU:CD	1:A:713:VAL:HG23	2.24	0.62
1:C:638:LYS:NZ	1:C:683:ASP:OD2	2.21	0.62
1:C:749:CYS:HA	1:C:960:LYS:HZ3	1.63	0.62
2:D:157:GLY:HA3	2:D:207:HIS:HE1	1.63	0.62
1:C:665:GLU:OE2	1:C:666:GLN:N	2.33	0.62
1:C:1023:LYS:HB3	1:C:1027:ALA:HB2	1.81	0.62
2:D:150:LYS:HD3	2:D:240:LEU:HB3	1.81	0.62
4:F:11:DT:C6	4:F:12:DT:H72	2.34	0.62
1:A:672:LEU:O	1:A:1022:GLN:NE2	2.33	0.62
2:B:338:THR:HG22	2:B:340:PRO:HA	1.80	0.62
2:D:284:ARG:NH2	2:D:288:THR:OG1	2.33	0.62
1:A:878:ARG:NH1	1:A:878:ARG:HB2	2.15	0.62
1:C:651:ILE:HD11	1:C:653:LEU:HB2	1.82	0.62
1:C:487:LEU:HD13	1:C:522:LEU:HB3	1.82	0.61
1:C:616:LYS:HZ1	1:C:978:TRP:C	2.07	0.61
1:A:430:LEU:HD21	1:C:434:VAL:HG13	1.82	0.61
1:A:665:GLU:OE2	1:A:667:LYS:N	2.25	0.61
2:B:278:GLN:HB3	2:B:284:ARG:HH12	1.65	0.61
1:C:412:ARG:HB2	1:C:426:ARG:HH12	1.64	0.61
1:C:493:THR:HG23	1:C:495:LEU:HG	1.82	0.61
1:C:418:LEU:HB2	1:C:423:GLN:HG3	1.82	0.61
1:C:555:ASP:OD2	1:C:557:LEU:HD23	2.01	0.61
2:D:137:ARG:NE	2:D:178:CYS:SG	2.73	0.61
2:B:16:GLN:NE2	2:B:73:ARG:HG3	2.15	0.61
1:A:735:ARG:HH12	1:A:741:GLU:C	2.08	0.60
1:A:835:GLY:HA3	1:A:851:TRP:CE2	2.35	0.60
2:B:293:ASP:OD1	2:B:294:ASP:N	2.34	0.60
2:B:331:ILE:O	2:B:343:TYR:HA	2.01	0.60
1:A:688:GLU:OE2	2:B:16:GLN:NE2	2.33	0.60
1:C:942:LEU:O	1:C:947:LYS:N	2.34	0.60
1:C:955:THR:HG1	1:C:957:TYR:HD1	1.49	0.60
1:C:562:VAL:HG23	1:C:569:ALA:HB3	1.82	0.60
2:D:226:SER:OG	2:D:228:CYS:SG	2.59	0.60
1:A:558:SER:OG	2:B:173:ASN:N	2.33	0.60
1:C:675:ARG:NH1	1:C:1014:TRP:CD2	2.69	0.60
3:E:19:DC:H4'	3:E:20:DA:H5'	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:26:DA:H2''	3:E:27:DC:OP2	2.00	0.60
2:B:293:ASP:HB3	2:B:296:GLY:H	1.67	0.60
2:D:4:GLN:OE1	2:D:347:GLN:NE2	2.34	0.60
3:E:25:DT:H2''	3:E:26:DA:OP2	2.00	0.60
4:F:20:DG:H2'	4:F:21:DT:C6	2.37	0.60
1:C:955:THR:OG1	1:C:957:TYR:HD1	1.85	0.59
1:C:502:LYS:O	1:C:506:THR:OG1	2.19	0.59
1:C:958:LEU:O	1:C:961:THR:HG22	2.01	0.59
1:C:1018:SER:HB3	1:C:1021:LEU:HD13	1.83	0.59
1:A:779:TYR:CE2	1:A:804:LYS:HB2	2.37	0.59
1:C:728:GLY:HA2	1:C:980:SER:HB3	1.83	0.59
1:C:752:CYS:SG	1:C:753:ASP:N	2.74	0.59
3:E:26:DA:OP2	3:E:26:DA:H8	1.86	0.59
1:A:863:MET:HG3	1:A:884:ALA:HA	1.84	0.59
1:A:753:ASP:HA	1:A:770:ARG:HH21	1.67	0.59
1:C:788:SER:HB2	2:D:65:ASN:HA	1.82	0.59
1:A:863:MET:HE2	1:A:884:ALA:HB2	1.85	0.59
2:D:308:THR:HB	2:D:311:ILE:HG22	1.84	0.59
2:B:28:VAL:HG13	2:B:48:VAL:HB	1.85	0.59
1:C:546:SER:O	1:C:577:ARG:NH2	2.35	0.59
1:C:969:VAL:HG12	1:C:975:ILE:HG13	1.84	0.59
2:D:16:GLN:HB3	2:D:34:LYS:HZ3	1.68	0.59
2:D:49:ARG:NH1	2:D:58:ARG:HD3	2.18	0.58
3:E:36:DA:H2''	3:E:37:DC:OP2	2.01	0.58
1:A:620:ASP:OD1	1:A:621:GLY:N	2.37	0.58
1:C:540:PRO:HD2	1:C:707:SER:HA	1.85	0.58
2:D:1:MET:HB3	2:D:305:PRO:HG3	1.84	0.58
2:D:132:ASP:OD2	2:D:193:THR:HA	2.03	0.58
1:A:713:VAL:HG13	1:A:718:ARG:CD	2.32	0.58
1:A:773:ASP:OD1	1:A:773:ASP:N	2.36	0.58
2:B:232:ARG:HA	2:B:255:GLY:N	2.19	0.58
1:A:538:TRP:CD2	1:A:542:LEU:HD21	2.38	0.58
1:A:571:THR:HG21	1:A:682:VAL:HG13	1.86	0.58
1:A:1011:LYS:O	1:A:1015:LEU:HG	2.04	0.58
2:B:283:LYS:HD2	2:B:317:TRP:HE1	1.67	0.58
2:D:249:CYS:SG	2:D:250:THR:N	2.76	0.58
2:B:78:ALA:HB3	2:B:91:LEU:HB2	1.86	0.58
1:C:587:LYS:NZ	1:C:712:SER:O	2.36	0.58
3:E:1:DG:H2''	3:E:2:DA:N7	2.18	0.58
2:B:132:ASP:OD2	2:B:194:ALA:N	2.28	0.58
2:B:66:SER:HB3	2:B:123:ARG:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:741:GLU:OE1	1:C:795:ARG:NH1	2.22	0.58
4:F:28:DC:H2"	4:F:29:DA:N7	2.19	0.58
1:C:893:PRO:O	1:C:898:ARG:NH2	2.34	0.57
3:E:9:DC:H2"	3:E:10:DT:OP2	2.04	0.57
1:A:502:LYS:O	1:A:506:THR:OG1	2.19	0.57
1:C:588:ASP:OD2	1:C:1018:SER:OG	2.18	0.57
1:C:1023:LYS:O	1:C:1027:ALA:HB3	2.04	0.57
4:F:11:DT:H2"	4:F:12:DT:OP2	2.04	0.57
4:F:23:DT:H2"	4:F:24:DG:C8	2.39	0.57
1:A:585:ALA:CB	1:A:675:ARG:HH12	2.17	0.57
2:B:249:CYS:SG	2:B:250:THR:N	2.75	0.57
1:C:520:HIS:NE2	4:F:23:DT:P	2.77	0.57
1:C:751:LEU:HD12	1:C:964:HIS:CG	2.40	0.57
2:D:96:ARG:NH1	2:D:138:TYR:CZ	2.69	0.57
2:B:108:MET:HE2	2:B:127:LYS:HD3	1.87	0.57
1:C:938:PHE:O	1:C:942:LEU:HG	2.04	0.57
1:C:795:ARG:NH1	2:D:39:ARG:NH1	2.52	0.57
1:A:872:ASN:OD1	3:E:18:DA:N6	2.38	0.57
2:B:284:ARG:NH1	2:B:284:ARG:HB2	2.20	0.57
3:E:38:DA:H2"	3:E:39:DA:H8	1.70	0.57
2:D:282:GLN:NE2	2:D:283:LYS:O	2.37	0.57
1:A:676:PRO:HG3	1:A:1013:HIS:CD2	2.40	0.57
1:A:912:LYS:HG3	1:A:913:PRO:HD3	1.87	0.57
2:B:71:PRO:HG2	2:B:98:PRO:HG3	1.86	0.57
2:D:159:ARG:HH12	2:D:206:PHE:HD2	1.53	0.57
2:D:167:ARG:HH11	2:D:172:TRP:CG	2.22	0.57
1:A:774:GLU:OE2	1:A:778:ARG:NH1	2.37	0.56
1:A:895:GLU:OE2	1:A:898:ARG:NH2	2.37	0.56
1:C:709:LEU:O	1:C:719:SER:HA	2.05	0.56
1:C:877:ARG:HE	1:C:916:ARG:NH1	1.97	0.56
2:D:47:GLY:H	2:D:60:ILE:HD11	1.69	0.56
1:C:575:ARG:NH1	1:C:577:ARG:HA	2.18	0.56
1:C:999:ARG:N	1:C:1000:GLN:HA	2.20	0.56
2:D:159:ARG:NH1	2:D:206:PHE:HD2	2.03	0.56
4:F:24:DG:H2"	4:F:25:DT:OP2	2.04	0.56
1:A:439:GLU:HA	1:A:444:GLY:H	1.70	0.56
1:A:534:HIS:CE1	1:A:587:LYS:NZ	2.74	0.56
1:C:750:THR:H	1:C:960:LYS:NZ	2.03	0.56
2:B:117:ASN:HB3	3:E:6:DG:H5"	1.87	0.56
2:B:148:ARG:N	2:B:149:GLY:HA2	2.21	0.56
2:D:33:GLN:NE2	2:D:35:GLY:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:269:HIS:HB3	2:D:292:LEU:HG	1.88	0.56
1:A:612:THR:N	1:A:650:SER:O	2.34	0.56
1:A:862:LYS:NZ	1:A:862:LYS:HB3	2.20	0.56
1:A:795:ARG:CZ	2:B:39:ARG:NH1	2.69	0.56
4:F:34:DG:H2''	4:F:35:DT:OP2	2.06	0.56
2:B:7:THR:N	2:B:53:GLY:O	2.38	0.56
2:B:168:THR:HG22	2:B:170:GLN:H	1.70	0.56
1:C:757:ALA:O	1:C:761:GLN:N	2.38	0.56
1:C:930:GLN:O	1:C:934:ASN:ND2	2.34	0.56
2:D:272:ILE:HD11	2:D:287:CYS:HB2	1.88	0.56
1:C:603:ASP:OD1	1:C:604:ASP:N	2.39	0.56
1:A:687:HIS:HD2	2:B:36:TRP:CD1	2.24	0.56
2:B:51:LYS:O	2:B:54:GLU:HB2	2.05	0.56
1:C:687:HIS:CD2	1:C:736:GLU:HG2	2.41	0.56
1:A:653:LEU:HD22	1:A:654:GLU:HA	1.89	0.55
2:B:273:ILE:HB	2:B:288:THR:OG1	2.05	0.55
4:F:2:DT:H2'	4:F:3:DG:C8	2.41	0.55
1:A:553:ILE:HG21	1:A:1007:GLU:HG3	1.88	0.55
2:B:221:GLY:HA2	2:B:258:ILE:O	2.06	0.55
2:D:330:ALA:HB1	2:D:343:TYR:HB3	1.89	0.55
2:D:339:PRO:HB2	2:D:341:GLU:N	2.21	0.55
3:E:41:DA:H8	3:E:41:DA:OP2	1.88	0.55
1:A:512:GLY:HA2	1:A:513:ARG:C	2.31	0.55
1:A:795:ARG:NH1	2:B:39:ARG:NH1	2.55	0.55
2:D:131:GLY:HA3	2:D:132:ASP:C	2.32	0.55
1:A:590:GLU:O	1:A:593:ILE:HG13	2.05	0.55
2:B:317:TRP:HB3	2:B:331:ILE:HD13	1.89	0.55
1:C:687:HIS:HD2	1:C:736:GLU:HG2	1.71	0.55
2:D:77:ILE:HG23	2:D:90:TYR:HE1	1.72	0.55
2:D:278:GLN:HB2	2:D:284:ARG:HB2	1.89	0.55
3:E:27:DC:H2''	3:E:28:DA:C8	2.41	0.55
2:B:219:LEU:HD11	2:B:256:LEU:N	2.21	0.55
1:C:492:ASN:CG	1:C:1025:MET:HE2	2.31	0.55
2:D:231:SER:O	2:D:255:GLY:N	2.34	0.55
1:A:509:ALA:HB1	1:C:1028:HIS:HB3	1.87	0.55
2:B:49:ARG:NH1	2:B:58:ARG:HB3	2.21	0.55
1:C:583:VAL:HG12	1:C:709:LEU:HD21	1.88	0.55
1:C:795:ARG:HH12	2:D:39:ARG:NH1	2.04	0.55
2:B:234:ILE:HD12	2:B:251:ILE:HA	1.89	0.55
1:C:577:ARG:HG3	1:C:579:ASP:OD1	2.06	0.55
1:C:619:CYS:HB3	1:C:642:PHE:HD1	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:156:PHE:HB2	2:D:182:VAL:HG12	1.88	0.55
1:A:558:SER:OG	1:A:558:SER:O	2.21	0.55
2:B:312:SER:OG	2:B:313:HIS:ND1	2.40	0.55
4:F:25:DT:H2''	4:F:26:DA:H8	1.72	0.55
1:C:621:GLY:HA2	1:C:640:VAL:HA	1.88	0.55
1:C:856:ASP:CG	1:C:867:PRO:HB3	2.31	0.55
3:E:3:DT:H2''	3:E:4:DC:C5	2.42	0.55
3:E:41:DA:OP2	3:E:41:DA:H2'	2.07	0.55
1:C:807:MET:SD	1:C:808:GLU:N	2.80	0.54
1:A:585:ALA:HB2	1:A:675:ARG:NH1	2.20	0.54
2:B:134:PRO:HA	2:B:183:TYR:CZ	2.43	0.54
1:C:683:ASP:OD1	1:C:684:GLU:N	2.40	0.54
1:A:540:PRO:HD2	1:A:707:SER:HA	1.89	0.54
1:A:534:HIS:CE1	1:A:587:LYS:HZ2	2.25	0.54
2:B:131:GLY:HA3	2:B:132:ASP:C	2.32	0.54
2:B:163:PRO:HB2	2:B:166:GLU:OE2	2.08	0.54
2:B:300:GLU:OE2	2:B:302:ARG:HG2	2.07	0.54
1:C:420:ARG:HA	1:C:423:GLN:HB2	1.89	0.54
1:A:748:ILE:HD12	1:A:749:CYS:N	2.23	0.54
2:B:233:LEU:HB3	2:B:252:LEU:HD23	1.89	0.54
1:A:811:PRO:HG2	1:A:971:ARG:HH12	1.72	0.54
1:C:553:ILE:HG13	1:C:576:PHE:HE1	1.71	0.54
1:C:557:LEU:O	2:D:173:ASN:ND2	2.40	0.54
2:D:229:ARG:HH12	2:D:280:GLU:N	2.06	0.54
2:B:118:ARG:NH1	4:F:48:DA:O3'	2.40	0.54
1:C:518:PRO:HB2	1:C:520:HIS:CE1	2.43	0.54
1:A:540:PRO:O	1:A:707:SER:OG	2.22	0.54
1:C:536:PHE:CE1	1:C:549:TRP:HB2	2.43	0.54
2:D:94:GLY:H	2:D:140:HIS:CE1	2.26	0.54
2:D:277:TYR:HH	2:D:317:TRP:CD1	2.25	0.54
1:C:574:ARG:NH2	1:C:1003:THR:O	2.41	0.54
1:A:831:GLN:NE2	1:A:848:ARG:O	2.41	0.53
1:C:590:GLU:HA	1:C:593:ILE:HG22	1.90	0.53
4:F:13:DT:H4'	4:F:14:DG:OP1	2.06	0.53
4:F:25:DT:H2''	4:F:26:DA:C8	2.43	0.53
1:A:823:ALA:HB1	1:A:879:LEU:HD23	1.89	0.53
1:C:412:ARG:HB2	1:C:426:ARG:NH1	2.23	0.53
1:C:858:GLN:HE21	1:C:888:VAL:HA	1.74	0.53
2:D:265:PRO:HB3	2:D:271:TYR:CE2	2.42	0.53
4:F:17:DC:H2''	4:F:18:DC:C6	2.43	0.53
1:A:508:LYS:HE3	1:A:514:GLN:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:840:LYS:HE3	1:A:847:GLU:OE2	2.08	0.53
1:A:980:SER:O	1:A:983:ASN:HB3	2.07	0.53
1:C:579:ASP:OD1	1:C:579:ASP:N	2.40	0.53
4:F:46:DA:H2"	4:F:47:DG:C8	2.44	0.53
1:A:603:ASP:OD1	1:A:605:SER:N	2.39	0.53
1:A:735:ARG:HB3	1:A:735:ARG:NH1	2.20	0.53
1:C:997:ASN:ND2	3:E:23:DG:OP1	2.42	0.53
1:A:735:ARG:HH12	1:A:740:LEU:C	2.17	0.53
2:B:212:ARG:NH1	2:B:293:ASP:HA	2.23	0.53
2:B:288:THR:HB	2:B:299:MET:HE1	1.89	0.53
1:C:1023:LYS:O	1:C:1027:ALA:CA	2.57	0.53
1:C:955:THR:OG1	1:C:957:TYR:CD1	2.62	0.53
2:B:257:THR:HG23	2:B:257:THR:O	2.09	0.53
2:B:286:GLU:OE1	2:B:286:GLU:N	2.40	0.53
3:E:3:DT:H2"	3:E:4:DC:C6	2.44	0.53
1:A:779:TYR:CZ	1:A:804:LYS:HB2	2.44	0.53
1:C:798:VAL:HG22	1:C:801:VAL:HB	1.91	0.53
4:F:7:DG:H2'	4:F:8:DG:C8	2.44	0.53
2:B:217:TYR:HB3	2:B:233:LEU:HD11	1.91	0.52
2:B:273:ILE:O	2:B:288:THR:OG1	2.19	0.52
1:C:671:GLU:OE2	1:C:986:GLY:N	2.43	0.52
2:B:47:GLY:N	2:B:60:ILE:HD11	2.24	0.52
1:C:871:MET:HG3	1:C:875:TYR:HB3	1.91	0.52
2:D:232:ARG:HD3	2:D:232:ARG:H	1.74	0.52
4:F:24:DG:OP2	4:F:24:DG:C8	2.62	0.52
2:B:104:SER:OG	2:B:134:PRO:O	2.28	0.52
2:D:16:GLN:HB3	2:D:34:LYS:NZ	2.25	0.52
1:A:479:PHE:CA	1:A:513:ARG:HH11	2.19	0.52
1:C:683:ASP:OD1	1:C:685:SER:N	2.38	0.52
2:D:338:THR:CG2	2:D:340:PRO:HA	2.30	0.52
3:E:27:DC:OP2	3:E:27:DC:H6	1.93	0.52
1:A:613:VAL:HB	1:A:722:PHE:CD2	2.45	0.52
1:A:753:ASP:HB3	1:A:770:ARG:HE	1.75	0.52
2:B:232:ARG:HB2	2:B:252:LEU:O	2.09	0.52
1:C:644:PHE:O	1:C:675:ARG:HB2	2.10	0.52
1:C:974:SER:OG	1:C:975:ILE:N	2.43	0.52
4:F:38:DG:H2"	4:F:39:DA:OP2	2.09	0.52
1:A:555:ASP:OD1	1:A:555:ASP:N	2.40	0.51
2:B:113:SER:N	2:B:121:THR:OG1	2.38	0.51
2:B:279:SER:HG	2:B:282:GLN:H	1.55	0.51
1:C:650:SER:HA	1:C:662:ILE:HG13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:863:MET:O	1:C:878:ARG:NH1	2.43	0.51
1:A:583:VAL:HG12	1:A:709:LEU:HD21	1.92	0.51
1:A:687:HIS:CG	1:A:736:GLU:OE2	2.63	0.51
1:A:733:MET:HG2	1:A:737:MET:HE2	1.92	0.51
1:C:538:TRP:CZ3	1:C:709:LEU:HB2	2.45	0.51
2:D:230:PRO:HB2	2:D:232:ARG:CD	2.41	0.51
1:A:558:SER:HG	2:B:173:ASN:H	1.56	0.51
1:C:649:ILE:HG22	1:C:663:PHE:HD2	1.75	0.51
1:C:1029:LYS:O	1:C:1029:LYS:HG2	2.11	0.51
2:D:159:ARG:NH1	2:D:206:PHE:CD2	2.78	0.51
3:E:16:DA:H2''	3:E:17:DC:H5'	1.92	0.51
4:F:9:DT:H2'	4:F:10:DT:C6	2.45	0.51
1:A:926:ASP:OD1	1:A:926:ASP:N	2.43	0.51
2:B:96:ARG:NH2	2:B:161:TYR:OH	2.44	0.51
2:B:211:ALA:HB2	2:B:216:VAL:HG13	1.93	0.51
1:A:731:GLU:HG3	1:A:735:ARG:HD2	1.92	0.51
1:A:735:ARG:HH11	1:A:735:ARG:CB	2.21	0.51
1:A:778:ARG:HB2	1:A:801:VAL:HG11	1.93	0.51
1:C:617:GLU:HA	1:C:644:PHE:HA	1.93	0.51
1:C:787:PHE:CE1	1:C:797:ARG:NH1	2.78	0.51
2:D:129:LEU:HB3	2:D:192:CYS:SG	2.50	0.51
1:A:671:GLU:OE1	1:A:671:GLU:N	2.43	0.51
1:A:834:ILE:HD12	1:A:891:LEU:HB2	1.92	0.51
2:D:206:PHE:HD1	2:D:260:SER:HB2	1.75	0.51
4:F:10:DT:H1'	4:F:11:DT:H5'	1.92	0.51
2:D:283:LYS:HD2	2:D:317:TRP:NE1	2.26	0.51
1:A:492:ASN:ND2	1:C:502:LYS:NZ	2.59	0.51
1:A:594:MET:O	1:A:598:ARG:HG3	2.10	0.51
1:C:751:LEU:HA	1:C:770:ARG:HB2	1.93	0.51
1:C:752:CYS:HB2	1:C:767:SER:O	2.11	0.51
3:E:5:DT:H1'	3:E:6:DG:C5	2.45	0.51
1:A:991:ARG:HH21	1:A:991:ARG:HB2	1.76	0.51
2:D:130:VAL:N	2:D:190:GLY:O	2.30	0.51
1:A:538:TRP:CZ3	1:A:709:LEU:HB2	2.46	0.50
1:A:546:SER:O	1:A:577:ARG:NH2	2.43	0.50
1:A:992:ARG:HH22	3:E:21:DG:H3'	1.77	0.50
1:C:579:ASP:OD1	1:C:580:VAL:N	2.44	0.50
3:E:37:DC:OP2	3:E:37:DC:H6	1.94	0.50
1:A:641:ARG:NH1	1:A:987:ASN:N	2.59	0.50
2:D:6:LEU:HD22	2:D:53:GLY:HA2	1.93	0.50
1:A:958:LEU:HA	1:A:961:THR:HG22	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:132:ASP:CG	2:B:194:ALA:H	2.14	0.50
2:D:180:PRO:HB3	2:D:202:ASP:C	2.36	0.50
3:E:44:DC:H4'	3:E:45:DC:OP1	2.11	0.50
2:B:258:ILE:HD13	2:B:284:ARG:HD2	1.94	0.50
1:C:912:LYS:HA	1:C:915:TRP:CZ3	2.45	0.50
1:C:1001:SER:O	1:C:1005:GLU:N	2.44	0.50
1:C:1025:MET:N	1:C:1025:MET:SD	2.85	0.50
1:A:557:LEU:O	1:A:560:TRP:HB2	2.12	0.50
1:A:795:ARG:NH1	2:B:39:ARG:HH11	2.10	0.50
2:B:47:GLY:H	2:B:60:ILE:HD11	1.76	0.50
1:C:650:SER:OG	1:C:651:ILE:N	2.42	0.50
1:C:856:ASP:OD2	1:C:867:PRO:HB3	2.11	0.50
1:C:951:ASP:OD1	1:C:951:ASP:N	2.43	0.50
3:E:34:DG:H1'	3:E:35:DA:H5'	1.93	0.50
3:E:47:DG:H2''	3:E:48:DC:C6	2.47	0.50
2:B:109:LEU:HD12	2:B:124:CYS:SG	2.51	0.50
2:D:106:LEU:HB2	2:D:129:LEU:HD11	1.93	0.50
2:D:321:SER:HA	2:D:327:ALA:HA	1.94	0.50
1:A:611:PHE:HA	1:A:651:ILE:HA	1.93	0.50
1:A:833:GLU:OE2	1:A:948:TYR:OH	2.16	0.50
1:A:865:LEU:HD21	1:A:878:ARG:HG2	1.93	0.50
3:E:35:DA:H2''	3:E:36:DA:C8	2.46	0.50
1:A:439:GLU:HA	1:A:444:GLY:N	2.27	0.50
2:B:229:ARG:HB3	2:B:257:THR:OG1	2.12	0.50
1:C:931:TYR:CD1	1:C:966:PRO:HG3	2.47	0.50
1:C:942:LEU:HD22	1:C:950:TYR:CE2	2.47	0.50
2:D:73:ARG:HH21	2:D:96:ARG:HD2	1.76	0.50
4:F:4:DC:H2''	4:F:5:DA:C8	2.46	0.50
2:B:8:ALA:HA	2:B:55:LEU:HB3	1.92	0.50
1:C:675:ARG:HD2	1:C:1014:TRP:CZ3	2.46	0.50
1:C:919:CYS:SG	1:C:922:ARG:NH1	2.85	0.50
2:D:159:ARG:HH21	2:D:224:LEU:HB2	1.77	0.50
1:A:882:ARG:NH1	1:A:906:ASP:CG	2.63	0.49
1:A:1002:LYS:O	1:A:1005:GLU:HG2	2.12	0.49
2:B:138:TYR:CE1	2:B:159:ARG:HB2	2.47	0.49
2:B:168:THR:O	2:B:172:TRP:N	2.46	0.49
2:D:147:SER:HB2	2:D:240:LEU:HB2	1.94	0.49
1:A:898:ARG:O	1:A:902:LEU:HG	2.12	0.49
1:C:520:HIS:CD2	4:F:23:DT:OP2	2.65	0.49
3:E:28:DA:H2''	3:E:29:DG:C8	2.47	0.49
1:A:735:ARG:NH1	1:A:741:GLU:C	2.70	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:696:PRO:HG3	2:D:172:TRP:HB3	1.94	0.49
2:D:197:LEU:HB2	2:D:200:LEU:HB2	1.94	0.49
2:B:293:ASP:HB3	2:B:298:HIS:HE1	1.78	0.49
4:F:12:DT:OP2	4:F:12:DT:H6	1.96	0.49
1:A:697:VAL:O	1:A:700:GLU:HG2	2.12	0.49
1:A:988:LYS:HE3	3:E:20:DA:H3'	1.94	0.49
1:A:820:ILE:HG23	1:A:871:MET:HG2	1.94	0.49
1:C:851:TRP:HA	1:C:854:THR:HG22	1.94	0.49
1:C:939:ALA:HA	1:C:942:LEU:HD12	1.94	0.49
1:C:946:PHE:HA	1:C:948:TYR:HD1	1.77	0.49
1:A:491:VAL:HG11	1:A:1015:LEU:HD13	1.94	0.49
1:A:577:ARG:HB3	1:A:580:VAL:HG23	1.94	0.49
1:A:579:ASP:O	1:A:583:VAL:HG13	2.12	0.49
1:A:727:THR:O	1:A:729:TYR:N	2.46	0.49
1:A:778:ARG:O	1:A:781:ILE:HG22	2.13	0.49
1:A:856:ASP:HA	1:A:859:LEU:HD12	1.94	0.49
1:C:577:ARG:NH1	1:C:577:ARG:HG2	2.28	0.49
1:C:667:LYS:HB3	1:C:670:SER:HB3	1.95	0.49
2:B:265:PRO:HB3	2:B:271:TYR:CE2	2.48	0.49
1:C:618:SER:HB2	1:C:728:GLY:HA3	1.93	0.49
1:C:686:ASP:OD2	1:C:689:THR:OG1	2.29	0.49
1:C:798:VAL:HG13	1:C:801:VAL:H	1.78	0.49
2:B:83:GLN:NE2	2:B:84:ASP:O	2.46	0.48
2:B:138:TYR:HE1	2:B:159:ARG:HB2	1.79	0.48
1:C:712:SER:O	1:C:712:SER:OG	2.30	0.48
1:C:779:TYR:CZ	1:C:804:LYS:HB2	2.48	0.48
1:C:877:ARG:HH21	1:C:916:ARG:HH12	1.59	0.48
1:A:747:TYR:HE2	1:A:799:LYS:HZ1	1.61	0.48
2:B:38:LYS:NZ	4:F:38:DG:H5''	2.28	0.48
1:C:421:ARG:NH2	4:F:14:DG:O6	2.46	0.48
2:D:134:PRO:HB2	2:D:137:ARG:NH1	2.28	0.48
1:C:708:ARG:HA	1:C:708:ARG:HD3	1.66	0.48
4:F:1:DC:H3'	4:F:2:DT:H71	1.96	0.48
1:A:843:PRO:HD2	1:A:848:ARG:NH1	2.29	0.48
1:A:898:ARG:O	1:A:901:LEU:HG	2.13	0.48
1:C:651:ILE:O	1:C:659:GLY:HA2	2.13	0.48
2:D:2:SER:O	2:D:348:VAL:HA	2.13	0.48
2:D:229:ARG:HD2	2:D:278:GLN:O	2.13	0.48
1:A:539:GLN:CD	1:A:710:ILE:HD11	2.38	0.48
2:B:182:VAL:HG22	2:B:195:HIS:HB2	1.96	0.48
1:C:762:ASN:HD21	1:C:765:LEU:CB	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:877:ARG:CZ	1:C:916:ARG:HH12	2.26	0.48
2:D:37:PRO:HB3	2:D:41:CYS:O	2.13	0.48
2:D:135:SER:OG	2:D:137:ARG:NH2	2.46	0.48
2:D:167:ARG:NH1	2:D:172:TRP:CD2	2.81	0.48
2:D:212:ARG:HB2	2:D:269:HIS:CD2	2.48	0.48
2:B:22:LEU:HD13	2:B:90:TYR:CG	2.48	0.48
2:B:115:GLY:H	2:B:116:CYS:HA	1.79	0.48
1:C:751:LEU:HD22	1:C:811:PRO:HB2	1.96	0.48
1:C:819:ASP:OD1	1:C:915:TRP:NE1	2.47	0.48
2:D:1:MET:HG2	2:D:350:PHE:HA	1.96	0.48
3:E:26:DA:OP2	3:E:26:DA:H2'	2.13	0.48
2:B:135:SER:N	2:B:137:ARG:HH12	2.12	0.48
2:B:211:ALA:HA	2:B:216:VAL:HA	1.95	0.48
1:C:523:ARG:HH12	3:E:25:DT:C7	2.22	0.48
2:D:148:ARG:N	2:D:149:GLY:HA2	2.29	0.48
1:A:465:LYS:NZ	4:F:23:DT:P	2.86	0.48
1:A:878:ARG:HB2	1:A:878:ARG:HH11	1.78	0.48
2:B:75:PRO:HG2	2:B:77:ILE:HD11	1.94	0.48
2:B:210:LEU:HD13	2:B:292:LEU:HD21	1.95	0.48
2:B:228:CYS:SG	2:B:230:PRO:HD3	2.54	0.48
2:B:266:ILE:HD13	2:B:350:PHE:CD2	2.49	0.48
1:C:657:ASP:OD1	1:C:657:ASP:N	2.46	0.48
2:D:87:PRO:HA	2:D:88:GLU:HA	1.53	0.48
3:E:20:DA:C4	3:E:21:DG:C6	3.02	0.48
1:A:818:CYS:SG	1:A:819:ASP:N	2.87	0.48
2:B:290:VAL:HG13	2:B:298:HIS:H	1.79	0.47
2:D:97:THR:HB	2:D:98:PRO:HD2	1.96	0.47
2:B:204:GLN:HG3	2:B:207:HIS:CD2	2.48	0.47
1:C:518:PRO:CB	1:C:520:HIS:CE1	2.96	0.47
1:C:774:GLU:CD	1:C:778:ARG:HE	2.14	0.47
1:C:410:ARG:NH1	3:E:41:DA:C4	2.80	0.47
1:C:696:PRO:HG3	2:D:172:TRP:CB	2.45	0.47
1:C:877:ARG:HH21	1:C:916:ARG:CZ	2.27	0.47
4:F:22:DC:OP2	4:F:22:DC:H2'	2.14	0.47
2:B:69:LEU:HD22	2:B:124:CYS:SG	2.54	0.47
1:C:877:ARG:NH2	1:C:916:ARG:HH12	2.11	0.47
3:E:41:DA:H2''	3:E:42:DA:C8	2.49	0.47
4:F:44:DC:H2''	4:F:45:DC:C6	2.49	0.47
1:A:760:SER:HB2	1:A:952:GLY:HA2	1.97	0.47
1:C:575:ARG:HB2	1:C:678:CYS:HB2	1.97	0.47
1:C:651:ILE:HB	1:C:662:ILE:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:961:THR:HA	1:C:965:VAL:HG23	1.97	0.47
2:D:146:ASN:HA	2:D:150:LYS:O	2.14	0.47
2:D:159:ARG:HH11	2:D:205:SER:HG	1.59	0.47
2:D:202:ASP:OD1	2:D:203:GLY:N	2.48	0.47
2:D:206:PHE:CD1	2:D:260:SER:HB2	2.50	0.47
2:D:229:ARG:HH12	2:D:280:GLU:H	1.62	0.47
1:A:492:ASN:O	1:C:502:LYS:NZ	2.47	0.47
1:A:828:LYS:HD3	1:A:949:ARG:HH22	1.79	0.47
1:A:835:GLY:HA3	1:A:851:TRP:CD2	2.49	0.47
2:B:306:GLN:N	2:B:306:GLN:OE1	2.48	0.47
1:C:590:GLU:O	1:C:593:ILE:HG22	2.15	0.47
1:A:542:LEU:HB2	1:A:545:VAL:HB	1.95	0.47
1:A:553:ILE:HD12	1:A:553:ILE:H	1.80	0.47
2:B:94:GLY:H	2:B:140:HIS:CE1	2.33	0.47
1:C:415:LEU:HD21	1:C:427:LEU:HD11	1.96	0.47
4:F:7:DG:H2'	4:F:8:DG:H8	1.80	0.47
1:A:698:VAL:HG23	1:A:701:ARG:NH2	2.30	0.47
1:A:742:ALA:O	4:F:39:DA:H5''	2.15	0.47
1:A:971:ARG:HE	1:A:972:ASP:CG	2.23	0.47
1:C:913:PRO:O	1:C:917:SER:N	2.48	0.47
1:A:675:ARG:HD2	1:A:1014:TRP:CZ3	2.50	0.47
1:C:428:ARG:O	1:C:432:ASN:ND2	2.44	0.47
1:C:924:CYS:HB2	1:C:927:GLN:HB2	1.95	0.47
2:D:164:PRO:HA	2:D:167:ARG:HB2	1.97	0.47
2:D:167:ARG:HH11	2:D:172:TRP:C	2.18	0.47
4:F:47:DG:C5	4:F:48:DA:C6	3.02	0.47
1:A:555:ASP:HA	1:A:574:ARG:HD3	1.97	0.46
2:B:232:ARG:HD2	2:B:232:ARG:O	2.15	0.46
1:A:511:SER:O	1:A:513:ARG:HB3	2.16	0.46
1:A:871:MET:O	3:E:18:DA:N6	2.47	0.46
1:A:957:TYR:OH	3:E:16:DA:OP1	2.32	0.46
2:B:114:ARG:HA	2:B:115:GLY:HA2	1.65	0.46
2:B:150:LYS:HE3	2:B:242:LEU:HD21	1.97	0.46
1:C:652:ARG:NH1	1:C:655:GLY:O	2.47	0.46
2:D:332:PRO:HA	2:D:342:ALA:O	2.15	0.46
4:F:27:DG:C5	4:F:28:DC:C4	3.04	0.46
1:A:645:THR:OG1	1:A:674:CYS:HA	2.15	0.46
1:A:748:ILE:HG21	1:A:756:ARG:HD3	1.97	0.46
1:A:897:ARG:NH1	1:A:948:TYR:HE2	2.09	0.46
1:C:742:ALA:HA	1:C:743:SER:HA	1.54	0.46
2:D:217:TYR:HD1	2:D:233:LEU:HD21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:849:ARG:HH22	1:A:852:ARG:HB3	1.81	0.46
2:B:242:LEU:HA	2:B:243:GLY:HA2	1.54	0.46
1:C:526:GLU:C	1:C:530:LEU:HG	2.39	0.46
1:A:590:GLU:HG3	1:A:713:VAL:CG2	2.44	0.46
1:C:645:THR:HG21	1:C:673:SER:HB2	1.96	0.46
1:A:989:LEU:HD22	1:A:1016:TYR:HE2	1.80	0.46
1:C:679:LEU:C	1:C:680:MET:HG3	2.40	0.46
2:D:229:ARG:HH22	2:D:280:GLU:HB2	1.80	0.46
1:A:742:ALA:HA	1:A:743:SER:HA	1.52	0.46
2:B:79:HIS:C	2:B:79:HIS:CD2	2.93	0.46
2:D:140:HIS:HB2	2:D:155:LEU:HD11	1.98	0.46
1:A:426:ARG:NE	1:C:442:GLU:OE1	2.41	0.46
2:B:290:VAL:HG23	2:B:299:MET:HE2	1.96	0.46
2:B:314:SER:HB3	2:B:331:ILE:HD12	1.98	0.46
1:C:913:PRO:HA	1:C:916:ARG:HB2	1.97	0.46
4:F:26:DA:H2"	4:F:27:DG:H8	1.80	0.46
1:A:603:ASP:OD2	1:A:606:MET:HB2	2.16	0.46
1:A:995:LYS:HB3	1:A:996:MET:SD	2.56	0.46
2:B:135:SER:O	2:B:137:ARG:HG2	2.15	0.46
2:B:168:THR:HB	2:B:171:ASN:HB2	1.98	0.46
1:C:579:ASP:O	1:C:583:VAL:HG13	2.15	0.46
1:C:643:SER:OG	1:C:644:PHE:N	2.49	0.46
1:C:749:CYS:HB2	1:C:959:HIS:NE2	2.31	0.46
2:D:39:ARG:HA	2:D:39:ARG:HD2	1.62	0.46
2:D:73:ARG:HH21	2:D:96:ARG:HH21	1.64	0.46
3:E:7:DG:N2	4:F:45:DC:O2	2.49	0.46
1:A:536:PHE:HB3	1:A:711:ILE:HD11	1.99	0.46
1:A:687:HIS:HD2	2:B:36:TRP:HD1	1.64	0.46
1:A:731:GLU:OE1	1:A:750:THR:OG1	2.34	0.46
1:A:876:ALA:HA	1:A:879:LEU:HB3	1.98	0.46
1:A:944:SER:OG	1:A:945:MET:N	2.48	0.46
1:C:557:LEU:HD12	1:C:560:TRP:HE3	1.81	0.46
1:C:750:THR:H	1:C:960:LYS:HZ3	1.64	0.46
1:C:993:PHE:HE2	1:C:1013:HIS:HA	1.81	0.46
2:D:3:LEU:HD21	2:D:306:GLN:O	2.16	0.46
2:D:66:SER:HB2	2:D:124:CYS:H	1.81	0.46
3:E:30:DA:OP2	3:E:30:DA:H8	1.99	0.46
1:A:687:HIS:ND1	1:A:736:GLU:OE2	2.48	0.45
1:A:927:GLN:CD	1:A:927:GLN:H	2.23	0.45
2:B:289:TYR:HD2	2:B:300:GLU:HG3	1.81	0.45
1:C:513[A]:ARG:CZ	1:C:513[A]:ARG:HB3	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:523:ARG:NH2	3:E:24:DC:H2'	2.31	0.45
1:A:795:ARG:NH1	4:F:40:DC:OP1	2.48	0.45
1:A:971:ARG:NE	1:A:972:ASP:OD1	2.43	0.45
2:B:231:SER:O	2:B:256:LEU:N	2.50	0.45
1:C:419:THR:HG23	4:F:13:DT:OP2	2.16	0.45
1:C:513[B]:ARG:CZ	1:C:513[B]:ARG:HB3	2.46	0.45
1:C:954:ILE:HG22	1:C:955:THR:N	2.30	0.45
3:E:28:DA:H2''	3:E:29:DG:H8	1.81	0.45
4:F:40:DC:C2	4:F:41:DA:N7	2.84	0.45
1:A:956:ASN:O	1:A:960:LYS:HG3	2.15	0.45
1:C:615:VAL:CG1	1:C:644:PHE:HD2	2.29	0.45
1:C:817:HIS:O	1:C:820:ILE:HG22	2.16	0.45
4:F:45:DC:H2''	4:F:46:DA:N7	2.32	0.45
1:A:435:LYS:HG3	1:A:439:GLU:OE2	2.16	0.45
1:A:566:ASP:OD1	1:A:567:VAL:N	2.41	0.45
1:A:590:GLU:HA	1:A:593:ILE:HG12	1.99	0.45
1:A:919:CYS:O	1:A:923:ASP:N	2.36	0.45
1:A:927:GLN:O	1:A:931:TYR:N	2.49	0.45
2:B:38:LYS:NZ	4:F:38:DG:P	2.90	0.45
2:B:135:SER:N	2:B:137:ARG:NH1	2.64	0.45
4:F:29:DA:C8	4:F:29:DA:OP2	2.69	0.45
1:A:539:GLN:HG2	1:A:710:ILE:HD11	1.98	0.45
1:A:594:MET:SD	1:A:718:ARG:NH1	2.89	0.45
2:B:12:GLY:O	2:B:341:GLU:HA	2.16	0.45
2:B:333:SER:OG	2:B:344:HIS:N	2.49	0.45
1:C:1001:SER:O	1:C:1005:GLU:HG3	2.16	0.45
3:E:21:DG:H4'	3:E:22:DT:OP1	2.16	0.45
1:A:560:TRP:CD1	2:B:173:ASN:HB3	2.51	0.45
1:A:749:CYS:HB2	1:A:959:HIS:CD2	2.50	0.45
1:C:936:GLN:O	1:C:936:GLN:NE2	2.48	0.45
3:E:29:DG:H2''	3:E:30:DA:C8	2.52	0.45
1:A:537:GLU:CD	1:A:710:ILE:HD12	2.41	0.45
1:A:1029:LYS:HB3	1:A:1029:LYS:HE2	1.78	0.45
2:B:293:ASP:HB3	2:B:298:HIS:CE1	2.51	0.45
1:C:785:ASN:CG	1:C:789:GLU:H	2.24	0.45
4:F:24:DG:OP2	4:F:24:DG:H2'	2.16	0.45
1:A:430:LEU:HD11	1:C:434:VAL:HG22	1.98	0.45
1:A:536:PHE:HB3	1:A:711:ILE:CD1	2.46	0.45
1:A:696:PRO:HG3	2:B:172:TRP:CG	2.51	0.45
1:A:860:ARG:HA	1:A:860:ARG:HD2	1.86	0.45
1:A:862:LYS:HB3	1:A:862:LYS:HZ3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:675:ARG:HD2	1:C:1014:TRP:CE3	2.51	0.45
2:B:316:THR:OG1	2:B:317:TRP:N	2.50	0.45
2:B:327:ALA:HB3	2:B:348:VAL:HG23	1.97	0.45
1:C:558:SER:O	1:C:558:SER:OG	2.34	0.45
2:D:144:VAL:HG22	2:D:153:CYS:SG	2.56	0.45
2:D:236:LEU:HD12	2:D:238:VAL:HG11	1.98	0.45
2:D:328:LEU:HD11	2:D:345:PHE:HD2	1.82	0.45
1:A:538:TRP:CZ2	1:A:709:LEU:HD13	2.52	0.45
1:A:640:VAL:HG23	1:A:682:VAL:O	2.17	0.45
1:C:538:TRP:HB3	1:C:707:SER:OG	2.17	0.45
1:C:883:GLU:OE1	1:C:883:GLU:N	2.45	0.45
1:C:922:ARG:NH1	1:C:922:ARG:HB3	2.32	0.45
4:F:49:DT:H2''	4:F:50:DC:C5	2.52	0.45
1:A:756:ARG:HH11	1:A:954:ILE:C	2.21	0.44
1:A:762:ASN:OD1	1:A:763:MET:N	2.50	0.44
2:B:235:ARG:HE	2:B:250:THR:HG21	1.82	0.44
2:D:93:HIS:HA	2:D:94:GLY:HA2	1.66	0.44
2:D:137:ARG:NH1	2:D:183:TYR:CE2	2.85	0.44
4:F:39:DA:C5	4:F:40:DC:C4	3.05	0.44
1:A:955:THR:OG1	1:A:958:LEU:HB2	2.18	0.44
2:B:36:TRP:HZ2	2:B:99:ASN:HB3	1.81	0.44
2:B:65:ASN:C	2:B:123:ARG:NH1	2.75	0.44
2:B:317:TRP:HB3	2:B:331:ILE:CD1	2.47	0.44
1:C:753:ASP:N	1:C:753:ASP:OD1	2.50	0.44
4:F:18:DC:H2'	4:F:19:DA:H8	1.81	0.44
2:B:80:PHE:HZ	2:B:83:GLN:HE21	1.65	0.44
1:C:523:ARG:HH22	3:E:24:DC:H2'	1.81	0.44
1:C:574:ARG:NE	1:C:1007:GLU:OE1	2.34	0.44
2:D:338:THR:HG22	2:D:340:PRO:CA	2.32	0.44
3:E:29:DG:H2''	3:E:30:DA:OP2	2.17	0.44
1:A:496:SER:H	1:A:499:GLN:CD	2.25	0.44
1:C:410:ARG:HG2	1:C:411:PRO:HD2	1.99	0.44
1:C:502:LYS:HA	1:C:505:ARG:NH1	2.33	0.44
1:C:646:ILE:H	1:C:646:ILE:HG13	1.63	0.44
2:D:230:PRO:HB2	2:D:232:ARG:HD2	2.00	0.44
1:A:751:LEU:HD22	1:A:811:PRO:HB2	1.99	0.44
2:B:49:ARG:CZ	2:B:58:ARG:HD2	2.47	0.44
2:B:70:PRO:HG2	2:B:72:LEU:HD21	1.99	0.44
2:B:322:LEU:N	2:B:326:THR:O	2.50	0.44
1:C:835:GLY:HA3	1:C:851:TRP:CZ2	2.52	0.44
2:D:218:PHE:CE1	2:D:236:LEU:HD21	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:40:DC:H2''	4:F:41:DA:OP2	2.16	0.44
1:A:804:LYS:NZ	2:B:101:GLU:OE2	2.50	0.44
1:A:430:LEU:HB2	1:C:437:PHE:CG	2.53	0.44
1:A:905:MET:O	1:A:909:LEU:HG	2.18	0.44
1:A:1012:HIS:HA	1:A:1015:LEU:HD12	2.00	0.44
2:B:39:ARG:HH11	2:B:39:ARG:HG3	1.82	0.44
1:C:419:THR:O	1:C:423:GLN:N	2.33	0.44
1:A:625:VAL:HG23	1:A:637:GLU:HB2	1.99	0.44
1:A:735:ARG:O	1:A:739:GLY:N	2.49	0.44
1:A:845:ARG:NH1	1:A:845:ARG:HB2	2.33	0.44
1:A:858:GLN:HB3	1:A:888:VAL:HG22	1.99	0.44
2:B:9:VAL:HG13	2:B:10:ASN:H	1.83	0.44
1:C:966:PRO:HA	1:C:969:VAL:HG22	2.00	0.44
1:A:834:ILE:HD13	1:A:834:ILE:HA	1.85	0.44
2:B:150:LYS:HE2	2:B:240:LEU:HB3	1.98	0.44
1:C:564:VAL:HG21	2:D:315:ARG:HH12	1.82	0.44
2:D:47:GLY:N	2:D:60:ILE:HD11	2.31	0.44
1:A:747:TYR:OH	1:A:796:ASP:HA	2.17	0.43
1:A:708:ARG:NH2	1:A:719:SER:OG	2.51	0.43
1:A:798:VAL:HG23	1:A:801:VAL:H	1.83	0.43
2:B:9:VAL:HG13	2:B:10:ASN:OD1	2.18	0.43
2:B:159:ARG:HH22	2:B:206:PHE:HE2	1.64	0.43
2:B:269:HIS:HA	2:B:271:TYR:HE1	1.84	0.43
2:B:310:GLU:OE2	2:B:344:HIS:CG	2.69	0.43
1:C:894:SER:O	1:C:898:ARG:HG3	2.18	0.43
4:F:30:DC:H2''	4:F:31:DT:C6	2.53	0.43
1:A:560:TRP:CZ3	1:A:569:ALA:HA	2.53	0.43
1:A:870:ARG:NH1	3:E:17:DC:H2''	2.33	0.43
2:B:115:GLY:N	2:B:116:CYS:HA	2.33	0.43
1:C:576:PHE:HB2	1:C:677:LEU:HD12	2.01	0.43
1:C:676:PRO:HG3	1:C:1013:HIS:CG	2.53	0.43
1:C:912:LYS:HA	1:C:915:TRP:CH2	2.53	0.43
3:E:4:DC:H1'	3:E:5:DT:C6	2.52	0.43
1:A:991:ARG:HB2	1:A:991:ARG:NH2	2.33	0.43
1:C:858:GLN:NE2	1:C:891:LEU:HG	2.34	0.43
2:D:3:LEU:HB3	2:D:348:VAL:HG12	2.01	0.43
2:D:299:MET:C	2:D:300:GLU:OE2	2.61	0.43
3:E:9:DC:C2	4:F:43:DG:N2	2.86	0.43
3:E:38:DA:H2''	3:E:39:DA:C8	2.51	0.43
4:F:15:DT:H2'	4:F:16:DT:C6	2.53	0.43
1:A:429:ASP:HB2	1:C:437:PHE:HE2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:LYS:HZ1	4:F:22:DC:H3'	1.84	0.43
1:A:674:CYS:H	1:A:1017:THR:HG21	1.83	0.43
2:B:75:PRO:HA	2:B:95:GLY:HA2	2.00	0.43
1:C:675:ARG:HD3	1:C:1017:THR:HG23	1.99	0.43
2:D:6:LEU:HD11	2:D:347:GLN:HB2	2.00	0.43
2:D:79:HIS:NE2	2:D:88:GLU:OE2	2.47	0.43
4:F:4:DC:H2''	4:F:5:DA:H8	1.84	0.43
1:A:735:ARG:NH1	1:A:740:LEU:C	2.76	0.43
1:A:783:ARG:HH21	1:A:784:LYS:HG2	1.83	0.43
1:C:762:ASN:HD21	1:C:765:LEU:CA	2.31	0.43
3:E:19:DC:O2	3:E:19:DC:H5'	2.18	0.43
1:A:533:PHE:HD2	1:A:534:HIS:CE1	2.37	0.43
1:A:544:ASN:HB3	2:B:167:ARG:O	2.19	0.43
1:A:619:CYS:HB2	1:A:642:PHE:CD2	2.54	0.43
2:B:87:PRO:HA	2:B:88:GLU:HA	1.69	0.43
4:F:29:DA:H1'	4:F:30:DC:O4'	2.18	0.43
4:F:48:DA:H1'	4:F:49:DT:O4'	2.18	0.43
1:A:849:ARG:NH1	1:A:853:SER:HB3	2.34	0.43
1:A:889:CYS:SG	1:A:902:LEU:HD21	2.58	0.43
2:B:86:LYS:HA	2:B:86:LYS:HD2	1.89	0.43
2:B:237:HIS:CD2	2:B:239:GLU:OE2	2.71	0.43
1:C:493:THR:O	1:C:493:THR:OG1	2.29	0.43
1:C:676:PRO:HG3	1:C:1013:HIS:CD2	2.54	0.43
1:C:810:GLN:O	1:C:812:THR:N	2.52	0.43
1:A:568:PRO:HB2	1:A:570:ASP:OD2	2.19	0.43
1:A:795:ARG:NE	2:B:39:ARG:HD3	2.33	0.43
1:A:810:GLN:OE1	1:A:971:ARG:NH1	2.52	0.43
1:A:814:ASP:OD2	1:A:817:HIS:N	2.46	0.43
1:A:849:ARG:NH2	1:A:852:ARG:HB3	2.34	0.43
2:B:180:PRO:HG3	2:B:202:ASP:HA	2.00	0.43
2:B:290:VAL:HG22	2:B:299:MET:HB2	2.01	0.43
1:C:615:VAL:HG11	1:C:644:PHE:HD2	1.84	0.43
1:C:785:ASN:ND2	1:C:789:GLU:H	2.16	0.43
1:C:903:LYS:HD2	1:C:906:ASP:OD2	2.19	0.43
2:D:167:ARG:NH1	2:D:172:TRP:CG	2.86	0.43
2:D:259:THR:H	2:D:277:TYR:H	1.65	0.43
1:A:415:LEU:HD13	1:A:426:ARG:NE	2.34	0.43
1:A:621:GLY:N	1:A:684:GLU:OE2	2.42	0.43
1:A:992:ARG:NH2	3:E:21:DG:O5'	2.52	0.43
1:C:534:HIS:ND1	1:C:587:LYS:HG2	2.34	0.43
1:C:555:ASP:OD1	1:C:555:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:716:LEU:HD12	1:C:718:ARG:NH2	2.34	0.43
1:C:739:GLY:CA	1:C:803:ALA:HB3	2.49	0.43
1:C:926:ASP:OD1	1:C:926:ASP:N	2.50	0.43
4:F:10:DT:OP2	4:F:10:DT:H6	2.02	0.43
2:B:102:LEU:HD12	2:B:102:LEU:HA	1.86	0.42
2:B:168:THR:HG22	2:B:170:GLN:N	2.34	0.42
1:C:587:LYS:NZ	1:C:712:SER:C	2.76	0.42
1:C:751:LEU:HD12	1:C:964:HIS:CD2	2.53	0.42
2:D:322:LEU:H	2:D:327:ALA:HA	1.84	0.42
2:B:145:ILE:HB	2:B:214:ASP:HA	2.00	0.42
2:B:159:ARG:HA	2:B:177:ASP:HA	2.00	0.42
2:D:43:THR:HG21	2:D:62:PHE:HE1	1.83	0.42
4:F:21:DT:H2''	4:F:22:DC:C5	2.53	0.42
1:A:603:ASP:OD1	1:A:604:ASP:N	2.52	0.42
2:B:82:ALA:HB2	2:B:88:GLU:HB2	2.01	0.42
2:B:188:GLU:HA	2:B:189:PHE:HA	1.64	0.42
1:C:786:PRO:HG2	1:C:787:PHE:CD1	2.54	0.42
1:C:787:PHE:CD1	1:C:797:ARG:NH1	2.88	0.42
2:D:179:PRO:O	2:D:181:GLN:N	2.52	0.42
1:A:993:PHE:HB3	1:A:1009:ILE:HG13	2.01	0.42
2:B:290:VAL:HG12	2:B:292:LEU:HD12	2.01	0.42
4:F:34:DG:N3	4:F:34:DG:H2'	2.35	0.42
1:A:610:GLY:C	1:A:651:ILE:HD12	2.45	0.42
1:A:912:LYS:C	1:A:912:LYS:HD2	2.44	0.42
1:A:1027:ALA:O	1:C:509:ALA:HB1	2.19	0.42
2:B:38:LYS:HZ1	4:F:38:DG:H5''	1.83	0.42
2:B:119:LYS:HB2	3:E:6:DG:O3'	2.19	0.42
2:B:134:PRO:HA	2:B:137:ARG:HH12	1.85	0.42
2:B:295:VAL:HB	2:B:298:HIS:CE1	2.54	0.42
1:C:764:VAL:HG11	1:C:936:GLN:HA	2.01	0.42
2:D:113:SER:N	2:D:121:THR:OG1	2.50	0.42
1:A:420:ARG:NH1	1:C:459:ARG:CZ	2.82	0.42
1:A:730:ASP:OD1	1:A:732:LYS:N	2.53	0.42
1:A:748:ILE:HG23	1:A:756:ARG:HB2	2.02	0.42
2:B:119:LYS:HE2	2:B:119:LYS:HB3	1.80	0.42
2:B:256:LEU:HD11	2:B:284:ARG:NH2	2.35	0.42
2:B:318:PHE:CE2	2:B:330:ALA:HB3	2.54	0.42
1:C:708:ARG:HB3	1:C:719:SER:OG	2.19	0.42
1:C:762:ASN:HD21	1:C:765:LEU:H	1.67	0.42
4:F:46:DA:C4	4:F:47:DG:C6	3.07	0.42
1:A:496:SER:HB3	1:A:499:GLN:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:877:ARG:NH2	1:A:916:ARG:NH1	2.67	0.42
2:B:127:LYS:NZ	2:B:187:LEU:O	2.40	0.42
2:B:322:LEU:HD21	2:B:328:LEU:HB3	2.02	0.42
1:C:895:GLU:OE1	1:C:895:GLU:N	2.46	0.42
2:D:228:CYS:SG	2:D:230:PRO:HD3	2.60	0.42
2:D:242:LEU:HA	2:D:243:GLY:HA2	1.51	0.42
1:A:487:LEU:HB2	1:A:522:LEU:HD22	2.02	0.42
1:A:647:MET:HE3	1:A:647:MET:HB3	1.68	0.42
1:A:732:LYS:HB3	1:A:732:LYS:HE2	1.69	0.42
1:A:878:ARG:HH11	1:A:878:ARG:HD3	1.65	0.42
1:A:946:PHE:HA	1:A:948:TYR:CE2	2.55	0.42
2:B:212:ARG:HG3	2:B:269:HIS:ND1	2.34	0.42
2:D:236:LEU:HA	2:D:249:CYS:HA	2.01	0.42
3:E:49:DA:H2	4:F:2:DT:H3	1.68	0.42
1:A:532:GLY:H	1:A:580:VAL:CG1	2.33	0.42
1:A:713:VAL:CG1	1:A:718:ARG:HD2	2.41	0.42
1:A:731:GLU:O	1:A:735:ARG:HG3	2.20	0.42
1:A:825:GLU:OE1	1:A:955:THR:HG21	2.19	0.42
1:A:1017:THR:HA	1:A:1022:GLN:NE2	2.35	0.42
2:B:197:LEU:HD23	2:B:197:LEU:HA	1.77	0.42
1:C:838:TYR:CZ	1:C:897:ARG:HG3	2.55	0.42
2:D:69:LEU:HD13	2:D:107:TYR:CZ	2.55	0.42
2:D:310:GLU:OE2	2:D:344:HIS:CE1	2.73	0.42
3:E:22:DT:H2''	3:E:23:DG:C8	2.55	0.42
4:F:3:DG:H2'	4:F:4:DC:C6	2.55	0.42
1:A:688:GLU:OE1	2:B:73:ARG:NH2	2.51	0.42
2:B:155:LEU:HB3	2:B:183:TYR:HB2	2.01	0.42
2:B:284:ARG:HH11	2:B:284:ARG:HB2	1.85	0.42
2:B:341:GLU:C	2:B:343:TYR:H	2.28	0.42
1:C:708:ARG:CZ	1:C:721:ARG:HG3	2.50	0.42
2:D:294:ASP:OD1	2:D:295:VAL:N	2.53	0.42
1:A:492:ASN:ND2	1:A:492:ASN:O	2.38	0.41
1:A:616:LYS:HE2	1:A:616:LYS:HB3	1.69	0.41
1:A:899:GLU:HA	1:A:902:LEU:HD12	2.02	0.41
2:B:1:MET:O	2:B:1:MET:HG2	2.19	0.41
2:B:258:ILE:HD11	2:B:276:GLY:HA3	2.02	0.41
1:C:693:ILE:O	1:C:696:PRO:HD2	2.20	0.41
1:C:1029:LYS:HZ1	1:C:1030:ASN:ND2	2.18	0.41
3:E:12:DT:H2''	3:E:13:DC:OP2	2.19	0.41
1:A:975:ILE:HG12	1:A:976:GLY:H	1.85	0.41
1:C:572:ILE:HD13	1:C:1002:LYS:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:16:GLN:HE22	2:D:32:GLY:C	2.28	0.41
2:D:166:GLU:O	2:D:168:THR:OG1	2.32	0.41
4:F:27:DG:C2	4:F:28:DC:C2	3.08	0.41
1:C:795:ARG:NH1	2:D:39:ARG:CZ	2.83	0.41
1:A:451:LEU:HB2	1:C:454:PHE:CE1	2.56	0.41
1:A:535:GLN:HA	1:A:549:TRP:CD2	2.56	0.41
1:A:608:THR:HB	1:A:718:ARG:HG2	2.01	0.41
1:C:985:SER:O	1:C:988:LYS:HB3	2.19	0.41
4:F:5:DA:H2''	4:F:6:DG:C8	2.55	0.41
4:F:38:DG:C2	4:F:39:DA:C5	3.08	0.41
1:A:870:ARG:HH11	3:E:17:DC:H2''	1.85	0.41
1:A:947:LYS:HE3	1:A:947:LYS:HB2	1.87	0.41
1:A:1013:HIS:O	1:A:1016:TYR:N	2.50	0.41
1:C:499:GLN:H	1:C:499:GLN:HG3	1.55	0.41
1:C:698:VAL:HG12	1:C:702:LYS:HE2	2.00	0.41
1:C:865:LEU:HG	1:C:878:ARG:HH11	1.80	0.41
1:A:500:TYR:HD2	1:A:519:LEU:HD23	1.85	0.41
1:A:869:MET:HG2	1:A:870:ARG:N	2.35	0.41
1:A:870:ARG:NH1	3:E:18:DA:C2	2.89	0.41
2:B:134:PRO:CA	2:B:137:ARG:HH12	2.33	0.41
1:C:564:VAL:CG2	2:D:315:ARG:HH12	2.33	0.41
3:E:16:DA:H2''	3:E:17:DC:C6	2.56	0.41
3:E:28:DA:OP2	3:E:28:DA:H2'	2.21	0.41
3:E:33:DG:OP2	3:E:33:DG:H8	2.04	0.41
4:F:41:DA:C6	4:F:42:DG:C6	3.09	0.41
1:A:716:LEU:HB3	1:A:718:ARG:HE	1.86	0.41
2:B:1:MET:SD	2:B:302:ARG:NH1	2.93	0.41
2:B:6:LEU:HD12	2:B:328:LEU:HD13	2.03	0.41
2:B:93:HIS:HA	2:B:94:GLY:HA2	1.64	0.41
1:C:840:LYS:O	1:C:843:PRO:HD3	2.20	0.41
1:A:709:LEU:O	1:A:719:SER:HA	2.21	0.41
1:A:735:ARG:CZ	1:A:742:ALA:HA	2.51	0.41
2:B:198:PRO:HB2	2:B:199:GLU:OE2	2.20	0.41
1:A:456:LEU:HD13	1:C:424:LYS:HG2	2.02	0.41
1:A:459:ARG:HH12	1:A:464:HIS:HD2	1.69	0.41
1:A:555:ASP:HB3	1:A:574:ARG:CZ	2.50	0.41
1:A:612:THR:O	1:A:650:SER:N	2.42	0.41
1:A:705:MET:HE3	1:A:705:MET:HB3	1.87	0.41
1:A:749:CYS:HB3	1:A:752:CYS:O	2.20	0.41
1:A:814:ASP:OD1	1:A:979:ALA:HB1	2.21	0.41
1:A:864:LYS:HB2	1:A:864:LYS:HE3	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1028:HIS:ND1	1:A:1029:LYS:HE3	2.36	0.41
2:B:289:TYR:HB3	2:B:300:GLU:OE2	2.20	0.41
2:B:331:ILE:HD13	2:B:331:ILE:HA	1.95	0.41
1:C:582:LEU:HD23	1:C:582:LEU:HA	1.89	0.41
1:C:814:ASP:OD1	1:C:816:LEU:N	2.51	0.41
1:C:829:ILE:O	1:C:833:GLU:HG2	2.21	0.41
1:C:908:TYR:CZ	1:C:915:TRP:HH2	2.39	0.41
3:E:18:DA:H2'	3:E:19:DC:O2	2.21	0.41
1:A:459:ARG:NH1	1:A:464:HIS:HD2	2.19	0.41
1:A:479:PHE:HD1	1:A:480:GLY:H	1.68	0.41
1:A:571:THR:CG2	1:A:682:VAL:HG13	2.50	0.41
1:A:871:MET:HE2	1:A:871:MET:HB2	1.94	0.41
1:A:1002:LYS:HA	1:A:1005:GLU:OE2	2.21	0.41
1:A:1018:SER:OG	1:A:1020:TYR:HB3	2.21	0.41
1:C:600:ARG:HD3	1:C:600:ARG:HA	1.67	0.41
1:C:751:LEU:O	1:C:770:ARG:N	2.34	0.41
2:D:16:GLN:NE2	2:D:32:GLY:O	2.53	0.41
2:B:7:THR:O	2:B:54:GLU:HA	2.21	0.40
2:B:65:ASN:C	2:B:123:ARG:HH11	2.28	0.40
1:C:766:HIS:HB2	1:C:963:ALA:HB1	2.03	0.40
2:D:9:VAL:HG13	2:D:10:ASN:H	1.86	0.40
1:A:680:MET:HE3	1:A:680:MET:HB2	1.82	0.40
1:A:990:PHE:CE1	1:A:1009:ILE:HD13	2.57	0.40
1:A:1025:MET:HG3	1:A:1026:GLU:OE2	2.21	0.40
2:B:229:ARG:HH22	2:B:280:GLU:HG3	1.87	0.40
2:D:106:LEU:HD22	2:D:127:LYS:HB3	2.02	0.40
2:D:217:TYR:CD1	2:D:235:ARG:HB2	2.55	0.40
3:E:39:DA:C6	3:E:40:DA:C6	3.09	0.40
1:A:882:ARG:O	1:A:886:GLU:HG2	2.22	0.40
1:A:1020:TYR:CE2	1:A:1024:PHE:HE2	2.40	0.40
2:B:277:TYR:OH	2:B:316:THR:OG1	2.33	0.40
1:C:543:LYS:O	1:C:545:VAL:HG23	2.21	0.40
1:C:915:TRP:NE1	1:C:916:ARG:HG2	2.37	0.40
2:D:213:GLN:O	2:D:214:ASP:OD1	2.40	0.40
3:E:27:DC:C2	3:E:28:DA:C5	3.09	0.40
1:C:533:PHE:C	1:C:549:TRP:HZ3	2.30	0.40
2:D:73:ARG:HE	2:D:96:ARG:HD2	1.85	0.40
2:D:82:ALA:HB2	2:D:88:GLU:HG3	2.03	0.40
2:D:142:LEU:HA	2:D:154:VAL:O	2.21	0.40
2:D:147:SER:CB	2:D:240:LEU:H	2.34	0.40
2:D:188:GLU:HA	2:D:189:PHE:HA	1.74	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	610/1159 (53%)	557 (91%)	53 (9%)	0	100	100
1	C	613/1159 (53%)	557 (91%)	56 (9%)	0	100	100
2	B	349/533 (66%)	316 (90%)	32 (9%)	1 (0%)	36	72
2	D	349/533 (66%)	324 (93%)	25 (7%)	0	100	100
All	All	1921/3384 (57%)	1754 (91%)	166 (9%)	1 (0%)	49	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	341	GLU

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	543/1000 (54%)	543 (100%)	0	100	100
1	C	546/1000 (55%)	542 (99%)	4 (1%)	76	79
2	B	303/465 (65%)	303 (100%)	0	100	100
2	D	303/465 (65%)	303 (100%)	0	100	100
All	All	1695/2930 (58%)	1691 (100%)	4 (0%)	85	86

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	513[A]	ARG
1	C	513[B]	ARG
1	C	956	ASN
1	C	957	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	492	ASN
1	A	517	GLN
1	A	775	ASN
1	A	956	ASN
2	B	83	GLN
2	B	99	ASN
2	B	222	HIS
1	C	517	GLN
1	C	858	GLN
1	C	997	ASN
1	C	1030	ASN
2	D	4	GLN
2	D	83	GLN
2	D	99	ASN
2	D	146	ASN
2	D	269	HIS
2	D	347	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

Of 6 ligands modelled in this entry, 6 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

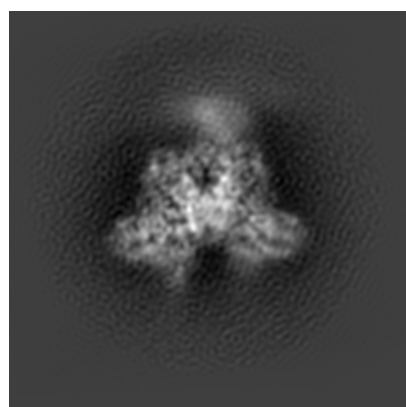
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7852. These allow visual inspection of the internal detail of the map and identification of artifacts.

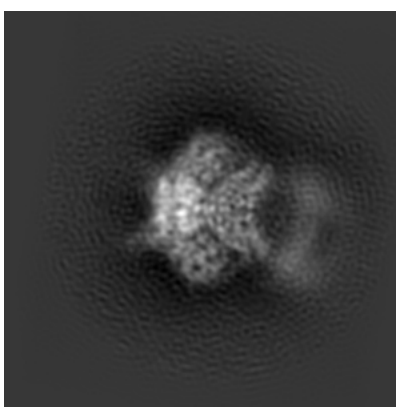
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

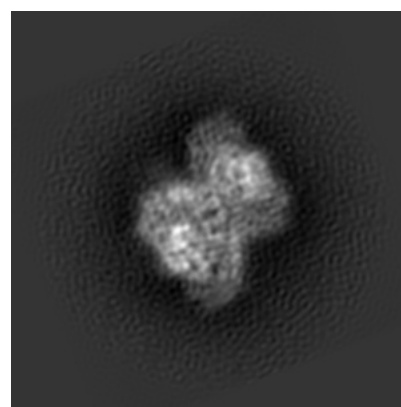
6.1.1 Primary map



X



Y

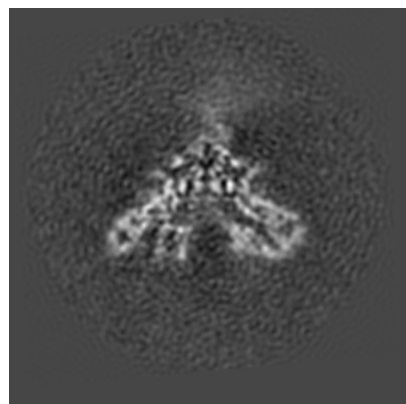


Z

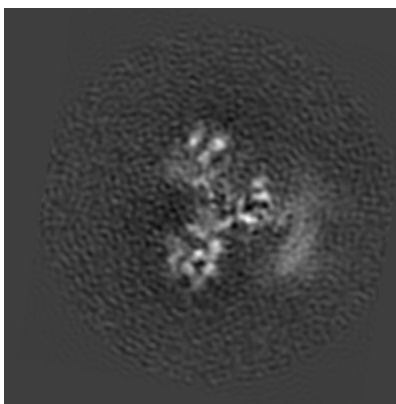
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

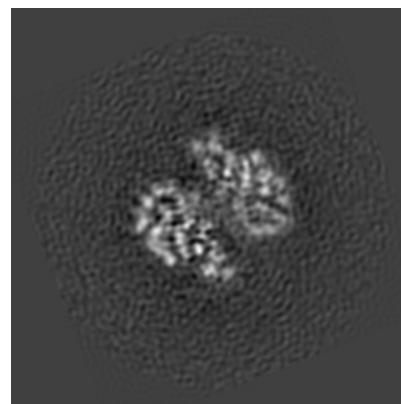
6.2.1 Primary map



X Index: 128



Y Index: 128

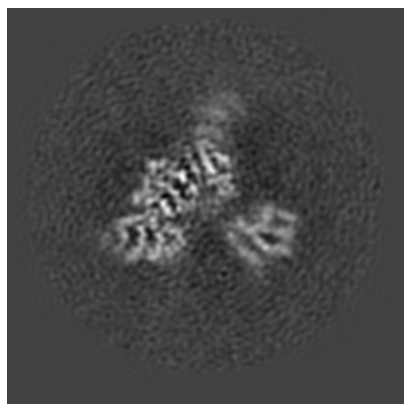


Z Index: 128

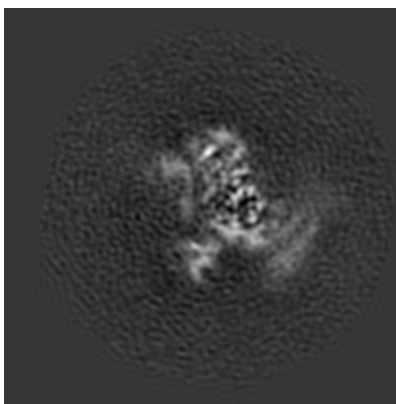
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

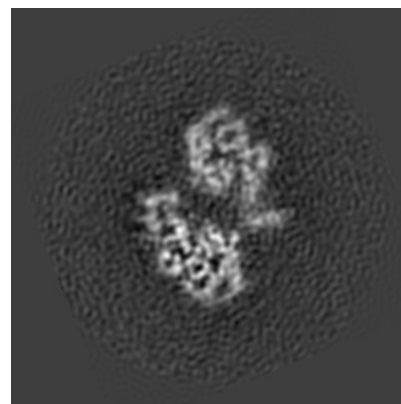
6.3.1 Primary map



X Index: 121



Y Index: 138

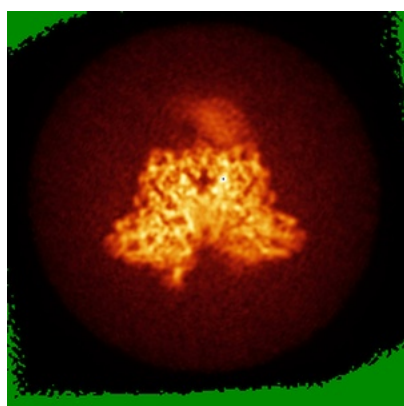


Z Index: 114

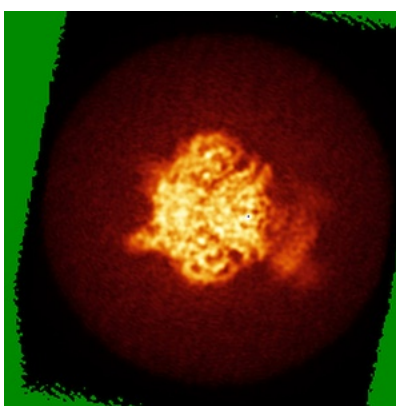
The images above show the largest variance slices of the map in three orthogonal directions.

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

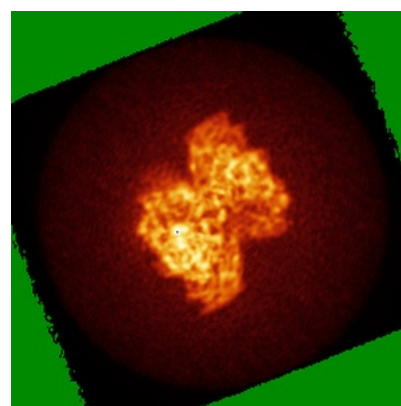
6.4.1 Primary map



X



Y

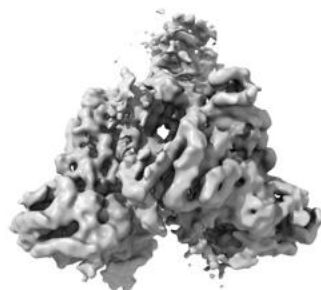


Z

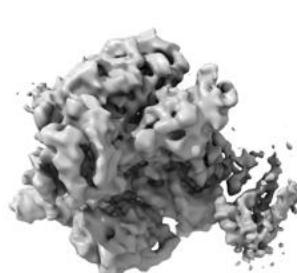
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

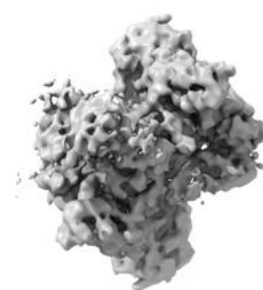
6.5.1 Primary map



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.

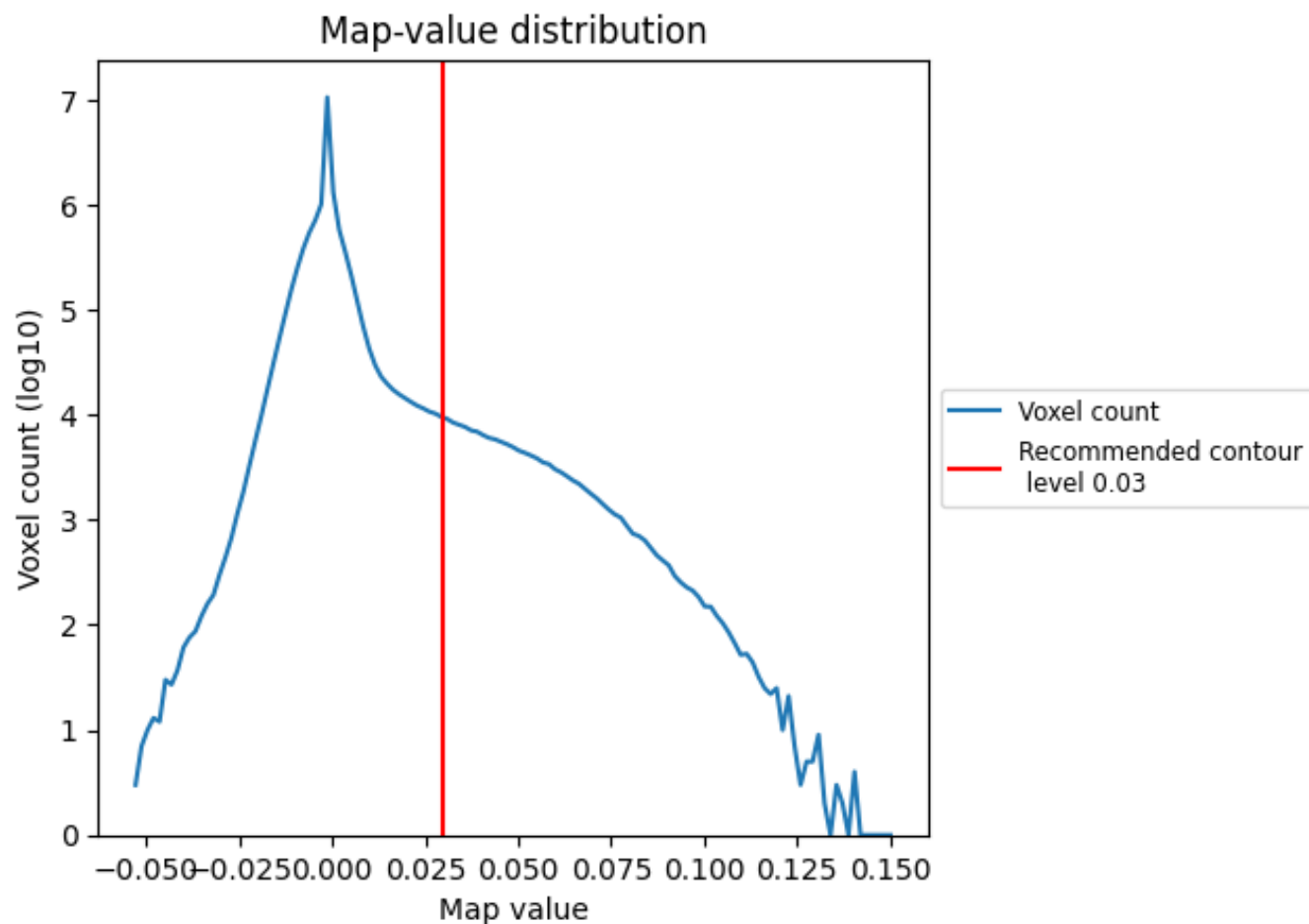
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

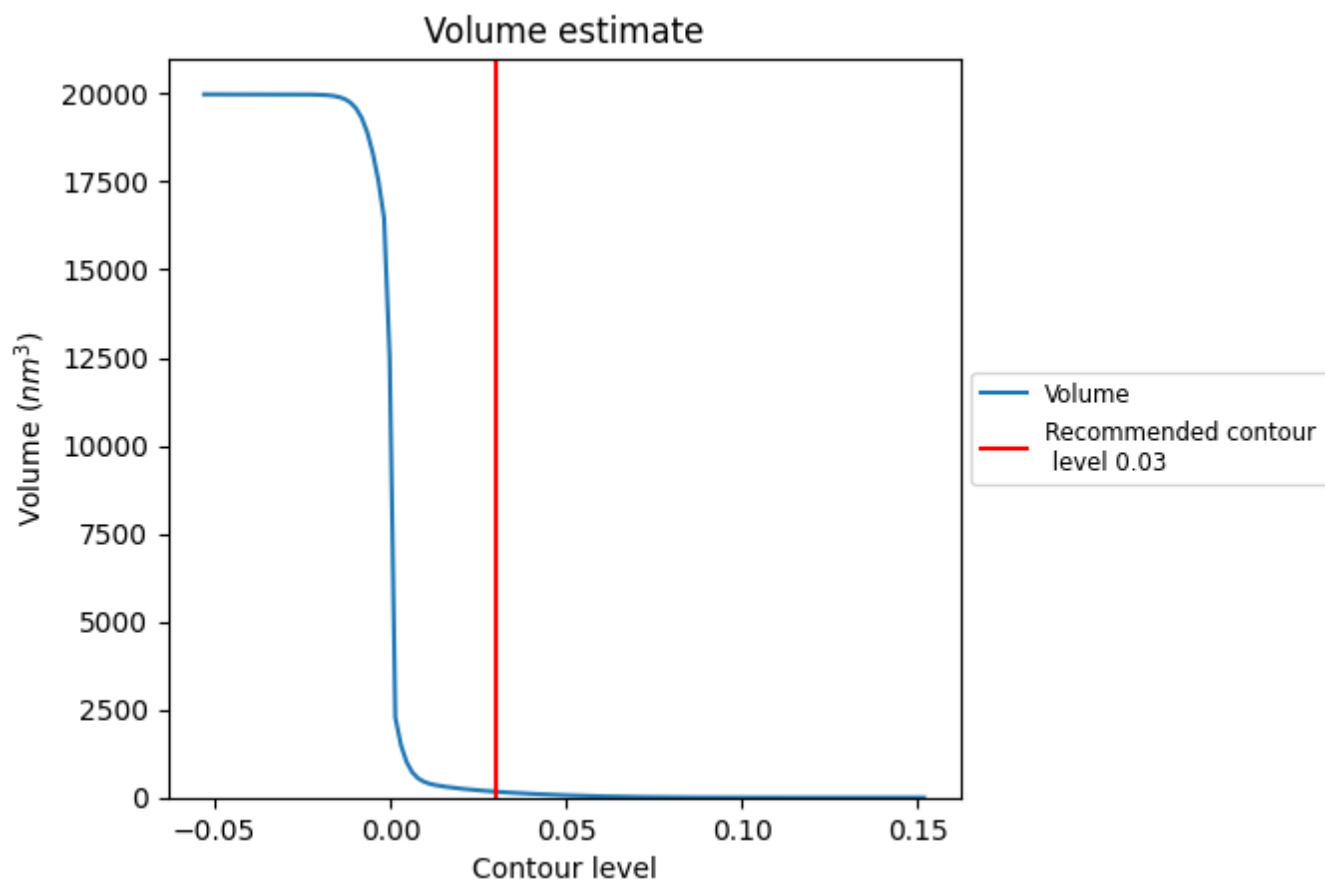
This section contains the results of statistical analysis of the map.

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.

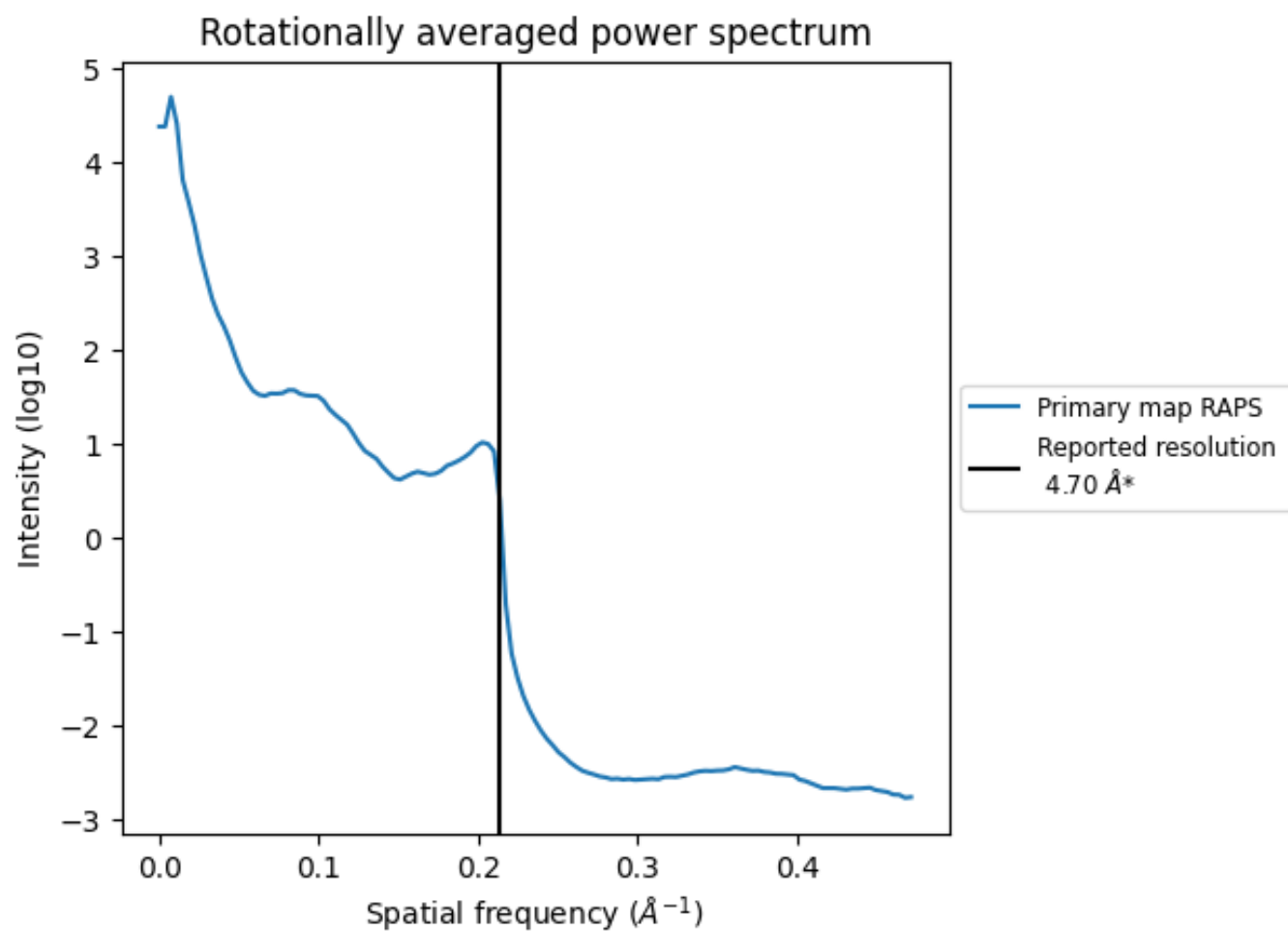
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 168 nm³; this corresponds to an approximate mass of 151 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.213 Å⁻¹

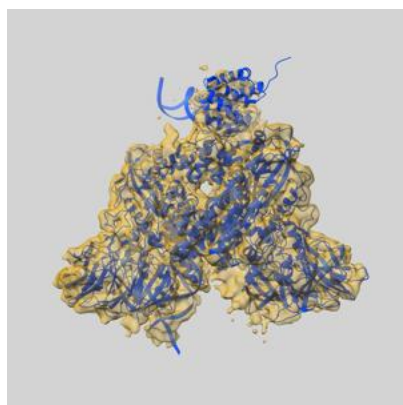
8 Fourier-Shell correlation

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

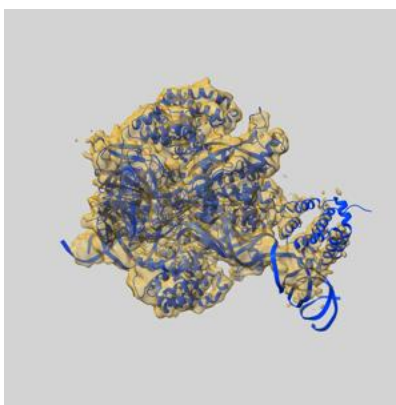
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7852 and PDB model 6DBW. Per-residue inclusion information can be found in section [3](#) on page [8](#).

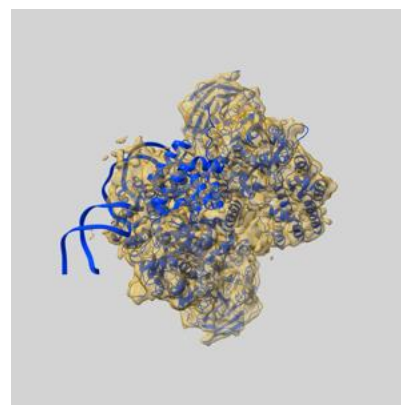
9.1 Map-model overlay [i](#)



X



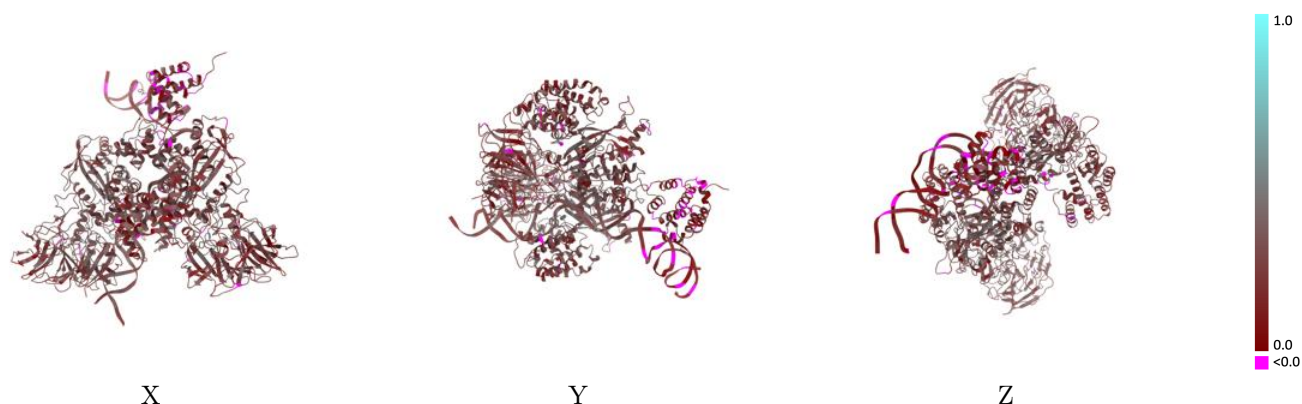
Y



Z

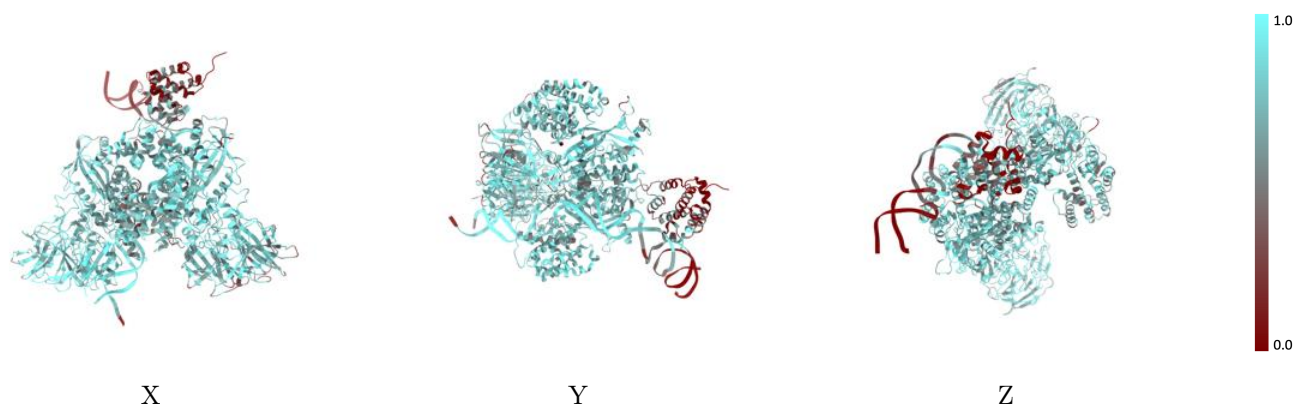
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



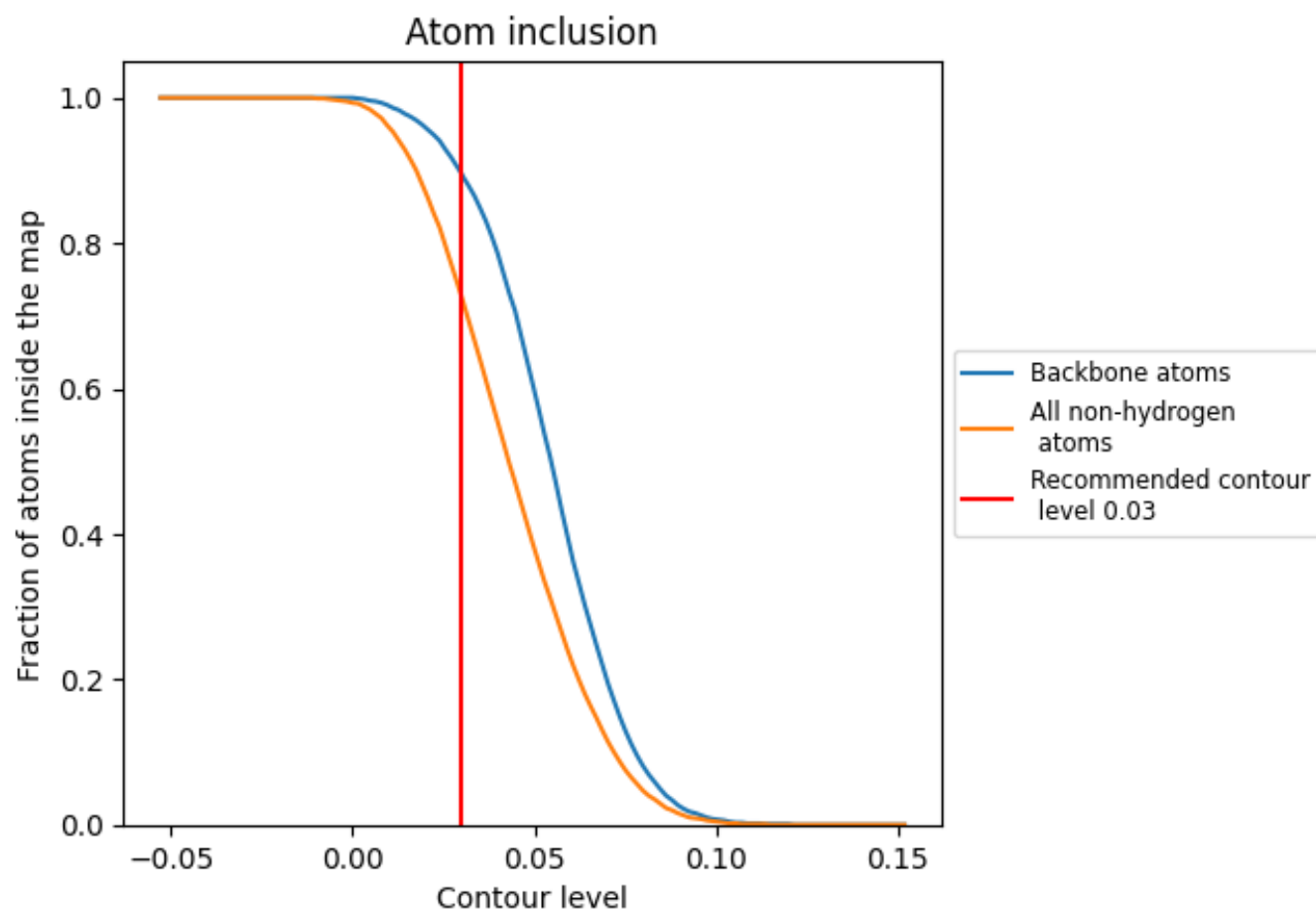
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 73% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7260	0.2650
A	0.7300	0.2810
B	0.8090	0.2970
C	0.6970	0.2550
D	0.7320	0.2570
E	0.6760	0.2170
F	0.6560	0.2190

1.0

0.0

<0.0