



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 05:09 AM UTC

PDB ID : 7DPA / pdb_00007dpa
EMDB ID : EMD-30802
Title : Cryo-EM structure of the human ELMO1-DOCK5-Rac1 complex
Authors : Kukimoto-Niino, M.; Katsura, K.; Kaushik, R.; Ehara, H.; Yokoyama, T.;
Uchikubo-Kamo, T.; Mishima-Tsumagari, C.; Yonemochi, M.; Ikeda, M.;
Hanada, K.; Zhang, K.Y.J.; Shirouzu, M.
Deposited on : 2020-12-18
Resolution : 3.80 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:

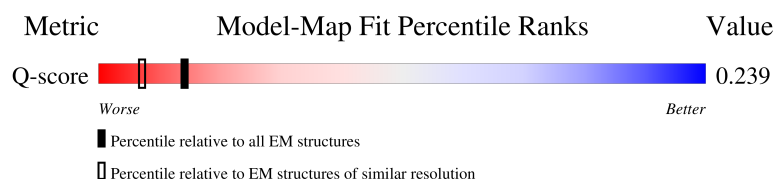
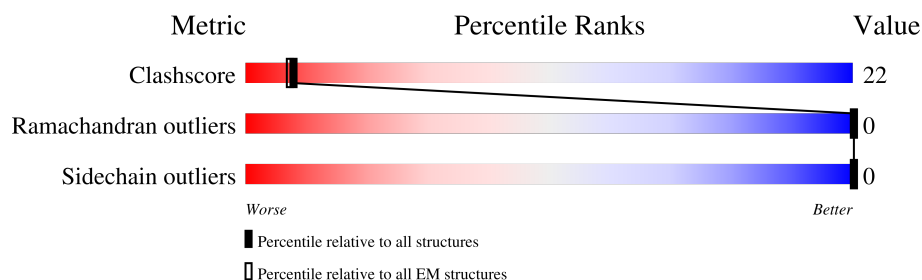
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.80 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	10198 (3.30 - 4.30)

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	1648	15% 55% 45%
1	D	1648	15% 55% 45%
2	B	184	5% 54% 42% .
2	E	184	. 53% 43% .

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Mol	Chain	Length	Quality of chain
3	C	733	15%12%73%
3	F	733	15%12%73%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 32858 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 Dedicator of cytokinesis protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1642	Total	C	N	O	S	0	0
			13436	8618	2264	2484	70		
1	D	1642	Total	C	N	O	S	0	0
			13436	8618	2264	2484	70		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q9H7D0
A	-4	GLY	-	expression tag	UNP Q9H7D0
A	-3	SER	-	expression tag	UNP Q9H7D0
A	-2	GLY	-	expression tag	UNP Q9H7D0
A	-1	GLY	-	expression tag	UNP Q9H7D0
A	0	SER	-	expression tag	UNP Q9H7D0
A	1285	ARG	LYS	variant	UNP Q9H7D0
D	-5	GLY	-	expression tag	UNP Q9H7D0
D	-4	GLY	-	expression tag	UNP Q9H7D0
D	-3	SER	-	expression tag	UNP Q9H7D0
D	-2	GLY	-	expression tag	UNP Q9H7D0
D	-1	GLY	-	expression tag	UNP Q9H7D0
D	0	SER	-	expression tag	UNP Q9H7D0
D	1285	ARG	LYS	variant	UNP Q9H7D0

- Molecule 2 is a protein called Ras-related C3 botulinum toxin substrate 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	177	Total	C	N	O	S	0	0
			1385	890	228	259	8		
2	E	177	Total	C	N	O	S	0	0
			1385	890	228	259	8		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	GLY	-	expression tag	UNP P63000
B	-5	SER	-	expression tag	UNP P63000
B	-4	SER	-	expression tag	UNP P63000
B	-3	GLY	-	expression tag	UNP P63000
B	-2	SER	-	expression tag	UNP P63000
B	-1	SER	-	expression tag	UNP P63000
B	0	GLY	-	expression tag	UNP P63000
B	15	ALA	GLY	engineered mutation	UNP P63000
E	-6	GLY	-	expression tag	UNP P63000
E	-5	SER	-	expression tag	UNP P63000
E	-4	SER	-	expression tag	UNP P63000
E	-3	GLY	-	expression tag	UNP P63000
E	-2	SER	-	expression tag	UNP P63000
E	-1	SER	-	expression tag	UNP P63000
E	0	GLY	-	expression tag	UNP P63000
E	15	ALA	GLY	engineered mutation	UNP P63000

- Molecule 3 is a protein called Engulfment and cell motility protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	198	Total	C	N	O	S	0	0
			1608	1018	277	303	10		
3	F	198	Total	C	N	O	S	0	0
			1608	1018	277	303	10		

There are 12 discrepancies between the modelled and reference sequences:

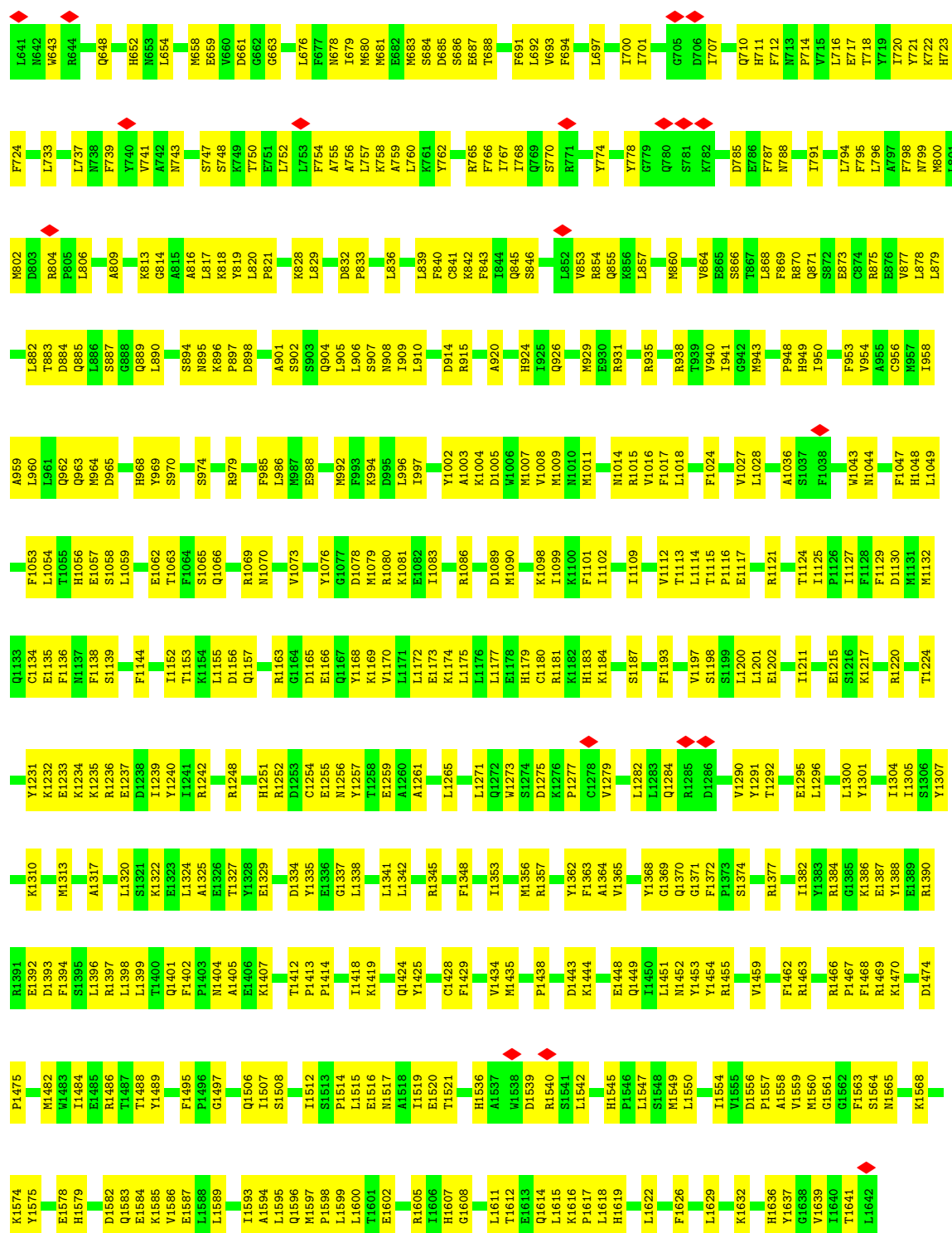
Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	GLY	-	expression tag	UNP Q92556
C	-4	GLY	-	expression tag	UNP Q92556
C	-3	SER	-	expression tag	UNP Q92556
C	-2	GLY	-	expression tag	UNP Q92556
C	-1	GLY	-	expression tag	UNP Q92556
C	0	SER	-	expression tag	UNP Q92556
F	-5	GLY	-	expression tag	UNP Q92556
F	-4	GLY	-	expression tag	UNP Q92556
F	-3	SER	-	expression tag	UNP Q92556
F	-2	GLY	-	expression tag	UNP Q92556
F	-1	GLY	-	expression tag	UNP Q92556
F	0	SER	-	expression tag	UNP Q92556

3 Residue-property plots [i](#)

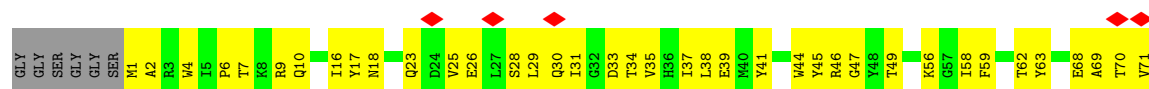
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Dedicator of cytokinesis protein 5

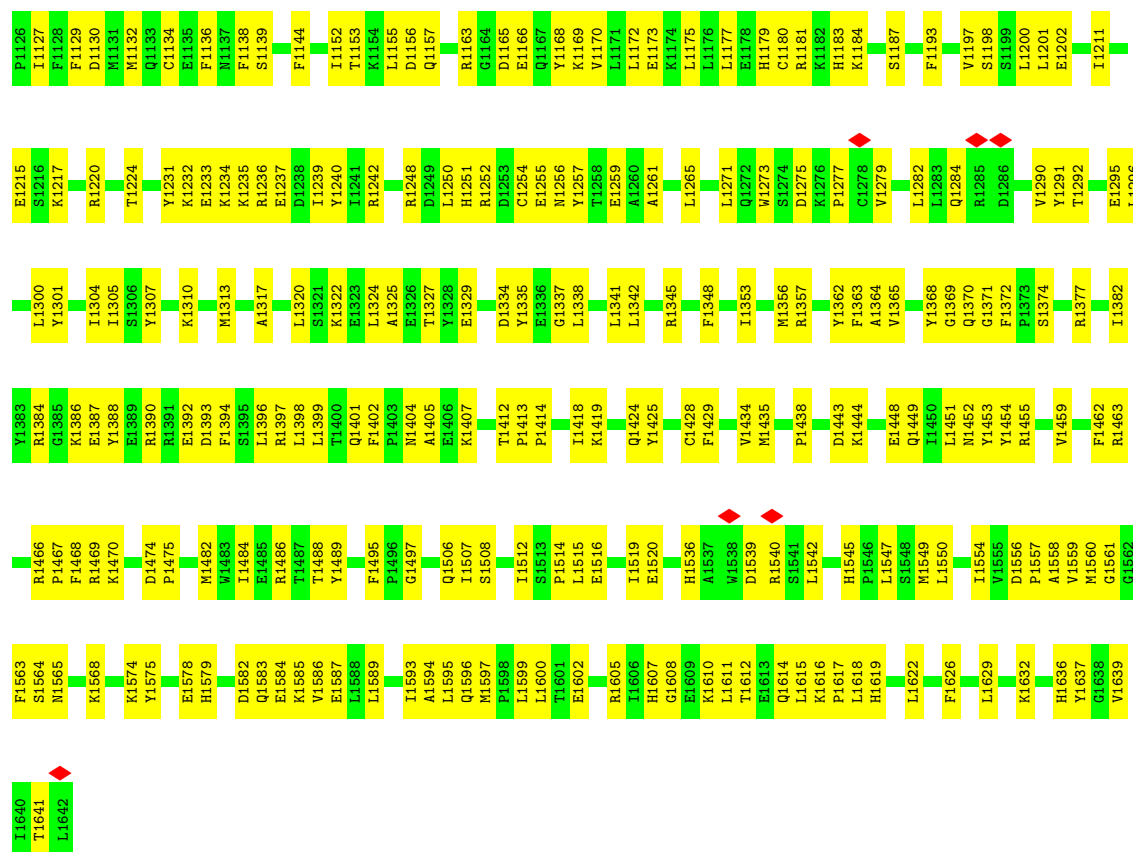




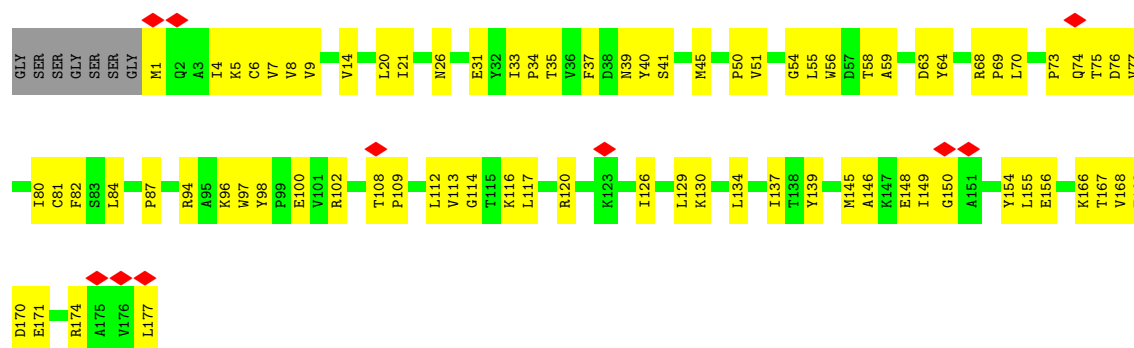
• Molecule 1: Dedicator of cytokinesis protein 5



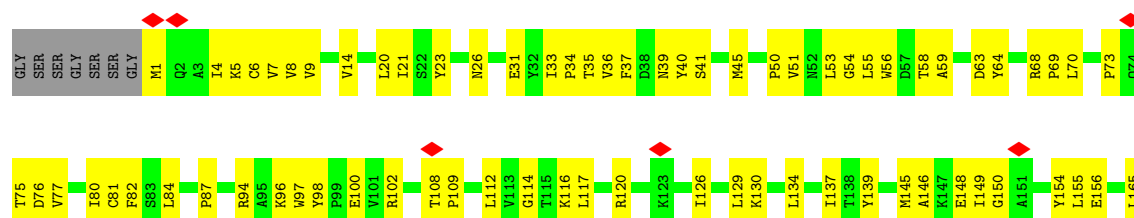
F1047	F1053	F1055	F1056	F1057	F1058	L1059	E1062	T1063	F1064	S1065	Q1066	E1067	K1068	R1069	N1070	V1073	Y1076	G1077	D1078	M1079	K1080	K1081	F1082	I1083	R1086	D1089	M1090	G1095	P1096	K1097	K1098	I1099	K1100	F1101	I1102	I1109	V1112	T1113	L1114	T1115	P1116	E1117	R1121	T1124	I1125										
H957	T958	A959	L960	L961	Q962	Q963	S964	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	Q1001	Q1002	Q1003	Q1004								
L879	L882	T883	D884	Q885	L886	S887	Q888	Q889	L890	S894	M895	K896	P897	D898	A901	S902	S903	Q904	L905	L906	S907	N908	L909	L910	D914	R915	A920	H924	I925	Q926	M929	E930	T931	Q1013	N1014	R1015	V1016	F1017	L1018	F1024	V1027	L1028	P948	H949	A1036	S1037	F1038	W1043	N1044	C956					
M802	D803	R804	P805	L806	A809	K813	Q814	A815	A816	L817	K818	Y819	L820	P821	W827	K828	L829	D832	P833	L836	F840	C841	K842	F843	T844	Q845	S846	Q851	L852	W853	R854	Q855	K856	L857	M860	V864	S865	T866	F867	N868	I791	L794	F795	L796	A797	F798	N799	M800	L801						
F724	L733	L737	N738	F739	Y740	W741	A742	N743	S747	L752	L753	F754	A755	A756	K757	L758	L759	L760	W761	Y762	L763	F764	F765	F766	W767	W768	R771	Y774	Y778	Q779	Q780	S781	L782	D785	E786	F787	N788	I791	L794	F795	L796	A797	F798	N799	M800	L801									
K573	G574	D575	N576	K577	K578	N579	E580	D581	A582	K583	F584	Y585	L586	T587	L588	P589	M590	K591	R592	M593	E594	M595	S596	E597	K598	E599	L600	Q601	A602	S603	K604	N605	L606	V607	T608	F609	S612	K613	D614	S615	T616	K617	D618	Q621	L622	A623	T624	C627	K630	L631	T632	L637	L638	G639	
L640	L641	N642	N643	R644	Q648	H652	H653	L654	E659	V660	D661	S662	G663	L676	F677	N678	L679	M680	E682	S684	D685	S686	E687	T688	F691	L692	V693	F694	L697	I700	I701	G705	D706	I707	Q710	H711	F712	F713	F714	V715	L716	E717	T718	Y719	I720	Y721	K722	H723							
F1047	F1053	F1055	F1056	F1057	F1058	L1059	E1062	T1063	F1064	S1065	Q1066	E1067	K1068	R1069	N1070	V1073	Y1076	G1077	D1078	M1079	K1080	K1081	F1082	I1083	R1086	D1089	M1090	G1095	P1096	K1097	K1098	I1099	K1100	F1101	I1102	I1109	V1112	T1113	L1114	T1115	P1116	E1117	R1121	T1124	I1125										
H154	G155	M158	L159	L163	V164	V165	R166	M169	G170	E171	N171	L172	L173	D174	P175	T180	I181	A182	L183	F184	K185	A186	H187	V189	R193	L194	K197	E200	E201	I204	L205	L208	D209	L210	L211	G212	Q213	S214	T215	F216	S217	T218	I219	H220	T221	Y222	G223	L224	N230						
F231	V232	C233	N234	I235	G236	E237	D238	A239	E240	L241	F242	M243	A244	L245	P248	D249	Q250	S251	T252	F253	I254	S255	E256	N257	T260	R261	V262	G263	S264	T265	G266	M267	P268	K269	E270	I271	E272	K273	N276	L277	V280	F281	T282	D283	L284	S285	S286	S287	D288	L289	T290	R291	P292	R293	V294
S295	L296	V297	C298	Q299	L300	V301	R302	E307	L308	K309	K312	K313	H314	T315	C316	R319	R320	P321	F322	G323	V324	A325	V326	M327	D328	I329	T330	D331	I332	I333	H334	G335	K336	V337	D338	E341	K342	Q343	H344	F345	I346	Q349	Q350	I351	A352	M353	E354	T355	Y356	I357	R358	Q359	R360	Q361	
L362	L363	M364	S365	P366	L367	L368	T369	S370	H371	L372	I373	G374	E375	N376	E377	P378	L379	T380	L383	N384	K385	V386	L387	A388	V392	N393	H394	K395	G396	Q397	G398	L399	W400	V401	S402	L403	K404	L405	L406	P407	G408	D409	L410	T411	Q414	K415	N416	H419	L420	R423	I427	A428	R429		
K430	M431	G432	F433	E435	I436	L437	L438	P439	G440	D441	V442	R443	T449	L450	H451	H452	G453	F455	D456	K457	G458	K459	K460	K461	T462	P463	E467	V468	T469	M470	S471	D474	E475	E476	G477	K478	L479	L480	E481	K482	A483	L484	H485	P486	G487	G492	L493	S494	E495	Y496	K497	Y501			
Y502	Q503	V504	K505	Q506	P507	C508	W509	Y510	I517	E520	E521	R524	C525	H526	T530	F531	R532	H533	R534	S535	S536	Q537	E538	T539	R540	D541	K542	S543	E544	R545	A546	F547	G548	V549	A550	K553	N556	P557	D558	G559	T560	L561	L562	Q563	D564	G565	R566	H567	D568	L569	V570	Y571	Y572		

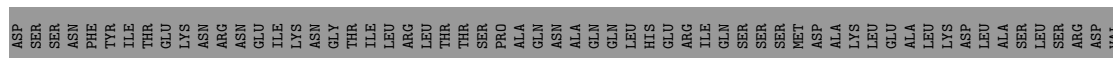


• Molecule 2: Ras-related C3 botulinum toxin substrate 1



• Molecule 2: Ras-related C3 botulinum toxin substrate 1







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	149846	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	0.5	Depositor
Maximum defocus (nm)	3.0	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.023	Depositor
Minimum map value	-0.008	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.004	Depositor
Map size ($\text{\AA}$)	431.6, 431.6, 431.6	wwPDB
Map dimensions	520, 520, 520	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.83, 0.83, 0.83	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.26	0/13722	0.50	0/18514
1	D	0.26	0/13722	0.50	0/18514
2	B	0.20	0/1415	0.43	0/1924
2	E	0.21	0/1415	0.43	0/1924
3	C	0.18	0/1641	0.44	0/2218
3	F	0.18	0/1641	0.44	0/2218
All	All	0.25	0/33556	0.49	0/45312

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	13436	0	13516	624	0
1	D	13436	0	13516	625	0
2	B	1385	0	1407	70	0
2	E	1385	0	1407	69	0
3	C	1608	0	1617	87	0
3	F	1608	0	1617	90	0
All	All	32858	0	33080	1474	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 22.

All (1474) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:166:ARG:HB2	1:D:174:ASP:HB2	1.50	0.93
1:A:1342:LEU:HD12	1:D:1342:LEU:HD12	1.51	0.92
1:A:166:ARG:HB2	1:A:174:ASP:HB2	1.50	0.91
1:A:10:GLN:HG3	1:A:37:ILE:HB	1.53	0.88
1:D:10:GLN:HG3	1:D:37:ILE:HB	1.53	0.88
1:D:739:PHE:HE2	1:D:794:LEU:HD12	1.37	0.88
1:A:739:PHE:HE2	1:A:794:LEU:HD12	1.37	0.87
1:A:1390:ARG:NH2	2:B:26:ASN:OD1	2.07	0.86
1:D:1396:LEU:HD21	3:F:606:ASP:HB3	1.56	0.86
1:A:1271:LEU:HD21	1:A:1296:LEU:HD23	1.58	0.85
1:A:393:ASN:HB3	1:A:401:VAL:HG21	1.58	0.85
1:D:393:ASN:HB3	1:D:401:VAL:HG21	1.58	0.84
1:D:958:ILE:HG23	1:D:1016:VAL:HG21	1.59	0.84
1:D:1271:LEU:HD21	1:D:1296:LEU:HD23	1.57	0.84
1:A:958:ILE:HG23	1:A:1016:VAL:HG21	1.60	0.84
1:D:1390:ARG:NH2	2:E:26:ASN:OD1	2.12	0.83
1:D:774:TYR:HA	1:D:778:TYR:HB2	1.61	0.83
1:D:1014:ASN:HB3	1:D:1079:MET:HE1	1.60	0.82
1:A:774:TYR:HA	1:A:778:TYR:HB2	1.61	0.82
1:A:1014:ASN:HB3	1:A:1079:MET:HE1	1.60	0.82
1:A:230:ASN:HB3	1:A:243:MET:HB2	1.63	0.81
1:D:1597:MET:HE1	1:D:1629:LEU:HB3	1.64	0.80
1:D:716:LEU:O	1:D:720:ILE:HB	1.82	0.80
1:A:1396:LEU:HD21	3:C:606:ASP:HB3	1.62	0.79
1:D:230:ASN:HB3	1:D:243:MET:HB2	1.63	0.79
1:A:716:LEU:O	1:A:720:ILE:HB	1.82	0.79
1:A:1597:MET:HE1	1:A:1629:LEU:HB3	1.63	0.79
1:D:240:GLU:OE2	1:D:261:ARG:NH2	2.17	0.77
1:D:95:LEU:HD13	1:D:98:TRP:HD1	1.48	0.77
1:A:33:ASP:OD1	3:C:697:ARG:NH2	2.17	0.77
1:A:95:LEU:HD13	1:A:98:TRP:HD1	1.48	0.77
3:F:610:VAL:HA	3:F:613:ILE:HG12	1.67	0.76
1:D:180:THR:OG1	1:D:962:GLN:OE1	2.04	0.76
1:A:240:GLU:OE2	1:A:261:ARG:NH2	2.17	0.76
1:D:1059:LEU:HA	1:D:1062:GLU:HB2	1.68	0.76
3:C:610:VAL:HA	3:C:613:ILE:HG12	1.67	0.76
1:A:943:MET:HE3	1:A:948:PRO:HB2	1.68	0.75
1:A:1402:PHE:O	3:C:584:LYS:NZ	2.20	0.75
3:C:550:GLN:HA	3:C:553:LEU:HD12	1.68	0.75
1:A:180:THR:HG21	1:A:958:ILE:HG22	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:550:GLN:HA	3:F:553:LEU:HD12	1.67	0.74
3:C:616:VAL:HG21	3:C:669:LEU:HD22	1.70	0.74
1:D:452:HIS:HB3	1:D:617:LYS:HE2	1.69	0.74
1:A:1059:LEU:HA	1:A:1062:GLU:HB2	1.68	0.74
2:E:96:LYS:HD2	2:E:100:GLU:HG3	1.69	0.74
1:A:384:ASN:HA	1:A:388:ALA:HB3	1.69	0.74
1:D:943:MET:HE3	1:D:948:PRO:HB2	1.68	0.74
1:D:180:THR:HG21	1:D:958:ILE:HG22	1.69	0.74
1:D:384:ASN:HA	1:D:388:ALA:HB3	1.69	0.74
1:D:405:LEU:HB3	1:D:414:GLN:HE22	1.53	0.74
1:D:1275:ASP:O	1:D:1292:THR:OG1	2.06	0.73
1:A:452:HIS:HB3	1:A:617:LYS:HE2	1.69	0.73
1:A:648:GLN:O	1:A:652:HIS:ND1	2.21	0.73
1:A:795:PHE:CZ	1:A:841:CYS:HB3	2.23	0.73
1:D:1233:GLU:O	1:D:1235:LYS:NZ	2.22	0.73
1:A:1362:TYR:HD2	1:A:1462:PHE:CE2	2.07	0.73
3:C:575:TRP:HZ3	3:C:588:TYR:HB2	1.54	0.73
1:A:98:TRP:O	1:A:101:ILE:HG22	1.89	0.72
1:A:1305:ILE:HD11	1:A:1320:LEU:HB2	1.70	0.72
1:D:795:PHE:CZ	1:D:841:CYS:HB3	2.23	0.72
3:F:616:VAL:HG21	3:F:669:LEU:HD22	1.70	0.72
1:D:854:ARG:NH1	1:D:855:GLN:OE1	2.22	0.72
2:B:96:LYS:HD2	2:B:100:GLU:HG3	1.69	0.72
1:D:98:TRP:O	1:D:101:ILE:HG22	1.89	0.72
1:D:648:GLN:O	1:D:652:HIS:ND1	2.21	0.72
1:D:879:LEU:HD22	1:D:924:HIS:CE1	2.25	0.72
1:A:180:THR:OG1	1:A:962:GLN:OE1	2.04	0.72
1:D:821:PRO:HB2	1:D:842:LYS:HZ3	1.55	0.72
1:A:785:ASP:OD1	1:A:788:ASN:ND2	2.23	0.72
1:A:221:THR:HB	1:A:249:ASP:HA	1.71	0.72
1:A:405:LEU:HB3	1:A:414:GLN:HE22	1.53	0.71
1:A:854:ARG:NH1	1:A:855:GLN:OE1	2.22	0.71
1:A:1275:ASP:O	1:A:1292:THR:OG1	2.07	0.71
1:D:1362:TYR:HD2	1:D:1462:PHE:CE2	2.07	0.71
3:F:575:TRP:HZ3	3:F:588:TYR:HB2	1.54	0.71
1:D:1305:ILE:HD11	1:D:1320:LEU:HB2	1.70	0.71
1:A:1233:GLU:O	1:A:1235:LYS:NZ	2.22	0.71
1:A:821:PRO:HB2	1:A:842:LYS:HZ3	1.55	0.71
1:A:879:LEU:HD22	1:A:924:HIS:CE1	2.25	0.71
1:D:718:THR:HB	1:D:768:ILE:HD13	1.73	0.71
1:D:785:ASP:OD1	1:D:788:ASN:ND2	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:VAL:HG22	1:A:325:ALA:H	1.56	0.71
1:A:915:ARG:HA	1:A:915:ARG:HH11	1.55	0.71
1:D:221:THR:HB	1:D:249:ASP:HA	1.71	0.71
2:B:20:LEU:HD13	2:B:55:LEU:HD13	1.73	0.70
1:D:324:VAL:HG22	1:D:325:ALA:H	1.56	0.70
1:D:506:GLN:HB3	1:D:617:LYS:HZ2	1.57	0.70
1:D:915:ARG:HA	1:D:915:ARG:HH11	1.55	0.70
1:D:1402:PHE:O	3:F:584:LYS:NZ	2.21	0.70
1:A:904:GLN:OE1	1:A:908:ASN:ND2	2.25	0.70
1:D:33:ASP:OD1	3:F:697:ARG:NH2	2.25	0.69
2:B:7:VAL:HG22	2:B:56:TRP:HD1	1.57	0.69
1:A:1121:ARG:O	1:A:1125:ILE:HD12	1.92	0.69
1:A:884:ASP:OD1	1:A:931:ARG:NH2	2.23	0.69
3:F:537:LYS:HG3	3:F:690:LEU:HG	1.75	0.69
1:A:718:THR:HB	1:A:768:ILE:HD13	1.73	0.69
1:A:890:LEU:HD11	1:A:938:ARG:HB3	1.75	0.69
1:A:1557:PRO:HB2	1:A:1561:GLY:HA2	1.75	0.69
1:D:1121:ARG:O	1:D:1125:ILE:HD12	1.92	0.69
1:D:1584:GLU:O	1:D:1587:GLU:HG2	1.93	0.69
2:E:20:LEU:HD13	2:E:55:LEU:HD13	1.73	0.69
3:F:670:ASN:ND2	3:F:676:ASP:O	2.26	0.69
1:A:679:ILE:HG23	1:A:733:LEU:HD12	1.74	0.69
3:C:537:LYS:HG3	3:C:690:LEU:HG	1.75	0.69
1:A:1066:GLN:O	1:A:1069:ARG:NH2	2.26	0.69
1:A:1584:GLU:O	1:A:1587:GLU:HG2	1.93	0.69
1:D:679:ILE:HG23	1:D:733:LEU:HD12	1.74	0.68
1:D:1561:GLY:O	1:D:1565:ASN:ND2	2.16	0.68
1:A:155:GLY:HA2	1:A:158:MET:SD	2.34	0.68
1:A:741:VAL:O	1:A:747:SER:OG	2.12	0.68
1:D:155:GLY:HA2	1:D:158:MET:SD	2.34	0.68
1:A:283:ASP:OD2	1:A:393:ASN:ND2	2.27	0.68
2:E:7:VAL:HG22	2:E:56:TRP:HD1	1.57	0.68
1:D:37:ILE:HA	1:D:47:GLY:HA3	1.76	0.68
1:A:409:ASP:HB2	1:A:414:GLN:HB2	1.76	0.68
1:D:890:LEU:HD11	1:D:938:ARG:HB3	1.75	0.68
1:A:1169:LYS:HE3	1:A:1202:GLU:HG2	1.76	0.68
3:C:670:ASN:ND2	3:C:676:ASP:O	2.26	0.68
1:D:1557:PRO:HB2	1:D:1561:GLY:HA2	1.75	0.68
1:A:762:TYR:HA	1:A:765:ARG:HB2	1.77	0.67
1:A:255:SER:HA	1:A:280:VAL:HG22	1.77	0.67
1:D:81:ILE:HD13	1:D:141:LEU:HD22	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:741:VAL:O	1:D:747:SER:OG	2.12	0.67
1:D:1066:GLN:O	1:D:1069:ARG:NH2	2.26	0.67
1:D:762:TYR:HA	1:D:765:ARG:HB2	1.77	0.67
1:D:757:LEU:HA	1:D:760:LEU:HB2	1.76	0.67
1:D:283:ASP:OD2	1:D:393:ASN:ND2	2.27	0.67
1:A:1059:LEU:O	1:A:1063:THR:OG1	2.07	0.67
1:D:255:SER:HA	1:D:280:VAL:HG22	1.76	0.67
1:D:680:MET:HA	1:D:683:MET:HG2	1.76	0.67
1:D:904:GLN:OE1	1:D:908:ASN:ND2	2.25	0.67
1:D:1482:MET:HE1	2:E:34:PRO:HD2	1.77	0.67
1:A:187:HIS:CD2	1:A:1009:MET:HB2	2.30	0.67
1:A:757:LEU:HA	1:A:760:LEU:HB2	1.76	0.67
1:A:1115:THR:O	1:A:1121:ARG:NH1	2.28	0.66
1:D:409:ASP:HB2	1:D:414:GLN:HB2	1.76	0.66
1:A:81:ILE:HD13	1:A:141:LEU:HD22	1.77	0.66
1:A:1168:TYR:CZ	1:A:1172:LEU:HD11	2.31	0.66
1:D:187:HIS:CD2	1:D:1009:MET:HB2	2.30	0.66
1:D:1169:LYS:HE3	1:D:1202:GLU:HG2	1.76	0.66
1:D:1443:ASP:OD1	1:D:1444:LYS:HD3	1.95	0.66
1:A:469:THR:HG21	1:A:532:ARG:HE	1.61	0.66
1:A:1371:GLY:O	1:A:1424:GLN:NE2	2.27	0.66
1:D:1115:THR:O	1:D:1121:ARG:NH1	2.28	0.66
1:A:37:ILE:HA	1:A:47:GLY:HA3	1.76	0.66
1:D:230:ASN:HD21	1:D:341:GLU:HB3	1.61	0.66
1:A:236:GLY:O	1:A:534:ARG:NH2	2.29	0.66
1:A:883:THR:HB	1:A:931:ARG:HH21	1.60	0.66
1:A:1561:GLY:O	1:A:1565:ASN:ND2	2.16	0.66
1:D:883:THR:HB	1:D:931:ARG:HH21	1.60	0.66
1:A:836:LEU:HD11	1:A:873:GLU:HB3	1.78	0.66
1:A:230:ASN:HD21	1:A:341:GLU:HB3	1.61	0.66
1:A:1443:ASP:OD1	1:A:1444:LYS:HD3	1.95	0.66
1:D:236:GLY:O	1:D:534:ARG:NH2	2.29	0.66
3:F:585:VAL:HG23	3:F:607:LYS:HZ3	1.61	0.66
1:A:680:MET:HA	1:A:683:MET:HG2	1.77	0.65
1:A:809:ALA:O	1:A:813:LYS:N	2.28	0.65
1:D:836:LEU:HD11	1:D:873:GLU:HB3	1.78	0.65
1:D:884:ASP:OD1	1:D:931:ARG:NH2	2.23	0.65
1:D:1232:LYS:HB2	1:D:1240:TYR:HE2	1.61	0.65
1:D:1371:GLY:O	1:D:1424:GLN:NE2	2.27	0.65
1:D:1168:TYR:CZ	1:D:1172:LEU:HD11	2.31	0.65
1:A:1467:PRO:HG3	2:B:33:ILE:HG13	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:GLN:HB3	1:A:617:LYS:HZ2	1.60	0.65
1:A:1063:THR:HG22	1:A:1069:ARG:HH11	1.61	0.65
1:A:1374:SER:HA	1:A:1377:ARG:HE	1.62	0.65
1:D:1467:PRO:HG3	2:E:33:ILE:HG13	1.79	0.65
3:F:669:LEU:HA	3:F:672:LEU:HD12	1.79	0.65
1:A:125:ILE:HD13	3:C:695:LYS:HD3	1.78	0.65
1:D:1063:THR:HG22	1:D:1069:ARG:HH11	1.61	0.65
1:D:16:ILE:HD13	3:F:707:PRO:HG2	1.78	0.64
1:D:560:THR:HG23	1:D:632:THR:HB	1.79	0.64
1:D:809:ALA:O	1:D:813:LYS:N	2.28	0.64
1:D:469:THR:HG21	1:D:532:ARG:HE	1.61	0.64
1:A:215:ILE:HG22	1:A:217:SER:H	1.62	0.64
1:A:1232:LYS:HB2	1:A:1240:TYR:HE2	1.61	0.64
1:D:1374:SER:HA	1:D:1377:ARG:HE	1.62	0.64
1:D:106:TYR:CZ	3:F:689:LEU:HD21	2.33	0.64
1:D:44:TRP:HZ2	3:F:713:ILE:HG23	1.63	0.64
1:D:106:TYR:CE2	3:F:689:LEU:HD21	2.32	0.64
3:C:553:LEU:HB3	3:C:583:HIS:CD2	2.33	0.64
1:D:215:ILE:HG22	1:D:217:SER:H	1.62	0.64
1:D:535:SER:OG	1:D:540:ARG:NH2	2.31	0.63
1:A:1607:HIS:O	1:A:1611:LEU:N	2.32	0.63
1:D:343:GLN:OE1	1:D:414:GLN:NE2	2.31	0.63
1:D:809:ALA:HB1	1:D:813:LYS:HG3	1.79	0.63
3:C:669:LEU:HA	3:C:672:LEU:HD12	1.79	0.63
3:F:588:TYR:OH	3:F:607:LYS:O	2.11	0.63
1:A:17:TYR:HA	3:C:536:LEU:HD21	1.81	0.63
1:A:98:TRP:HH2	1:A:155:GLY:HA3	1.64	0.63
1:A:343:GLN:OE1	1:A:414:GLN:NE2	2.31	0.63
1:D:313:LYS:N	1:D:353:MET:SD	2.72	0.63
1:D:561:THR:OG1	1:D:630:LYS:O	2.17	0.63
3:F:553:LEU:HB3	3:F:583:HIS:CD2	2.33	0.63
1:A:106:TYR:CE2	3:C:689:LEU:HD21	2.33	0.63
1:A:482:LYS:HD3	1:A:486:PRO:HG2	1.81	0.63
1:A:535:SER:OG	1:A:540:ARG:NH2	2.31	0.63
1:A:1:MET:HG2	3:C:720:TYR:HA	1.81	0.63
1:D:1607:HIS:O	1:D:1611:LEU:N	2.32	0.62
1:A:809:ALA:HB1	1:A:813:LYS:HG3	1.79	0.62
1:D:44:TRP:CE3	1:D:58:ILE:HG22	2.35	0.62
1:A:806:LEU:HD11	1:A:813:LYS:HD2	1.81	0.62
2:B:120:ARG:HH22	2:B:139:TYR:HB2	1.64	0.62
1:D:929:MET:HE1	1:D:968:HIS:HB3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ILE:HD13	3:C:707:PRO:HG2	1.82	0.62
1:A:871:GLN:NE2	1:A:875:ARG:HD3	2.15	0.62
1:A:929:MET:HE1	1:A:968:HIS:HB3	1.82	0.62
1:A:1177:LEU:O	1:A:1181:ARG:HG2	2.00	0.62
1:A:474:ASP:HB3	1:A:478:LYS:H	1.65	0.62
1:D:871:GLN:NE2	1:D:875:ARG:HD3	2.15	0.62
1:D:889:GLN:O	1:D:895:ASN:ND2	2.32	0.62
3:C:622:CYS:HB2	3:C:625:MET:HB2	1.81	0.62
1:D:806:LEU:HD11	1:D:813:LYS:HD2	1.81	0.61
1:A:204:ILE:HA	1:A:208:LEU:HB2	1.81	0.61
1:A:44:TRP:CE3	1:A:58:ILE:HG22	2.35	0.61
1:A:560:THR:HG23	1:A:632:THR:HB	1.79	0.61
1:D:98:TRP:HH2	1:D:155:GLY:HA3	1.64	0.61
1:D:814:GLY:O	1:D:818:LYS:NZ	2.30	0.61
2:E:120:ARG:HH22	2:E:139:TYR:HB2	1.64	0.61
1:A:313:LYS:N	1:A:353:MET:SD	2.72	0.61
1:D:10:GLN:HB2	1:D:37:ILE:HD12	1.83	0.61
1:D:1116:PRO:HA	1:D:1121:ARG:HH12	1.65	0.61
3:F:616:VAL:HG11	3:F:669:LEU:HD13	1.82	0.61
1:A:7:THR:HG22	1:A:9:ARG:H	1.66	0.61
1:A:871:GLN:HE21	1:A:875:ARG:HD3	1.65	0.61
1:D:1063:THR:HG22	1:D:1069:ARG:HD3	1.82	0.61
1:A:889:GLN:O	1:A:895:ASN:ND2	2.32	0.61
3:C:616:VAL:HG11	3:C:669:LEU:HD13	1.82	0.61
1:D:871:GLN:HE21	1:D:875:ARG:HD3	1.65	0.61
1:D:759:ALA:HA	1:D:762:TYR:HB2	1.83	0.61
1:D:1177:LEU:O	1:D:1181:ARG:HG2	2.00	0.61
1:D:7:THR:HG22	1:D:9:ARG:H	1.66	0.61
1:D:474:ASP:HB3	1:D:478:LYS:H	1.65	0.61
1:A:95:LEU:HD13	1:A:98:TRP:CD1	2.35	0.61
1:D:204:ILE:HA	1:D:208:LEU:HB2	1.81	0.61
1:D:1056:HIS:ND1	1:D:1057:GLU:OE2	2.32	0.61
1:A:561:THR:OG1	1:A:630:LYS:O	2.17	0.60
1:A:1063:THR:HG22	1:A:1069:ARG:HD3	1.82	0.60
3:F:622:CYS:HB2	3:F:625:MET:HB2	1.81	0.60
1:A:10:GLN:HB2	1:A:37:ILE:HD12	1.83	0.60
3:F:578:ARG:NH2	3:F:600:PRO:HA	2.16	0.60
1:D:482:LYS:HD3	1:D:486:PRO:HG2	1.81	0.60
1:A:1559:VAL:HG22	2:B:59:ALA:HA	1.84	0.60
1:D:83:GLY:O	1:D:145:LYS:NZ	2.34	0.60
1:A:476:GLU:OE1	1:A:524:ARG:NH2	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:GLY:O	1:A:145:LYS:NZ	2.34	0.60
1:A:44:TRP:HZ2	3:C:713:ILE:HG23	1.65	0.60
1:A:131:ILE:HD11	1:A:144:LEU:HG	1.84	0.60
1:A:508:CYS:SG	1:A:509:TRP:N	2.73	0.60
1:A:759:ALA:HA	1:A:762:TYR:HB2	1.83	0.60
1:A:889:GLN:NE2	1:A:898:ASP:OD2	2.35	0.60
1:A:1251:HIS:O	1:A:1255:GLU:N	2.35	0.60
1:A:257:ASN:ND2	1:A:281:PHE:O	2.34	0.60
1:A:1116:PRO:HA	1:A:1121:ARG:HH12	1.65	0.60
1:A:1056:HIS:ND1	1:A:1057:GLU:OE2	2.32	0.59
1:A:1488:THR:HB	1:A:1508:SER:HB2	1.85	0.59
3:C:588:TYR:OH	3:C:607:LYS:O	2.11	0.59
1:D:95:LEU:HA	1:D:98:TRP:CD1	2.37	0.59
1:D:261:ARG:HH22	1:D:302:ARG:HH12	1.48	0.59
1:D:181:ILE:HD13	1:D:907:SER:HA	1.85	0.59
1:D:257:ASN:ND2	1:D:281:PHE:O	2.34	0.59
1:D:889:GLN:NE2	1:D:898:ASP:OD2	2.35	0.59
1:D:1251:HIS:O	1:D:1255:GLU:N	2.35	0.59
3:F:625:MET:HE1	3:F:638:LEU:HD12	1.84	0.59
1:A:95:LEU:HA	1:A:98:TRP:CD1	2.37	0.59
1:A:756:ALA:O	1:A:760:LEU:N	2.33	0.59
1:A:1290:VAL:HG23	1:A:1291:TYR:H	1.67	0.59
3:C:625:MET:HE1	3:C:638:LEU:HD12	1.84	0.59
1:D:901:ALA:O	1:D:905:LEU:HG	2.02	0.59
1:A:37:ILE:HD13	1:A:45:TYR:HB3	1.85	0.59
1:A:1506:GLN:OE1	1:A:1507:ILE:N	2.34	0.59
1:D:1617:PRO:HB2	2:E:70:LEU:HD13	1.85	0.59
1:A:261:ARG:HH22	1:A:302:ARG:HH12	1.48	0.59
1:A:1549:MET:SD	2:B:56:TRP:CZ3	2.96	0.59
3:C:663:CYS:O	3:C:666:THR:HG22	2.03	0.59
1:D:756:ALA:O	1:D:760:LEU:N	2.33	0.59
1:A:747:SER:HA	1:A:750:THR:HG22	1.84	0.59
1:A:901:ALA:O	1:A:905:LEU:HG	2.02	0.59
1:A:929:MET:HE2	1:A:964:MET:SD	2.43	0.59
1:D:131:ILE:HD11	1:D:144:LEU:HG	1.84	0.59
1:D:1290:VAL:HG23	1:D:1291:TYR:H	1.68	0.59
1:D:1466:ARG:NH1	2:E:31:GLU:OE2	2.35	0.59
1:A:717:GLU:O	1:A:723:HIS:NE2	2.36	0.59
1:A:1582:ASP:HB3	1:A:1585:LYS:HZ1	1.68	0.59
1:D:929:MET:HE2	1:D:964:MET:SD	2.43	0.59
1:A:1575:TYR:O	1:A:1579:HIS:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1617:PRO:HB2	2:B:70:LEU:HD13	1.85	0.59
1:D:414:GLN:HG3	1:D:416:ASN:H	1.68	0.59
1:A:181:ILE:HD13	1:A:907:SER:HA	1.85	0.58
1:D:37:ILE:HD13	1:D:45:TYR:HB3	1.85	0.58
3:C:585:VAL:HG23	3:C:607:LYS:HZ3	1.68	0.58
1:D:1:MET:HG2	3:F:720:TYR:HA	1.85	0.58
1:D:1488:THR:HB	1:D:1508:SER:HB2	1.85	0.58
3:C:578:ARG:NH2	3:C:600:PRO:HA	2.16	0.58
1:D:1211:ILE:HD13	1:D:1220:ARG:HG2	1.85	0.58
1:D:1261:ALA:HB2	1:D:1307:TYR:CB	2.33	0.58
1:A:414:GLN:HG3	1:A:416:ASN:H	1.68	0.58
1:A:1549:MET:CE	2:B:39:ASN:HB3	2.33	0.58
1:D:87:LEU:HD12	1:D:145:LYS:HG3	1.85	0.58
1:A:480:LEU:HA	1:A:484:ILE:HD12	1.86	0.58
2:B:21:ILE:HD13	2:B:34:PRO:HA	1.86	0.58
2:E:21:ILE:HD13	2:E:34:PRO:HA	1.86	0.58
1:A:1261:ALA:HB2	1:A:1307:TYR:CB	2.33	0.58
1:D:1:MET:N	3:F:717:PRO:O	2.37	0.58
1:D:747:SER:HA	1:D:750:THR:HG22	1.84	0.58
1:A:320:ARG:HH12	1:A:322:PHE:HD2	1.52	0.58
1:D:240:GLU:OE2	1:D:302:ARG:NH1	2.37	0.58
1:D:1356:MET:SD	1:D:1452:ASN:ND2	2.77	0.57
1:A:87:LEU:HD12	1:A:145:LYS:HG3	1.85	0.57
1:A:1356:MET:SD	1:A:1452:ASN:ND2	2.77	0.57
3:C:663:CYS:O	3:C:679:SER:OG	2.22	0.57
1:D:717:GLU:O	1:D:723:HIS:NE2	2.36	0.57
1:D:1003:ALA:O	1:D:1004:LYS:HG3	2.04	0.57
3:F:663:CYS:O	3:F:679:SER:OG	2.22	0.57
1:D:480:LEU:HA	1:D:484:ILE:HD12	1.86	0.57
1:D:1279:VAL:HG23	1:D:1282:LEU:HD23	1.86	0.57
1:A:91:LEU:HD11	1:A:124:LEU:HD11	1.86	0.57
1:A:165:VAL:HG23	1:A:175:PRO:HD3	1.87	0.57
1:A:1438:PRO:HB3	1:A:1454:TYR:HE2	1.69	0.57
1:D:91:LEU:HD11	1:D:124:LEU:HD11	1.87	0.57
1:D:556:ASN:N	1:D:560:THR:O	2.36	0.57
3:F:663:CYS:O	3:F:666:THR:HG22	2.03	0.57
1:A:1438:PRO:HB3	1:A:1454:TYR:CE2	2.40	0.57
1:D:165:VAL:HG23	1:D:175:PRO:HD3	1.87	0.57
1:D:423:ARG:HH11	1:D:427:ILE:HD12	1.69	0.57
1:A:240:GLU:OE2	1:A:302:ARG:NH1	2.37	0.57
1:A:556:ASN:N	1:A:560:THR:O	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:802:MET:SD	1:A:817:LEU:HD12	2.45	0.57
1:A:1211:ILE:HD13	1:A:1220:ARG:HG2	1.85	0.57
1:D:320:ARG:HH12	1:D:322:PHE:HD2	1.52	0.57
1:D:1506:GLN:OE1	1:D:1507:ILE:N	2.34	0.57
1:D:1575:TYR:O	1:D:1579:HIS:N	2.36	0.57
2:E:171:GLU:HA	2:E:174:ARG:HG2	1.87	0.57
1:A:1396:LEU:HD13	3:C:607:LYS:HB2	1.86	0.57
1:D:802:MET:SD	1:D:817:LEU:HD12	2.45	0.57
1:D:1637:TYR:HB3	1:D:1639:VAL:HG13	1.86	0.57
1:A:1362:TYR:HD2	1:A:1462:PHE:HE2	1.53	0.57
2:B:171:GLU:HA	2:B:174:ARG:HG2	1.87	0.57
3:C:627:GLU:HG2	3:C:631:LEU:HB2	1.87	0.57
1:A:330:THR:HB	1:A:344:HIS:CE1	2.40	0.57
1:A:621:GLN:HE22	1:A:623:ALA:HB2	1.70	0.57
1:A:1003:ALA:O	1:A:1004:LYS:HG3	2.04	0.57
1:D:678:ASN:H	1:D:681:MET:HE2	1.70	0.57
1:D:1217:LYS:HD2	1:D:1254:CYS:SG	2.45	0.57
1:A:356:TYR:OH	1:A:367:LEU:O	2.19	0.57
1:D:1438:PRO:HB3	1:D:1454:TYR:HE2	1.69	0.57
1:D:1582:ASP:HB3	1:D:1585:LYS:HZ1	1.70	0.57
1:A:1412:THR:HB	1:A:1413:PRO:HD3	1.87	0.56
1:D:1412:THR:HB	1:D:1413:PRO:HD3	1.87	0.56
1:A:678:ASN:H	1:A:681:MET:HE2	1.70	0.56
1:A:685:ASP:OD1	1:A:686:SER:N	2.38	0.56
1:A:931:ARG:O	1:A:935:ARG:NH1	2.39	0.56
1:A:1390:ARG:O	1:A:1393:ASP:N	2.38	0.56
1:A:1637:TYR:HB3	1:A:1639:VAL:HG13	1.86	0.56
1:D:621:GLN:HE22	1:D:623:ALA:HB2	1.70	0.56
1:D:685:ASP:OD1	1:D:686:SER:N	2.38	0.56
1:D:1015:ARG:HH12	1:D:1076:TYR:HD1	1.53	0.56
1:D:1390:ARG:O	1:D:1393:ASP:N	2.38	0.56
2:E:45:MET:HB3	2:E:50:PRO:HA	1.88	0.56
1:D:351:ILE:HG13	1:D:352:ALA:H	1.70	0.56
1:D:1632:LYS:O	1:D:1636:HIS:HB3	2.06	0.56
1:A:106:TYR:CZ	3:C:689:LEU:HD21	2.40	0.56
1:D:1284:GLN:H	1:D:1284:GLN:CD	2.13	0.56
1:D:1368:TYR:HE2	1:D:1414:PRO:HB3	1.71	0.56
1:D:330:THR:HB	1:D:344:HIS:CE1	2.40	0.56
1:D:621:GLN:NE2	1:D:622:ILE:O	2.39	0.56
1:A:84:GLU:O	1:A:87:LEU:N	2.33	0.56
1:A:423:ARG:HH11	1:A:427:ILE:HD12	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1279:VAL:HG23	1:A:1282:LEU:HD23	1.86	0.56
2:B:45:MET:HB3	2:B:50:PRO:HA	1.88	0.56
1:D:508:CYS:SG	1:D:509:TRP:N	2.73	0.56
1:A:17:TYR:HB2	3:C:536:LEU:HD11	1.86	0.56
1:A:35:VAL:HG12	1:A:49:THR:HA	1.87	0.56
1:A:1217:LYS:HD2	1:A:1254:CYS:SG	2.45	0.56
1:D:931:ARG:O	1:D:935:ARG:NH1	2.39	0.56
1:D:1438:PRO:HB3	1:D:1454:TYR:CE2	2.40	0.56
2:E:94:ARG:NH2	2:E:148:GLU:OE2	2.38	0.56
1:A:684:SER:O	1:A:688:THR:HG22	2.06	0.56
1:A:1284:GLN:H	1:A:1284:GLN:CD	2.13	0.55
1:D:857:LEU:HB3	1:D:905:LEU:HD11	1.89	0.55
1:A:438:LEU:HB3	1:A:439:PRO:HD3	1.88	0.55
1:A:739:PHE:CE2	1:A:794:LEU:HD12	2.29	0.55
1:A:960:LEU:O	1:A:964:MET:HE3	2.07	0.55
1:A:1397:ARG:NH1	3:C:606:ASP:OD2	2.38	0.55
3:F:693:GLU:O	3:F:697:ARG:HG2	2.06	0.55
1:A:860:MET:HE3	1:A:905:LEU:HD22	1.88	0.55
1:A:1549:MET:HE1	2:B:39:ASN:HB3	1.89	0.55
1:A:1632:LYS:O	1:A:1636:HIS:HB3	2.06	0.55
3:C:661:GLU:HA	3:C:664:ILE:HD12	1.89	0.55
1:D:315:THR:OG1	1:D:349:GLN:O	2.18	0.55
1:D:438:LEU:HB3	1:D:439:PRO:HD3	1.88	0.55
1:D:1516:GLU:HA	1:D:1519:ILE:HD12	1.88	0.55
3:F:627:GLU:HG2	3:F:631:LEU:HB2	1.87	0.55
1:A:315:THR:OG1	1:A:349:GLN:O	2.18	0.55
1:A:474:ASP:HA	1:A:525:CYS:HA	1.88	0.55
1:A:621:GLN:NE2	1:A:622:ILE:O	2.39	0.55
1:A:1183:HIS:HB3	1:A:1187:SER:OG	2.07	0.55
1:D:1467:PRO:HG2	2:E:31:GLU:C	2.31	0.55
1:A:443:ARG:NH1	1:A:627:CYS:O	2.40	0.55
1:A:548:GLY:HA3	1:A:573:LYS:HA	1.89	0.55
1:D:35:VAL:HG12	1:D:49:THR:HA	1.87	0.55
1:D:1098:LYS:O	1:D:1101:PHE:N	2.38	0.55
1:A:714:PRO:HB2	1:A:717:GLU:HB3	1.87	0.55
1:A:1368:TYR:HE2	1:A:1414:PRO:HB3	1.71	0.55
3:C:693:GLU:O	3:C:697:ARG:HG2	2.06	0.55
1:D:85:LEU:O	1:D:88:VAL:HG22	2.07	0.55
1:D:95:LEU:HD13	1:D:98:TRP:CD1	2.35	0.55
1:D:443:ARG:NH1	1:D:627:CYS:O	2.40	0.55
1:A:1261:ALA:HB2	1:A:1307:TYR:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:469:THR:HB	1:D:530:THR:HB	1.89	0.55
1:D:714:PRO:HB2	1:D:717:GLU:HB3	1.88	0.55
1:D:1261:ALA:HB2	1:D:1307:TYR:HB2	1.88	0.55
2:E:129:LEU:HD22	2:E:134:LEU:HD12	1.88	0.55
1:A:857:LEU:HB3	1:A:905:LEU:HD11	1.89	0.55
1:D:739:PHE:CE2	1:D:794:LEU:HD12	2.29	0.55
1:D:960:LEU:O	1:D:964:MET:HE3	2.07	0.55
1:A:964:MET:HG3	1:A:969:TYR:CE2	2.42	0.55
1:D:272:GLU:HB2	1:D:362:LEU:HD23	1.89	0.55
1:D:860:MET:HE3	1:D:905:LEU:HD22	1.88	0.55
1:A:351:ILE:HG13	1:A:352:ALA:H	1.70	0.54
2:B:129:LEU:HD22	2:B:134:LEU:HD12	1.88	0.54
1:D:1396:LEU:HD13	3:F:607:LYS:HB2	1.89	0.54
1:A:4:TRP:HB3	1:A:39:GLU:HB3	1.88	0.54
1:A:469:THR:HB	1:A:530:THR:HB	1.89	0.54
1:A:1015:ARG:HH12	1:A:1076:TYR:HD1	1.53	0.54
1:A:1098:LYS:O	1:A:1101:PHE:N	2.38	0.54
1:A:1155:LEU:HD21	1:A:1201:LEU:HD21	1.89	0.54
1:D:320:ARG:HB2	1:D:321:PRO:HD2	1.88	0.54
1:D:1183:HIS:HB3	1:D:1187:SER:OG	2.07	0.54
1:A:832:ASP:O	1:A:836:LEU:HG	2.08	0.54
1:D:476:GLU:OE1	1:D:524:ARG:NH2	2.32	0.54
1:D:964:MET:HG3	1:D:969:TYR:CE2	2.42	0.54
1:D:684:SER:O	1:D:688:THR:HG22	2.06	0.54
1:D:1559:VAL:HG22	2:E:59:ALA:HA	1.89	0.54
1:A:272:GLU:HB2	1:A:362:LEU:HD23	1.89	0.54
1:A:563:GLN:NE2	1:A:632:THR:O	2.41	0.54
1:A:1114:LEU:HD22	1:A:1163:ARG:HB3	1.89	0.54
3:F:564:LYS:HZ1	3:F:590:ASP:HA	1.73	0.54
1:A:85:LEU:O	1:A:88:VAL:HG22	2.07	0.54
1:A:481:GLU:HG2	1:A:483:ALA:H	1.73	0.54
1:D:87:LEU:HD21	1:D:148:VAL:HG11	1.88	0.54
1:A:94:THR:HG21	1:A:152:ILE:HG12	1.89	0.54
1:A:313:LYS:HE2	1:A:316:CYS:HB3	1.90	0.54
1:A:320:ARG:HB2	1:A:321:PRO:HD2	1.88	0.54
1:D:94:THR:HG21	1:D:152:ILE:HG12	1.89	0.54
1:D:1090:MET:HE3	1:D:1090:MET:HA	1.89	0.54
1:A:1265:LEU:HB2	1:A:1304:ILE:HD13	1.90	0.54
2:E:40:TYR:O	2:E:55:LEU:HB2	2.08	0.54
1:A:6:PRO:HD3	3:C:724:TYR:HB2	1.89	0.54
2:B:40:TYR:O	2:B:55:LEU:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:PHE:O	1:D:118:GLN:HG3	2.08	0.54
1:D:548:GLY:HA3	1:D:573:LYS:HA	1.89	0.54
1:D:767:ILE:HG13	1:D:768:ILE:N	2.23	0.54
1:D:950:ILE:O	1:D:954:VAL:HG23	2.07	0.54
1:D:1549:MET:SD	2:E:56:TRP:CZ3	3.01	0.54
1:A:62:THR:OG1	3:C:711:PRO:HB3	2.06	0.54
1:D:63:TYR:CZ	3:F:711:PRO:HD2	2.43	0.54
1:D:474:ASP:HA	1:D:525:CYS:HA	1.88	0.54
3:F:661:GLU:HA	3:F:664:ILE:HD12	1.89	0.54
1:A:106:TYR:O	3:C:551:GLN:HG3	2.08	0.53
1:A:260:ILE:HD11	1:A:307:GLU:HB3	1.89	0.53
1:A:1392:GLU:CD	2:B:166:LYS:HE3	2.33	0.53
1:A:1516:GLU:HA	1:A:1519:ILE:HD12	1.88	0.53
1:D:1:MET:H2	3:F:717:PRO:HB2	1.73	0.53
1:D:25:VAL:HG21	1:D:58:ILE:HD12	1.90	0.53
1:D:260:ILE:HD11	1:D:307:GLU:HB3	1.89	0.53
1:D:1397:ARG:NH1	3:F:606:ASP:OD2	2.41	0.53
1:A:87:LEU:HD21	1:A:148:VAL:HG11	1.88	0.53
1:A:943:MET:HE1	1:A:949:HIS:CD2	2.43	0.53
1:A:950:ILE:O	1:A:954:VAL:HG23	2.07	0.53
1:D:125:ILE:HD13	3:F:695:LYS:HD3	1.91	0.53
1:D:832:ASP:O	1:D:836:LEU:HG	2.08	0.53
1:D:943:MET:HE1	1:D:949:HIS:CD2	2.43	0.53
1:D:1155:LEU:HD21	1:D:1201:LEU:HD21	1.89	0.53
1:A:114:PHE:O	1:A:118:GLN:HG3	2.08	0.53
1:A:1536:HIS:CD2	1:A:1542:LEU:HD23	2.43	0.53
1:D:356:TYR:OH	1:D:367:LEU:O	2.19	0.53
1:D:836:LEU:HD22	1:D:877:VAL:HG11	1.91	0.53
1:A:639:GLY:HA2	1:A:643:TRP:HB3	1.90	0.53
1:D:1114:LEU:HD22	1:D:1163:ARG:HB3	1.89	0.53
1:D:1484:ILE:O	1:D:1512:ILE:N	2.42	0.53
3:F:551:GLN:HE22	3:F:552:ARG:HH21	1.57	0.53
1:A:767:ILE:HG13	1:A:768:ILE:N	2.23	0.53
1:D:4:TRP:HB3	1:D:39:GLU:HB3	1.88	0.53
1:A:25:VAL:HG21	1:A:58:ILE:HD12	1.90	0.53
1:A:455:PHE:HZ	1:A:547:PHE:H	1.57	0.53
1:A:836:LEU:HD22	1:A:877:VAL:HG11	1.91	0.53
1:A:1090:MET:HE3	1:A:1090:MET:HA	1.89	0.53
1:D:187:HIS:CE1	1:D:1008:VAL:HB	2.44	0.53
1:D:313:LYS:HE2	1:D:316:CYS:HB3	1.90	0.53
1:A:1484:ILE:O	1:A:1512:ILE:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:563:GLN:NE2	1:D:632:THR:O	2.41	0.53
1:D:1265:LEU:HB2	1:D:1304:ILE:HD13	1.90	0.53
1:D:1536:HIS:CD2	1:D:1542:LEU:HD23	2.43	0.53
1:D:722:LYS:HE2	1:D:724:PHE:HB2	1.91	0.53
1:D:791:ILE:O	1:D:794:LEU:HB3	2.09	0.53
2:B:94:ARG:NH2	2:B:148:GLU:OE2	2.38	0.53
1:D:455:PHE:HZ	1:D:547:PHE:H	1.57	0.53
1:D:481:GLU:HG2	1:D:483:ALA:H	1.73	0.53
1:A:791:ILE:O	1:A:794:LEU:HB3	2.08	0.52
1:A:1452:ASN:OD1	1:A:1453:TYR:N	2.42	0.52
2:B:75:THR:HG22	2:B:76:ASP:H	1.73	0.52
1:D:84:GLU:O	1:D:87:LEU:N	2.33	0.52
1:A:562:LEU:HD21	1:A:622:ILE:HD11	1.91	0.52
1:A:1024:PHE:HA	1:A:1027:VAL:HG12	1.91	0.52
1:D:1024:PHE:HA	1:D:1027:VAL:HG12	1.91	0.52
1:A:575:ASP:OD2	1:A:577:LYS:NZ	2.37	0.52
3:C:563:ARG:C	3:C:575:TRP:HE1	2.18	0.52
1:D:18:ASN:ND2	1:D:28:SER:HB3	2.24	0.52
1:A:18:ASN:ND2	1:A:28:SER:HB3	2.24	0.52
3:F:666:THR:HG21	3:F:678:MET:HE2	1.91	0.52
2:B:82:PHE:HE2	2:B:84:LEU:HD23	1.75	0.52
1:D:201:GLU:O	1:D:205:LEU:HB3	2.10	0.52
1:D:639:GLY:HA2	1:D:643:TRP:HB3	1.90	0.52
1:A:187:HIS:CE1	1:A:1008:VAL:HB	2.44	0.52
1:A:941:ILE:HA	1:A:992:MET:HE1	1.92	0.52
1:A:1301:TYR:O	1:A:1305:ILE:HG12	2.10	0.52
1:A:1539:ASP:OD1	1:A:1540:ARG:N	2.43	0.52
2:B:120:ARG:NH2	3:C:649:ASN:OD1	2.43	0.52
2:B:146:ALA:O	2:B:150:GLY:N	2.41	0.52
2:B:174:ARG:HA	2:B:177:LEU:HB2	1.92	0.52
3:C:692:MET:SD	3:C:695:LYS:HD2	2.50	0.52
1:D:1166:GLU:O	1:D:1169:LYS:HG2	2.10	0.52
1:D:1539:ASP:OD1	1:D:1540:ARG:N	2.43	0.52
2:E:82:PHE:HE2	2:E:84:LEU:HD23	1.75	0.52
2:E:155:LEU:HD13	2:E:168:VAL:HA	1.91	0.52
1:A:816:ALA:O	1:A:819:TYR:HB3	2.10	0.52
2:B:87:PRO:HG2	2:B:134:LEU:HD22	1.91	0.52
3:C:666:THR:HG21	3:C:678:MET:HE2	1.91	0.52
1:D:697:LEU:HA	1:D:700:ILE:HB	1.92	0.52
1:D:1452:ASN:OD1	1:D:1453:TYR:N	2.42	0.52
1:A:212:GLY:HA2	1:A:219:ILE:HD13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:965:ASP:O	1:A:969:TYR:N	2.33	0.51
2:B:7:VAL:HG22	2:B:56:TRP:CD1	2.43	0.51
1:A:1404:ASN:CG	1:A:1424:GLN:HB2	2.36	0.51
1:A:1482:MET:HE1	2:B:34:PRO:HD2	1.92	0.51
1:D:485:HIS:HB3	1:D:486:PRO:HD3	1.92	0.51
3:F:687:ASP:OD1	3:F:688:THR:N	2.43	0.51
1:A:697:LEU:HA	1:A:700:ILE:HB	1.92	0.51
2:B:155:LEU:HD13	2:B:168:VAL:HA	1.91	0.51
3:C:551:GLN:HE22	3:C:552:ARG:HH21	1.57	0.51
2:E:75:THR:HG22	2:E:76:ASP:H	1.73	0.51
3:F:692:MET:SD	3:F:695:LYS:HD2	2.50	0.51
1:A:41:TYR:HD2	1:A:44:TRP:HB2	1.75	0.51
3:C:687:ASP:OD1	3:C:688:THR:N	2.43	0.51
1:D:1404:ASN:CG	1:D:1424:GLN:HB2	2.36	0.51
2:E:87:PRO:HG2	2:E:134:LEU:HD22	1.91	0.51
1:A:539:THR:HG22	1:A:541:ASP:H	1.75	0.51
1:A:1399:LEU:HD21	1:A:1407:LYS:HE3	1.93	0.51
1:D:344:HIS:CE1	1:D:346:ILE:HB	2.45	0.51
1:D:562:LEU:HD21	1:D:622:ILE:HD11	1.91	0.51
1:D:915:ARG:HA	1:D:915:ARG:NH1	2.25	0.51
3:F:637:VAL:HB	3:F:640:LEU:HD12	1.91	0.51
1:A:722:LYS:HE2	1:A:724:PHE:HB2	1.92	0.51
1:D:31:ILE:HG21	3:F:698:LEU:HA	1.93	0.51
1:D:41:TYR:HD2	1:D:44:TRP:HB2	1.75	0.51
1:D:1301:TYR:O	1:D:1305:ILE:HG12	2.10	0.51
1:A:485:HIS:HB3	1:A:486:PRO:HD3	1.92	0.51
3:F:563:ARG:C	3:F:575:TRP:HE1	2.18	0.51
1:A:1080:ARG:HA	1:A:1083:ILE:HD12	1.93	0.51
1:A:1166:GLU:O	1:A:1169:LYS:HG2	2.10	0.51
1:A:1277:PRO:HG3	1:A:1292:THR:HA	1.93	0.51
2:B:9:VAL:HB	2:B:97:TRP:CZ3	2.46	0.51
1:D:1277:PRO:HG3	1:D:1292:THR:HA	1.93	0.51
2:E:174:ARG:HA	2:E:177:LEU:HB2	1.92	0.51
1:A:766:PHE:CE1	1:A:828:LYS:HG3	2.46	0.51
1:A:1059:LEU:HD21	1:A:1117:GLU:HG2	1.93	0.51
1:A:1585:LYS:O	1:A:1589:LEU:HG	2.11	0.51
3:C:637:VAL:HB	3:C:640:LEU:HD12	1.92	0.51
1:D:450:LEU:HB2	1:D:510:TYR:CG	2.46	0.51
1:A:281:PHE:HD1	1:A:388:ALA:HB2	1.76	0.50
1:A:1018:LEU:HD21	1:A:1083:ILE:HG12	1.93	0.50
3:C:577:CYS:HA	3:C:588:TYR:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:212:GLY:HA2	1:D:219:ILE:HD13	1.91	0.50
1:D:941:ILE:HA	1:D:992:MET:HE1	1.92	0.50
1:A:344:HIS:CE1	1:A:346:ILE:HB	2.46	0.50
1:D:1369:GLY:HA2	1:D:1418:ILE:HG22	1.93	0.50
1:A:1273:TRP:CE2	1:A:1327:THR:HG21	2.46	0.50
1:D:1356:MET:O	1:D:1357:ARG:HD2	2.11	0.50
2:E:146:ALA:O	2:E:150:GLY:N	2.41	0.50
1:A:330:THR:HA	1:A:333:ILE:HG22	1.94	0.50
1:A:1594:ALA:HB1	1:A:1641:THR:HB	1.93	0.50
1:D:816:ALA:O	1:D:819:TYR:HB3	2.10	0.50
1:D:1585:LYS:O	1:D:1589:LEU:HG	2.11	0.50
1:A:343:GLN:HB3	1:A:406:LEU:HD21	1.94	0.50
1:A:762:TYR:HD1	1:A:765:ARG:HG3	1.76	0.50
1:A:814:GLY:O	1:A:818:LYS:NZ	2.30	0.50
1:A:1234:LYS:HD2	1:A:1234:LYS:N	2.26	0.50
1:D:1362:TYR:HD2	1:D:1462:PHE:HE2	1.53	0.50
2:E:9:VAL:HB	2:E:97:TRP:CZ3	2.46	0.50
1:A:201:GLU:O	1:A:205:LEU:HB3	2.10	0.50
1:A:748:SER:O	1:A:752:LEU:HB2	2.12	0.50
1:A:915:ARG:HA	1:A:915:ARG:NH1	2.25	0.50
1:A:1353:ILE:HG13	1:D:1335:TYR:HB2	1.94	0.50
1:A:1356:MET:O	1:A:1357:ARG:HD2	2.11	0.50
1:A:1404:ASN:OD1	1:A:1424:GLN:HB2	2.11	0.50
2:B:41:SER:HA	2:B:54:GLY:HA2	1.93	0.50
1:D:1018:LEU:HD21	1:D:1083:ILE:HG12	1.93	0.50
2:E:8:VAL:O	2:E:58:THR:OG1	2.28	0.50
1:A:86:PRO:HA	1:A:89:GLN:HG2	1.93	0.50
1:A:875:ARG:HG2	1:A:924:HIS:CD2	2.46	0.50
1:A:994:LYS:HA	1:A:997:ILE:HG22	1.93	0.50
1:D:309:LYS:HE3	1:D:355:THR:HA	1.94	0.50
1:D:539:THR:HG22	1:D:541:ASP:H	1.76	0.50
1:D:994:LYS:HA	1:D:997:ILE:HG22	1.92	0.50
1:D:1080:ARG:HA	1:D:1083:ILE:HD12	1.93	0.50
1:D:1273:TRP:CE2	1:D:1327:THR:HG21	2.46	0.50
1:D:1384:ARG:HB2	1:D:1495:PHE:CD2	2.47	0.50
1:D:1399:LEU:HD13	1:D:1405:ALA:HB1	1.94	0.50
1:A:1335:TYR:HB2	1:D:1353:ILE:HG13	1.93	0.50
1:A:1612:THR:HG23	1:A:1614:GLN:H	1.77	0.50
1:D:762:TYR:HD1	1:D:765:ARG:HG3	1.76	0.50
1:D:766:PHE:CE1	1:D:828:LYS:HG3	2.46	0.50
1:A:450:LEU:HB2	1:A:510:TYR:CG	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:659:GLU:OE2	1:D:663:GLY:N	2.44	0.50
1:D:875:ARG:HG2	1:D:924:HIS:CD2	2.46	0.50
1:D:1011:MET:HG2	1:D:1076:TYR:CG	2.47	0.50
1:A:309:LYS:HE3	1:A:355:THR:HA	1.94	0.49
1:A:840:PHE:O	1:A:843:PHE:HB2	2.12	0.49
1:A:1384:ARG:HB2	1:A:1495:PHE:CD2	2.47	0.49
1:A:1474:ASP:OD1	1:A:1474:ASP:N	2.45	0.49
1:D:1152:ILE:HB	1:D:1236:ARG:HH12	1.77	0.49
1:D:1324:LEU:HB3	1:D:1341:LEU:HD21	1.94	0.49
1:A:7:THR:O	1:A:10:GLN:NE2	2.30	0.49
1:A:722:LYS:HG2	1:A:724:PHE:H	1.78	0.49
1:D:281:PHE:HD1	1:D:388:ALA:HB2	1.76	0.49
1:D:343:GLN:HB3	1:D:406:LEU:HD21	1.94	0.49
1:D:840:PHE:O	1:D:843:PHE:HB2	2.12	0.49
1:D:1399:LEU:HD21	1:D:1407:LYS:HE3	1.93	0.49
3:F:577:CYS:HA	3:F:588:TYR:HB3	1.94	0.49
1:A:319:ARG:HG2	1:A:327:MET:HB2	1.95	0.49
1:D:1404:ASN:OD1	1:D:1424:GLN:HB2	2.11	0.49
1:D:1594:ALA:HB1	1:D:1641:THR:HB	1.93	0.49
1:A:994:LYS:NZ	1:A:1048:HIS:HB3	2.27	0.49
1:A:1434:VAL:HG22	1:A:1463:ARG:NH2	2.27	0.49
1:D:319:ARG:HG2	1:D:327:MET:HB2	1.95	0.49
1:D:1466:ARG:O	1:D:1484:ILE:HA	2.12	0.49
1:D:1474:ASP:N	1:D:1474:ASP:OD1	2.45	0.49
1:A:153:ASP:HB3	1:A:164:VAL:HG22	1.95	0.49
1:A:566:ARG:NE	1:A:568:ASP:OD1	2.39	0.49
1:A:1011:MET:HG2	1:A:1076:TYR:CG	2.47	0.49
1:A:1466:ARG:O	1:A:1484:ILE:HA	2.12	0.49
1:D:7:THR:O	1:D:10:GLN:NE2	2.30	0.49
1:D:1434:VAL:HG22	1:D:1463:ARG:NH2	2.27	0.49
1:D:1612:THR:HG23	1:D:1614:GLN:H	1.77	0.49
1:A:31:ILE:HG21	3:C:698:LEU:HA	1.93	0.49
1:A:906:LEU:HD12	1:A:909:ILE:HD11	1.94	0.49
1:A:1152:ILE:HB	1:A:1236:ARG:HH12	1.77	0.49
1:A:1369:GLY:HA2	1:A:1418:ILE:HG22	1.93	0.49
1:D:86:PRO:HA	1:D:89:GLN:HG2	1.93	0.49
1:D:906:LEU:HD12	1:D:909:ILE:HD11	1.94	0.49
1:D:1059:LEU:HD21	1:D:1117:GLU:HG2	1.93	0.49
1:D:1362:TYR:CD2	1:D:1462:PHE:CE2	2.96	0.49
2:E:6:CYS:O	2:E:56:TRP:CD1	2.65	0.49
2:E:75:THR:HG22	2:E:76:ASP:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:659:GLU:OE2	1:A:663:GLY:N	2.44	0.49
1:A:392:VAL:O	1:A:395:LYS:HG2	2.12	0.49
1:A:1324:LEU:HB3	1:A:1341:LEU:HD21	1.94	0.49
2:B:6:CYS:O	2:B:56:TRP:CD1	2.65	0.49
2:B:75:THR:HG22	2:B:76:ASP:N	2.27	0.49
1:D:31:ILE:HG22	3:F:701:LEU:HD23	1.94	0.49
1:D:392:VAL:O	1:D:395:LYS:HG2	2.12	0.49
1:D:748:SER:O	1:D:752:LEU:HB2	2.12	0.49
1:D:879:LEU:HD22	1:D:924:HIS:HE1	1.77	0.49
1:D:1234:LYS:HD2	1:D:1234:LYS:N	2.26	0.49
1:D:1334:ASP:O	1:D:1337:GLY:N	2.46	0.49
1:D:1058:SER:HA	1:D:1080:ARG:NH1	2.28	0.49
1:D:1173:GLU:OE1	1:D:1198:SER:HB2	2.13	0.49
1:A:1058:SER:HA	1:A:1080:ARG:NH1	2.28	0.49
1:D:166:ARG:HD3	1:D:174:ASP:CG	2.38	0.49
1:D:153:ASP:HB3	1:D:164:VAL:HG22	1.95	0.48
1:D:575:ASP:N	1:D:575:ASP:OD1	2.46	0.48
1:D:722:LYS:HG2	1:D:724:PHE:H	1.77	0.48
1:A:654:LEU:HB3	1:A:692:LEU:HD21	1.95	0.48
1:A:1399:LEU:HD13	1:A:1405:ALA:HB1	1.94	0.48
1:D:287:MET:HE3	1:D:419:HIS:HA	1.95	0.48
1:D:330:THR:HA	1:D:333:ILE:HG22	1.94	0.48
2:E:7:VAL:HG22	2:E:56:TRP:CD1	2.43	0.48
1:A:9:ARG:HD2	1:A:68:GLU:HG2	1.95	0.48
1:A:287:MET:HE3	1:A:419:HIS:HA	1.96	0.48
1:A:1173:GLU:OE1	1:A:1198:SER:HB2	2.13	0.48
3:C:617:VAL:HB	3:C:621:ASP:HB2	1.96	0.48
1:D:654:LEU:HB3	1:D:692:LEU:HD21	1.95	0.48
1:D:1583:GLN:O	1:D:1586:VAL:HG12	2.13	0.48
1:A:101:ILE:HD12	1:A:159:LEU:HD21	1.95	0.48
1:A:242:PHE:CZ	1:A:244:ALA:HB2	2.48	0.48
1:A:474:ASP:OD1	1:A:475:GLU:N	2.45	0.48
1:A:1370:GLN:C	1:A:1372:PHE:H	2.20	0.48
1:D:743:ASN:N	1:D:747:SER:OG	2.46	0.48
1:D:1370:GLN:C	1:D:1372:PHE:H	2.20	0.48
2:E:41:SER:HA	2:E:54:GLY:HA2	1.93	0.48
1:D:814:GLY:O	1:D:818:LYS:HG2	2.14	0.48
1:D:994:LYS:NZ	1:D:1048:HIS:HB3	2.27	0.48
3:F:548:ILE:O	3:F:552:ARG:HG2	2.14	0.48
3:F:661:GLU:O	3:F:665:TRP:CE3	2.66	0.48
1:A:575:ASP:N	1:A:575:ASP:OD1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:743:ASN:N	1:A:747:SER:OG	2.46	0.48
1:A:1516:GLU:O	1:A:1519:ILE:HB	2.14	0.48
3:C:548:ILE:O	3:C:552:ARG:HG2	2.13	0.48
3:C:661:GLU:O	3:C:665:TRP:CE3	2.66	0.48
1:D:868:LEU:HG	1:D:871:GLN:NE2	2.29	0.48
1:A:181:ILE:HG13	1:A:959:ALA:HB2	1.95	0.48
1:A:814:GLY:O	1:A:818:LYS:HG2	2.14	0.48
1:A:868:LEU:HG	1:A:871:GLN:NE2	2.29	0.48
1:A:1112:VAL:HG13	1:A:1124:THR:HG21	1.95	0.48
1:A:1168:TYR:CE1	1:A:1172:LEU:HD11	2.48	0.48
1:A:1231:TYR:O	1:A:1235:LYS:N	2.46	0.48
1:A:420:LEU:HD11	1:A:423:ARG:HE	1.79	0.48
1:A:799:ASN:OD1	1:A:845:GLN:HB3	2.14	0.48
1:A:1583:GLN:O	1:A:1586:VAL:HG12	2.13	0.48
1:D:1112:VAL:HG13	1:D:1124:THR:HG21	1.95	0.48
1:D:1452:ASN:O	1:D:1455:ARG:HB2	2.14	0.48
1:D:1516:GLU:O	1:D:1519:ILE:HB	2.14	0.48
2:E:120:ARG:NH2	3:F:649:ASN:OD1	2.47	0.48
1:A:796:LEU:HA	1:A:799:ASN:ND2	2.28	0.48
1:D:101:ILE:HD12	1:D:159:LEU:HD21	1.95	0.48
1:D:1168:TYR:CE1	1:D:1172:LEU:HD11	2.48	0.48
1:A:1:MET:N	3:C:717:PRO:O	2.47	0.47
1:A:1121:ARG:O	1:A:1124:THR:N	2.44	0.47
1:A:1317:ALA:HB1	1:A:1348:PHE:CE2	2.49	0.47
1:A:1362:TYR:CD2	1:A:1462:PHE:CE2	2.96	0.47
1:A:1514:PRO:HD2	1:A:1515:LEU:H	1.79	0.47
1:D:504:VAL:HG12	1:D:506:GLN:H	1.79	0.47
1:D:1136:PHE:HA	1:D:1139:SER:OG	2.13	0.47
1:D:1564:SER:O	1:D:1568:LYS:HG3	2.14	0.47
1:A:379:LEU:HD11	1:A:428:ALA:O	2.13	0.47
1:A:992:MET:O	1:A:996:LEU:HD23	2.15	0.47
1:A:1386:LYS:HG3	1:A:1387:GLU:OE1	2.14	0.47
2:B:167:THR:O	2:B:171:GLU:HG2	2.14	0.47
1:D:676:LEU:HA	1:D:681:MET:HE1	1.97	0.47
1:D:1466:ARG:HH11	2:E:31:GLU:CD	2.22	0.47
1:A:166:ARG:HD3	1:A:174:ASP:CG	2.39	0.47
1:A:676:LEU:HA	1:A:681:MET:HE1	1.97	0.47
1:A:845:GLN:HG3	1:A:846:SER:H	1.78	0.47
1:A:1121:ARG:HD2	1:A:1168:TYR:HD2	1.78	0.47
1:A:1452:ASN:O	1:A:1455:ARG:HB2	2.14	0.47
1:A:1468:PHE:CD2	1:A:1470:LYS:HG3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1564:SER:O	1:A:1568:LYS:HG3	2.14	0.47
3:C:661:GLU:HG3	3:C:665:TRP:HZ3	1.80	0.47
1:D:38:LEU:HB3	3:F:724:TYR:HE2	1.79	0.47
1:D:242:PHE:CZ	1:D:244:ALA:HB2	2.48	0.47
1:D:379:LEU:HD11	1:D:428:ALA:O	2.13	0.47
1:D:1121:ARG:HD2	1:D:1168:TYR:HD2	1.78	0.47
2:E:167:THR:O	2:E:171:GLU:HG2	2.14	0.47
3:F:557:VAL:HA	3:F:579:LEU:HB3	1.96	0.47
1:A:504:VAL:HG12	1:A:506:GLN:H	1.80	0.47
1:A:1156:ASP:OD1	1:A:1200:LEU:HD21	2.15	0.47
2:B:21:ILE:HD11	2:B:35:THR:H	1.80	0.47
2:B:80:ILE:HG23	2:B:112:LEU:HD13	1.96	0.47
3:C:624:HIS:HB3	3:C:653:ASN:ND2	2.29	0.47
1:D:9:ARG:HD2	1:D:68:GLU:HG2	1.95	0.47
1:D:845:GLN:HG3	1:D:846:SER:H	1.78	0.47
1:D:866:SER:C	1:D:868:LEU:H	2.22	0.47
1:D:1018:LEU:HD11	1:D:1079:MET:HE3	1.97	0.47
1:A:63:TYR:CZ	3:C:711:PRO:HD2	2.49	0.47
1:A:979:ARG:HH12	1:A:1036:ALA:HA	1.79	0.47
1:A:1018:LEU:HD11	1:A:1079:MET:HE3	1.96	0.47
1:A:1136:PHE:HA	1:A:1139:SER:OG	2.13	0.47
2:B:1:MET:HE1	2:B:51:VAL:HA	1.96	0.47
1:D:17:TYR:HA	3:F:536:LEU:HD21	1.97	0.47
1:D:181:ILE:HG13	1:D:959:ALA:HB2	1.95	0.47
1:D:463:PRO:O	1:D:505:LYS:NZ	2.40	0.47
1:D:926:GLN:O	1:D:929:MET:HB3	2.15	0.47
1:D:1121:ARG:HD2	1:D:1168:TYR:CD2	2.50	0.47
1:D:1317:ALA:HB1	1:D:1348:PHE:CE2	2.49	0.47
1:D:1386:LYS:HG3	1:D:1387:GLU:OE1	2.14	0.47
2:E:8:VAL:HG13	2:E:81:CYS:SG	2.55	0.47
3:F:555:ARG:O	3:F:558:GLU:HG3	2.15	0.47
1:A:1484:ILE:HB	1:A:1512:ILE:HB	1.97	0.47
3:C:719:ASN:ND2	3:C:721:ASP:OD2	2.34	0.47
1:D:1121:ARG:O	1:D:1124:THR:N	2.44	0.47
1:D:1514:PRO:HD2	1:D:1515:LEU:H	1.79	0.47
2:E:1:MET:HE1	2:E:51:VAL:HA	1.96	0.47
3:F:624:HIS:HB3	3:F:653:ASN:ND2	2.29	0.47
1:A:896:LYS:CG	1:A:897:PRO:HD3	2.45	0.47
1:A:1575:TYR:HA	1:A:1578:GLU:HB2	1.97	0.47
1:A:1602:GLU:HA	1:A:1605:ARG:HD2	1.97	0.47
2:B:8:VAL:O	2:B:58:THR:OG1	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:VAL:HG13	2:B:81:CYS:SG	2.55	0.47
1:D:34:THR:OG1	3:F:700:ASP:OD2	2.25	0.47
1:D:189:VAL:O	1:D:193:ARG:HG2	2.15	0.47
1:D:550:ALA:HB2	1:D:571:VAL:HA	1.96	0.47
1:D:796:LEU:HA	1:D:799:ASN:ND2	2.28	0.47
1:D:799:ASN:OD1	1:D:845:GLN:HB3	2.14	0.47
1:D:1098:LYS:O	1:D:1102:ILE:HD12	2.15	0.47
1:D:1156:ASP:OD1	1:D:1200:LEU:HD21	2.15	0.47
3:F:616:VAL:HG22	3:F:644:ILE:HA	1.96	0.47
1:A:463:PRO:HB2	1:A:505:LYS:HG2	1.96	0.47
1:A:463:PRO:O	1:A:505:LYS:NZ	2.40	0.47
1:A:1374:SER:HA	1:A:1377:ARG:NE	2.29	0.47
1:A:1550:LEU:O	1:A:1554:ILE:HG12	2.15	0.47
1:D:965:ASP:O	1:D:969:TYR:N	2.33	0.47
1:D:1362:TYR:CD2	1:D:1462:PHE:HE2	2.33	0.47
1:D:1468:PHE:CD2	1:D:1470:LYS:HG3	2.49	0.47
1:D:1575:TYR:HA	1:D:1578:GLU:HB2	1.97	0.47
2:E:80:ILE:HG23	2:E:112:LEU:HD13	1.96	0.47
2:E:112:LEU:HD23	2:E:154:TYR:HD1	1.79	0.47
1:A:189:VAL:O	1:A:193:ARG:HG2	2.15	0.47
1:A:197:LYS:HA	1:A:200:GLU:HG2	1.96	0.47
1:A:550:ALA:HB2	1:A:571:VAL:HA	1.96	0.47
1:A:1121:ARG:HD2	1:A:1168:TYR:CD2	2.50	0.47
2:B:117:LEU:HD13	2:B:156:GLU:HB3	1.97	0.47
1:D:463:PRO:HB2	1:D:505:LYS:HG2	1.96	0.47
1:D:800:MET:HA	1:D:804:ARG:HE	1.80	0.47
1:D:1595:LEU:O	1:D:1599:LEU:HG	2.15	0.47
1:D:1602:GLU:HA	1:D:1605:ARG:HD2	1.97	0.47
3:F:617:VAL:HB	3:F:621:ASP:HB2	1.96	0.47
3:F:719:ASN:ND2	3:F:721:ASP:OD2	2.34	0.47
1:A:232:VAL:HB	1:A:241:LEU:HB3	1.97	0.47
1:A:387:ILE:HG23	1:A:392:VAL:HG11	1.96	0.47
1:A:1612:THR:O	1:A:1616:LYS:N	2.48	0.47
2:B:112:LEU:HD23	2:B:154:TYR:HD1	1.79	0.47
1:D:896:LYS:CG	1:D:897:PRO:HD3	2.45	0.47
1:D:1384:ARG:HB2	1:D:1495:PHE:CE2	2.50	0.47
1:A:181:ILE:HG22	1:A:185:LYS:NZ	2.30	0.46
1:A:530:THR:HA	1:A:549:VAL:HG12	1.96	0.46
1:A:1057:GLU:O	1:A:1080:ARG:HD3	2.14	0.46
1:A:1127:ILE:HA	1:A:1130:ASP:OD2	2.15	0.46
1:A:1364:ALA:HB3	1:A:1429:PHE:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:557:VAL:HA	3:C:579:LEU:HB3	1.96	0.46
1:D:230:ASN:ND2	1:D:341:GLU:HB3	2.30	0.46
1:D:561:THR:HG21	1:D:630:LYS:HB3	1.97	0.46
1:D:575:ASP:OD2	1:D:577:LYS:NZ	2.37	0.46
1:D:1127:ILE:HA	1:D:1130:ASP:OD2	2.15	0.46
1:D:1484:ILE:HB	1:D:1512:ILE:HB	1.97	0.46
1:D:1550:LEU:O	1:D:1554:ILE:HG12	2.14	0.46
2:E:41:SER:OG	2:E:53:LEU:O	2.30	0.46
1:A:125:ILE:CD1	3:C:695:LYS:HD3	2.44	0.46
1:A:678:ASN:N	1:A:681:MET:HE2	2.30	0.46
1:A:1334:ASP:O	1:A:1337:GLY:N	2.46	0.46
3:C:578:ARG:NH1	3:C:598:GLU:OE1	2.38	0.46
3:C:616:VAL:HG22	3:C:644:ILE:HA	1.96	0.46
3:C:677:MET:HB2	3:C:682:THR:HG21	1.97	0.46
1:D:307:GLU:CD	1:D:313:LYS:HE3	2.40	0.46
1:D:1386:LYS:HG3	1:D:1387:GLU:H	1.80	0.46
3:F:579:LEU:HA	3:F:586:LEU:HD13	1.98	0.46
1:A:324:VAL:HG12	1:A:327:MET:HE3	1.98	0.46
1:A:1098:LYS:O	1:A:1102:ILE:HD12	2.15	0.46
1:D:181:ILE:HG22	1:D:185:LYS:NZ	2.30	0.46
1:D:387:ILE:HG23	1:D:392:VAL:HG11	1.96	0.46
1:D:566:ARG:NE	1:D:568:ASP:OD1	2.39	0.46
1:D:902:SER:OG	1:D:953:PHE:HZ	1.98	0.46
1:D:1057:GLU:O	1:D:1080:ARG:HD3	2.14	0.46
1:D:1364:ALA:HB3	1:D:1429:PHE:CE1	2.50	0.46
2:E:21:ILE:HD11	2:E:35:THR:H	1.80	0.46
2:E:63:ASP:OD1	2:E:64:TYR:N	2.48	0.46
3:F:661:GLU:HG3	3:F:665:TRP:HZ3	1.80	0.46
1:A:4:TRP:CH2	1:A:46:ARG:HG2	2.51	0.46
1:A:136:LEU:HD12	1:A:140:GLU:HG2	1.98	0.46
1:A:277:LEU:HD23	1:A:277:LEU:H	1.80	0.46
1:A:307:GLU:CD	1:A:313:LYS:HE3	2.40	0.46
1:A:438:LEU:HG	1:A:630:LYS:HZ3	1.80	0.46
1:A:1198:SER:O	1:A:1202:GLU:HG3	2.16	0.46
1:A:1618:LEU:O	1:A:1622:LEU:HG	2.16	0.46
1:D:197:LYS:HA	1:D:200:GLU:HG2	1.96	0.46
1:D:992:MET:O	1:D:996:LEU:HD23	2.15	0.46
1:D:1003:ALA:C	1:D:1005:ASP:H	2.24	0.46
1:D:1183:HIS:CG	1:D:1184:LYS:H	2.33	0.46
1:A:430:LYS:HG3	1:A:433:PHE:CE1	2.51	0.46
1:A:866:SER:C	1:A:868:LEU:H	2.22	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1003:ALA:C	1:A:1005:ASP:H	2.24	0.46
1:A:1589:LEU:O	1:A:1593:ILE:HG12	2.15	0.46
3:C:640:LEU:HD13	3:C:656:ALA:O	2.15	0.46
1:D:70:THR:HG22	1:D:71:VAL:H	1.81	0.46
1:D:256:GLU:OE2	1:D:370:SER:OG	2.26	0.46
1:D:420:LEU:HD11	1:D:423:ARG:HE	1.79	0.46
1:D:606:LEU:HD12	1:D:609:PHE:HD2	1.81	0.46
1:D:701:ILE:HD11	1:D:712:PHE:CG	2.51	0.46
1:D:979:ARG:HH12	1:D:1036:ALA:HA	1.79	0.46
1:D:1078:ASP:HB3	1:D:1081:LYS:HD3	1.97	0.46
1:D:1231:TYR:O	1:D:1235:LYS:N	2.46	0.46
1:D:1545:HIS:HD2	2:E:5:LYS:HE3	1.80	0.46
1:D:1618:LEU:O	1:D:1622:LEU:HG	2.16	0.46
3:F:537:LYS:HB2	3:F:694:ILE:HG13	1.98	0.46
1:A:46:ARG:HB3	1:A:58:ILE:HG23	1.98	0.46
1:A:1078:ASP:HB3	1:A:1081:LYS:HD3	1.97	0.46
3:C:555:ARG:O	3:C:558:GLU:HG3	2.15	0.46
1:D:1070:ASN:HA	1:D:1073:VAL:HG12	1.98	0.46
1:D:1248:ARG:HH22	1:D:1252:ARG:HH11	1.63	0.46
1:D:1589:LEU:O	1:D:1593:ILE:HG12	2.15	0.46
3:F:640:LEU:HD13	3:F:656:ALA:O	2.15	0.46
1:A:41:TYR:HB3	1:A:44:TRP:O	2.16	0.46
1:A:70:THR:HG22	1:A:71:VAL:H	1.81	0.46
1:A:1183:HIS:CG	1:A:1184:LYS:H	2.33	0.46
1:A:1394:PHE:HD2	1:A:1428:CYS:HG	1.61	0.46
1:A:1414:PRO:HB2	1:A:1419:LYS:HE3	1.98	0.46
1:A:1595:LEU:O	1:A:1599:LEU:HG	2.15	0.46
3:C:532:PRO:O	3:C:536:LEU:HD13	2.16	0.46
1:D:4:TRP:CH2	1:D:46:ARG:HG2	2.51	0.46
1:D:277:LEU:H	1:D:277:LEU:HD23	1.80	0.46
1:D:400:TRP:CG	1:D:401:VAL:H	2.33	0.46
1:D:755:ALA:O	1:D:820:LEU:HD23	2.15	0.46
1:D:1098:LYS:HD2	1:D:1134:CYS:SG	2.56	0.46
1:D:1557:PRO:HG3	1:D:1563:PHE:CE2	2.51	0.46
1:D:1612:THR:O	1:D:1616:LYS:N	2.48	0.46
1:A:6:PRO:HG3	3:C:724:TYR:CD1	2.50	0.46
1:A:453:GLY:HA2	1:A:618:ASP:HA	1.98	0.46
1:A:606:LEU:HD12	1:A:609:PHE:HD2	1.81	0.46
1:A:701:ILE:HD11	1:A:712:PHE:CG	2.51	0.46
1:A:1386:LYS:HG3	1:A:1387:GLU:H	1.80	0.46
1:A:1404:ASN:ND2	1:A:1424:GLN:HB2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:281:PHE:HE1	1:D:383:LEU:HD22	1.81	0.46
1:D:1384:ARG:HD2	1:D:1495:PHE:HD2	1.81	0.46
1:D:1404:ASN:ND2	1:D:1424:GLN:HB2	2.31	0.46
2:E:117:LEU:HD13	2:E:156:GLU:HB3	1.97	0.46
1:A:400:TRP:CG	1:A:401:VAL:H	2.33	0.46
1:A:755:ALA:O	1:A:820:LEU:HD23	2.15	0.46
1:A:926:GLN:O	1:A:929:MET:HB3	2.15	0.46
1:A:1536:HIS:ND1	1:A:1547:LEU:HD11	2.31	0.46
1:D:449:THR:OG1	1:D:621:GLN:OE1	2.24	0.46
1:D:938:ARG:HA	1:D:941:ILE:HB	1.98	0.46
1:D:997:ILE:HG12	1:D:1053:PHE:HD1	1.81	0.46
1:D:1414:PRO:HB2	1:D:1419:LYS:HE3	1.98	0.46
1:A:1259:GLU:HG3	1:A:1497:GLY:O	2.16	0.46
1:A:1384:ARG:HB2	1:A:1495:PHE:CE2	2.50	0.46
1:A:1557:PRO:HG3	1:A:1563:PHE:CE2	2.51	0.46
2:B:63:ASP:OD1	2:B:64:TYR:N	2.48	0.46
1:D:41:TYR:HB3	1:D:44:TRP:O	2.16	0.46
1:D:232:VAL:HB	1:D:241:LEU:HB3	1.97	0.46
1:D:438:LEU:HG	1:D:630:LYS:HZ3	1.81	0.46
3:F:677:MET:HB2	3:F:682:THR:HG21	1.97	0.46
1:A:97:GLU:CD	1:A:1065:SER:HB2	2.41	0.45
1:A:938:ARG:HA	1:A:941:ILE:HB	1.98	0.45
1:A:1193:PHE:O	1:A:1197:VAL:HG23	2.16	0.45
1:A:1329:GLU:HB3	1:A:1338:LEU:HD21	1.98	0.45
1:A:1362:TYR:CD2	1:A:1462:PHE:HE2	2.33	0.45
1:D:289:LEU:HD13	1:D:291:ARG:HD2	1.98	0.45
1:D:887:SER:O	1:D:890:LEU:HB3	2.16	0.45
1:D:1109:ILE:O	1:D:1112:VAL:HG12	2.16	0.45
1:D:1329:GLU:HB3	1:D:1338:LEU:HD21	1.98	0.45
1:D:1560:MET:HE3	1:D:1565:ASN:ND2	2.31	0.45
1:A:887:SER:O	1:A:890:LEU:HB3	2.16	0.45
1:A:902:SER:OG	1:A:953:PHE:HZ	1.98	0.45
1:A:1248:ARG:HH22	1:A:1252:ARG:HH11	1.64	0.45
1:D:97:GLU:CD	1:D:1065:SER:HB2	2.41	0.45
1:D:423:ARG:NH1	1:D:427:ILE:HD12	2.31	0.45
1:D:430:LYS:HG3	1:D:433:PHE:CE1	2.51	0.45
1:D:530:THR:HA	1:D:549:VAL:HG12	1.96	0.45
2:E:114:GLY:HA3	2:E:156:GLU:HG2	1.98	0.45
1:A:59:PHE:CE2	1:A:63:TYR:HB3	2.52	0.45
1:A:329:ILE:O	1:A:332:ILE:HG22	2.17	0.45
1:A:800:MET:HA	1:A:804:ARG:HE	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:879:LEU:HD12	1:A:882:LEU:HD22	1.98	0.45
1:A:1239:ILE:HD13	1:A:1242:ARG:HE	1.80	0.45
3:C:590:ASP:C	3:C:591:LEU:HD22	2.42	0.45
1:D:1462:PHE:HB2	1:D:1489:TYR:HB2	1.98	0.45
1:D:1536:HIS:ND1	1:D:1547:LEU:HD11	2.31	0.45
1:A:287:MET:HE2	1:A:420:LEU:HB2	1.99	0.45
1:A:449:THR:OG1	1:A:621:GLN:OE1	2.24	0.45
1:A:1070:ASN:HA	1:A:1073:VAL:HG12	1.98	0.45
1:A:1545:HIS:HD2	2:B:5:LYS:HE3	1.81	0.45
1:D:6:PRO:HD3	3:F:724:TYR:HB2	1.99	0.45
1:D:18:ASN:CG	3:F:536:LEU:HG	2.42	0.45
1:D:18:ASN:OD1	3:F:536:LEU:HG	2.16	0.45
1:D:25:VAL:HG11	1:D:56:LYS:HG3	1.99	0.45
1:D:320:ARG:CZ	1:D:322:PHE:HB2	2.46	0.45
1:D:474:ASP:OD1	1:D:475:GLU:N	2.45	0.45
1:D:1239:ILE:HD13	1:D:1242:ARG:HE	1.80	0.45
3:F:590:ASP:C	3:F:591:LEU:HD22	2.42	0.45
1:A:997:ILE:HG12	1:A:1053:PHE:HD1	1.81	0.45
1:A:1622:LEU:O	1:A:1626:PHE:HB2	2.17	0.45
3:C:537:LYS:HB2	3:C:694:ILE:HG13	1.98	0.45
3:C:579:LEU:HA	3:C:586:LEU:HD13	1.97	0.45
1:D:46:ARG:HB3	1:D:58:ILE:HG23	1.98	0.45
1:D:697:LEU:HD22	1:D:700:ILE:HD12	1.98	0.45
1:D:879:LEU:HD12	1:D:882:LEU:HD22	1.98	0.45
1:A:169:ASN:ND2	1:A:173:LEU:HD12	2.32	0.45
1:A:281:PHE:HE1	1:A:383:LEU:HD22	1.81	0.45
1:A:767:ILE:HG13	1:A:768:ILE:H	1.82	0.45
1:A:985:PHE:CD2	1:A:986:LEU:HD12	2.52	0.45
1:A:1109:ILE:O	1:A:1112:VAL:HG12	2.16	0.45
1:A:1384:ARG:HD2	1:A:1495:PHE:HD2	1.81	0.45
1:A:1560:MET:HE3	1:A:1565:ASN:ND2	2.31	0.45
2:B:114:GLY:HA3	2:B:156:GLU:HG2	1.98	0.45
1:D:59:PHE:CE2	1:D:63:TYR:HB3	2.51	0.45
1:D:890:LEU:HD11	1:D:938:ARG:HD3	1.98	0.45
1:D:1259:GLU:HG3	1:D:1497:GLY:O	2.16	0.45
1:D:1557:PRO:HB2	1:D:1560:MET:O	2.17	0.45
1:A:697:LEU:HD22	1:A:700:ILE:HD12	1.98	0.45
1:A:1098:LYS:HD2	1:A:1134:CYS:SG	2.56	0.45
1:A:1138:PHE:O	1:A:1138:PHE:CG	2.70	0.45
1:A:1153:THR:HG22	1:A:1157:GLN:OE1	2.17	0.45
3:C:564:LYS:HZ1	3:C:590:ASP:HA	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:ILE:HG13	1:A:352:ALA:N	2.31	0.45
1:A:561:THR:HG21	1:A:630:LYS:HB3	1.97	0.45
1:A:1435:MET:SD	1:A:1455:ARG:HG2	2.57	0.45
1:A:1557:PRO:HB2	1:A:1560:MET:O	2.17	0.45
1:D:169:ASN:ND2	1:D:173:LEU:HD12	2.32	0.45
1:D:806:LEU:HD21	1:D:809:ALA:HB3	1.99	0.45
1:D:829:LEU:HD23	1:D:829:LEU:H	1.82	0.45
1:D:1622:LEU:O	1:D:1626:PHE:HB2	2.17	0.45
1:A:25:VAL:HG11	1:A:56:LYS:HG3	1.99	0.45
1:A:860:MET:SD	1:A:882:LEU:HG	2.57	0.45
1:D:1153:THR:HG22	1:D:1157:GLN:OE1	2.17	0.45
1:A:386:VAL:HG23	1:A:387:ILE:HG13	1.99	0.45
1:A:1144:PHE:CZ	1:A:1193:PHE:HD2	2.35	0.45
3:C:642:PHE:CZ	3:C:654:PHE:HB2	2.52	0.45
1:D:136:LEU:HD12	1:D:140:GLU:HG2	1.98	0.45
1:D:243:MET:HB3	1:D:245:LEU:HG	1.98	0.45
1:D:280:VAL:O	1:D:380:THR:OG1	2.26	0.45
1:D:324:VAL:HG12	1:D:327:MET:HE3	1.98	0.45
1:D:517:ILE:HG12	1:D:521:GLU:HB3	2.00	0.45
1:D:970:SER:O	1:D:974:SER:OG	2.34	0.45
1:D:1198:SER:O	1:D:1202:GLU:HG3	2.16	0.45
1:D:1435:MET:SD	1:D:1455:ARG:HG2	2.57	0.45
2:E:14:VAL:HG13	2:E:116:LYS:NZ	2.32	0.45
2:E:170:ASP:O	2:E:174:ARG:HG2	2.17	0.45
1:A:25:VAL:HG23	1:A:26:GLU:HG2	1.99	0.44
1:A:423:ARG:NH1	1:A:427:ILE:HD12	2.31	0.44
1:A:517:ILE:HG12	1:A:521:GLU:HB3	1.99	0.44
1:A:1237:GLU:O	1:A:1240:TYR:HB3	2.18	0.44
1:A:1300:LEU:O	1:A:1304:ILE:HG13	2.17	0.44
1:A:1399:LEU:HD12	3:C:607:LYS:HD3	1.99	0.44
1:A:1549:MET:SD	2:B:56:TRP:HZ3	2.38	0.44
3:C:564:LYS:NZ	3:C:590:ASP:HA	2.32	0.44
1:D:63:TYR:CE1	3:F:711:PRO:HB2	2.53	0.44
1:D:187:HIS:CE1	1:D:1009:MET:H	2.35	0.44
1:D:453:GLY:HA2	1:D:618:ASP:HA	1.98	0.44
1:D:795:PHE:CE2	1:D:841:CYS:HB3	2.52	0.44
1:D:1300:LEU:O	1:D:1304:ILE:HG13	2.17	0.44
1:A:181:ILE:HD11	1:A:956:CYS:HA	1.99	0.44
1:A:230:ASN:ND2	1:A:341:GLU:HB3	2.29	0.44
1:A:243:MET:HB3	1:A:245:LEU:HG	1.98	0.44
1:A:795:PHE:CE2	1:A:841:CYS:HB3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:879:LEU:HD22	1:A:924:HIS:HE1	1.77	0.44
1:A:890:LEU:HD11	1:A:938:ARG:HD3	1.98	0.44
1:A:1313:MET:HA	1:A:1453:TYR:OH	2.18	0.44
1:A:1325:ALA:O	1:A:1329:GLU:HG3	2.17	0.44
2:B:14:VAL:HG13	2:B:116:LYS:NZ	2.32	0.44
1:D:80:VAL:HG22	1:D:85:LEU:HD11	2.00	0.44
1:D:351:ILE:HG13	1:D:352:ALA:N	2.31	0.44
1:D:386:VAL:HG23	1:D:387:ILE:HG13	1.99	0.44
1:D:1193:PHE:O	1:D:1197:VAL:HG23	2.17	0.44
1:D:1325:ALA:O	1:D:1329:GLU:HG3	2.17	0.44
1:D:1374:SER:HA	1:D:1377:ARG:NE	2.29	0.44
1:A:187:HIS:CE1	1:A:1009:MET:H	2.35	0.44
1:A:320:ARG:CZ	1:A:322:PHE:HB2	2.46	0.44
1:A:1449:GLN:OE1	1:A:1449:GLN:N	2.45	0.44
1:D:767:ILE:HG13	1:D:768:ILE:H	1.82	0.44
1:D:985:PHE:HA	1:D:988:GLU:OE1	2.17	0.44
1:D:1449:GLN:OE1	1:D:1449:GLN:N	2.45	0.44
1:A:970:SER:O	1:A:974:SER:OG	2.34	0.44
1:A:1028:LEU:HB3	1:A:1043:TRP:CZ2	2.53	0.44
1:A:1607:HIS:HE2	1:A:1619:HIS:HB2	1.82	0.44
1:D:25:VAL:HG23	1:D:26:GLU:HG2	1.99	0.44
1:D:329:ILE:O	1:D:332:ILE:HG22	2.17	0.44
1:D:1002:TYR:OH	1:D:1009:MET:HE2	2.17	0.44
1:D:1138:PHE:O	1:D:1138:PHE:CG	2.70	0.44
1:D:1257:TYR:CE2	1:D:1310:LYS:HD3	2.52	0.44
1:A:693:VAL:HG12	1:A:757:LEU:HD11	2.00	0.44
1:A:806:LEU:HD21	1:A:809:ALA:HB3	1.99	0.44
1:A:1007:MET:HE3	1:A:1007:MET:HB3	1.69	0.44
1:A:1257:TYR:CE2	1:A:1310:LYS:HD3	2.52	0.44
1:A:1462:PHE:HB2	1:A:1489:TYR:HB2	1.98	0.44
1:D:91:LEU:O	1:D:95:LEU:HD23	2.18	0.44
1:D:570:VAL:HB	1:D:612:SER:H	1.83	0.44
1:D:1418:ILE:HG21	1:D:1425:TYR:CG	2.53	0.44
3:F:532:PRO:O	3:F:536:LEU:HD13	2.16	0.44
1:A:80:VAL:HG22	1:A:85:LEU:HD11	2.00	0.44
1:A:985:PHE:HA	1:A:988:GLU:OE1	2.17	0.44
3:C:607:LYS:HZ3	3:C:608:LEU:H	1.65	0.44
1:D:166:ARG:HB3	1:D:171:ASN:HA	2.00	0.44
1:D:864:VAL:HG21	1:D:909:ILE:HG22	2.00	0.44
1:D:879:LEU:HD12	1:D:882:LEU:HB2	2.00	0.44
1:D:1313:MET:HA	1:D:1453:TYR:OH	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4:ILE:HD11	2:E:51:VAL:HG21	2.00	0.44
2:E:114:GLY:H	2:E:156:GLU:HA	1.82	0.44
1:A:289:LEU:HD13	1:A:291:ARG:HD2	1.98	0.44
1:A:1608:GLY:HA2	1:A:1611:LEU:HB3	1.99	0.44
1:D:23:GLN:OE1	1:D:58:ILE:HB	2.18	0.44
1:D:158:MET:HG2	1:D:159:LEU:HD12	1.99	0.44
1:D:678:ASN:N	1:D:681:MET:HE2	2.31	0.44
1:D:985:PHE:CD2	1:D:986:LEU:HD12	2.52	0.44
3:F:578:ARG:NH1	3:F:598:GLU:OE1	2.38	0.44
1:A:91:LEU:HD13	1:A:152:ILE:HD11	2.00	0.44
1:A:1174:LYS:HB3	1:A:1174:LYS:HE2	1.75	0.44
1:D:693:VAL:HG12	1:D:757:LEU:HD11	2.00	0.44
1:D:722:LYS:HG3	1:D:724:PHE:CD2	2.53	0.44
1:D:755:ALA:HB1	1:D:819:TYR:CE2	2.53	0.44
1:D:1015:ARG:NH1	1:D:1076:TYR:HD1	2.15	0.44
1:D:1144:PHE:CZ	1:D:1193:PHE:HD2	2.35	0.44
1:D:1365:VAL:HG11	1:D:1398:LEU:HD23	2.00	0.44
1:D:1556:ASP:O	1:D:1558:ALA:N	2.50	0.44
1:D:1608:GLY:HA2	1:D:1611:LEU:HB3	1.99	0.44
1:A:140:GLU:O	1:A:144:LEU:HD23	2.17	0.44
1:A:438:LEU:HD13	1:A:661:ASP:HA	2.00	0.44
1:A:994:LYS:HA	1:A:1049:LEU:HD13	2.00	0.44
1:A:1015:ARG:NH1	1:A:1076:TYR:HD1	2.16	0.44
1:A:1180:CYS:O	1:A:1187:SER:HB3	2.18	0.44
1:A:1418:ILE:HG21	1:A:1425:TYR:CG	2.53	0.44
3:C:551:GLN:NE2	3:C:552:ARG:HH21	2.16	0.44
1:D:140:GLU:O	1:D:144:LEU:HD23	2.18	0.44
1:D:181:ILE:HD11	1:D:956:CYS:HA	1.99	0.44
1:D:1044:ASN:HA	1:D:1101:PHE:HZ	1.83	0.44
1:D:1180:CYS:O	1:D:1187:SER:HB3	2.18	0.44
2:E:8:VAL:HG21	2:E:20:LEU:HD11	1.99	0.44
1:A:91:LEU:O	1:A:95:LEU:HD23	2.18	0.43
1:A:1556:ASP:O	1:A:1558:ALA:N	2.50	0.43
1:A:1579:HIS:HD2	1:A:1582:ASP:HB2	1.83	0.43
1:D:287:MET:HE2	1:D:420:LEU:HB2	1.99	0.43
1:D:875:ARG:NH1	1:D:920:ALA:O	2.46	0.43
1:D:1392:GLU:CD	2:E:166:LYS:HE3	2.43	0.43
1:D:1463:ARG:HD3	1:D:1486:ARG:HH11	1.84	0.43
1:D:1554:ILE:HA	2:E:37:PHE:CD1	2.53	0.43
1:A:1:MET:N	1:A:1:MET:SD	2.90	0.43
1:A:755:ALA:HB1	1:A:819:TYR:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1365:VAL:HG11	1:A:1398:LEU:HD23	2.00	0.43
2:B:8:VAL:HG21	2:B:20:LEU:HD11	1.99	0.43
3:C:652:LEU:HD23	3:C:652:LEU:HA	1.82	0.43
1:D:659:GLU:HG2	1:D:711:HIS:CD2	2.53	0.43
1:D:860:MET:SD	1:D:882:LEU:HG	2.57	0.43
1:D:931:ARG:HG2	1:D:935:ARG:HH12	1.83	0.43
1:D:1362:TYR:HE2	1:D:1459:VAL:HG21	1.83	0.43
2:E:82:PHE:CE1	2:E:154:TYR:HE1	2.36	0.43
3:F:551:GLN:NE2	3:F:552:ARG:HH21	2.16	0.43
3:F:564:LYS:NZ	3:F:590:ASP:HA	2.32	0.43
1:A:864:VAL:HG21	1:A:909:ILE:HG22	2.00	0.43
1:D:796:LEU:HD23	1:D:799:ASN:HD22	1.83	0.43
1:D:994:LYS:HA	1:D:1049:LEU:HD13	2.00	0.43
1:D:1028:LEU:HB3	1:D:1043:TRP:CZ2	2.53	0.43
1:D:1079:MET:HB3	1:D:1079:MET:HE2	1.59	0.43
1:A:124:LEU:HA	1:A:127:TRP:CE3	2.54	0.43
1:A:722:LYS:HG3	1:A:724:PHE:CD2	2.53	0.43
1:A:1044:ASN:HA	1:A:1101:PHE:HZ	1.83	0.43
1:D:122:TYR:HE1	3:F:695:LYS:HE3	1.82	0.43
1:D:467:GLU:HG3	1:D:509:TRP:HB3	1.99	0.43
1:D:1237:GLU:O	1:D:1240:TYR:HB3	2.18	0.43
1:A:18:ASN:HA	1:A:29:LEU:O	2.18	0.43
1:A:158:MET:HG2	1:A:159:LEU:HD12	1.99	0.43
1:A:285:SER:O	1:A:420:LEU:HB3	2.19	0.43
1:A:467:GLU:HG3	1:A:509:TRP:HB3	1.99	0.43
1:A:1362:TYR:HE2	1:A:1459:VAL:HG21	1.83	0.43
1:D:91:LEU:HD13	1:D:152:ILE:HD11	1.99	0.43
1:D:262:TRP:CZ2	1:D:358:ARG:HB3	2.54	0.43
1:D:1300:LEU:HD23	1:D:1300:LEU:HA	1.82	0.43
3:F:642:PHE:CZ	3:F:654:PHE:HB2	2.53	0.43
1:A:869:PHE:HD2	1:A:870:ARG:NH1	2.17	0.43
1:A:940:VAL:HG13	1:A:992:MET:SD	2.59	0.43
1:A:1166:GLU:O	1:A:1170:VAL:HG23	2.18	0.43
1:A:1215:GLU:O	1:A:1215:GLU:HG3	2.18	0.43
1:A:1220:ARG:O	1:A:1224:THR:HG22	2.19	0.43
2:B:4:ILE:HD11	2:B:51:VAL:HG21	2.00	0.43
3:C:622:CYS:HB3	3:C:624:HIS:CE1	2.53	0.43
1:D:243:MET:HE1	1:D:289:LEU:HD23	1.99	0.43
1:D:869:PHE:HD2	1:D:870:ARG:NH1	2.17	0.43
1:D:994:LYS:HZ2	1:D:1048:HIS:HB3	1.83	0.43
1:D:1394:PHE:HD2	1:D:1428:CYS:HG	1.63	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ARG:HB3	1:A:171:ASN:HA	2.00	0.43
1:A:243:MET:HE1	1:A:289:LEU:HD23	1.99	0.43
1:A:379:LEU:HD12	1:A:379:LEU:HA	1.84	0.43
1:A:405:LEU:HB3	1:A:414:GLN:NE2	2.29	0.43
1:A:829:LEU:H	1:A:829:LEU:HD23	1.82	0.43
1:A:938:ARG:HG3	1:A:941:ILE:HD12	2.01	0.43
1:A:1002:TYR:OH	1:A:1009:MET:HE2	2.17	0.43
1:A:1463:ARG:HD3	1:A:1486:ARG:HH11	1.83	0.43
2:B:170:ASP:O	2:B:174:ARG:HG2	2.17	0.43
1:D:438:LEU:HD13	1:D:661:ASP:HA	2.00	0.43
1:D:564:ASP:HA	1:D:624:THR:H	1.83	0.43
1:D:1215:GLU:O	1:D:1215:GLU:HG3	2.18	0.43
1:A:931:ARG:HG2	1:A:935:ARG:HH12	1.83	0.43
1:A:1099:ILE:HD11	1:A:1134:CYS:O	2.19	0.43
1:A:1256:ASN:O	1:A:1259:GLU:N	2.52	0.43
1:D:18:ASN:HA	1:D:29:LEU:O	2.18	0.43
1:D:940:VAL:HG13	1:D:992:MET:SD	2.59	0.43
1:D:1166:GLU:O	1:D:1170:VAL:HG23	2.18	0.43
1:D:1220:ARG:O	1:D:1224:THR:HG22	2.19	0.43
2:E:68:ARG:N	2:E:69:PRO:HD3	2.34	0.43
1:A:69:ALA:HB2	1:A:78:GLU:HG2	2.00	0.43
1:A:79:THR:HA	1:A:85:LEU:HD22	2.00	0.43
1:A:313:LYS:NZ	1:A:354:GLU:OE2	2.52	0.43
1:A:570:VAL:HB	1:A:612:SER:H	1.83	0.43
1:D:404:LYS:HE3	1:D:404:LYS:HB3	1.87	0.43
1:D:1099:ILE:HD11	1:D:1134:CYS:O	2.19	0.43
1:D:1607:HIS:HE2	1:D:1619:HIS:HB2	1.82	0.43
1:A:659:GLU:HG2	1:A:711:HIS:CD2	2.53	0.43
1:A:687:GLU:HA	1:A:754:PHE:HZ	1.84	0.43
1:A:857:LEU:HD13	1:A:905:LEU:HD11	2.01	0.43
1:A:1054:LEU:HD21	1:A:1112:VAL:CG2	2.49	0.43
1:A:1291:TYR:HA	1:A:1295:GLU:OE2	2.18	0.43
2:B:114:GLY:H	2:B:156:GLU:HA	1.82	0.43
1:D:9:ARG:HA	1:D:9:ARG:HD3	1.82	0.43
1:D:124:LEU:HA	1:D:127:TRP:CE3	2.53	0.43
1:D:260:ILE:HD13	1:D:309:LYS:HD3	2.01	0.43
1:D:832:ASP:OD1	1:D:833:PRO:HD3	2.19	0.43
1:A:23:GLN:OE1	1:A:58:ILE:HB	2.18	0.42
1:A:142:ALA:O	1:A:146:LYS:HG3	2.18	0.42
1:A:796:LEU:HD23	1:A:799:ASN:HD22	1.83	0.42
1:A:909:ILE:HG13	1:A:910:LEU:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1016:VAL:HG23	1:A:1017:PHE:HD1	1.83	0.42
2:B:82:PHE:CE1	2:B:154:TYR:HE1	2.36	0.42
1:D:69:ALA:HB2	1:D:78:GLU:HG2	2.00	0.42
1:D:1363:PHE:O	1:D:1382:ILE:HG23	2.19	0.42
1:D:1516:GLU:O	1:D:1520:GLU:OE1	2.37	0.42
1:D:1549:MET:CE	2:E:39:ASN:HB3	2.49	0.42
1:D:1594:ALA:O	1:D:1597:MET:HB2	2.19	0.42
2:E:171:GLU:HA	2:E:174:ARG:CG	2.49	0.42
1:A:832:ASP:OD1	1:A:833:PRO:HD3	2.19	0.42
1:A:906:LEU:HA	1:A:909:ILE:HG12	2.00	0.42
1:A:1469:ARG:HD3	1:A:1469:ARG:HA	1.91	0.42
1:A:1554:ILE:HA	2:B:37:PHE:CE1	2.54	0.42
1:D:79:THR:HA	1:D:85:LEU:HD22	2.01	0.42
1:D:285:SER:O	1:D:420:LEU:HB3	2.19	0.42
1:A:260:ILE:HD13	1:A:309:LYS:HD3	2.01	0.42
1:A:262:TRP:CH2	1:A:358:ARG:HB3	2.55	0.42
1:A:875:ARG:NH1	1:A:920:ALA:O	2.46	0.42
1:A:1363:PHE:O	1:A:1382:ILE:HG23	2.19	0.42
1:A:1387:GLU:HG2	1:A:1388:TYR:N	2.34	0.42
1:D:106:TYR:O	3:F:551:GLN:HG3	2.19	0.42
1:D:313:LYS:NZ	1:D:354:GLU:OE2	2.52	0.42
1:D:697:LEU:HA	1:D:700:ILE:HD12	2.01	0.42
1:D:909:ILE:HG13	1:D:910:LEU:N	2.34	0.42
1:D:1291:TYR:HA	1:D:1295:GLU:OE2	2.18	0.42
1:D:1579:HIS:HD2	1:D:1582:ASP:HB2	1.83	0.42
2:E:70:LEU:C	2:E:73:PRO:HD2	2.44	0.42
3:F:622:CYS:HB3	3:F:624:HIS:CE1	2.53	0.42
2:B:145:MET:O	2:B:149:ILE:HG23	2.18	0.42
2:B:171:GLU:HA	2:B:174:ARG:CG	2.49	0.42
3:C:677:MET:CB	3:C:682:THR:HG21	2.49	0.42
1:D:1:MET:N	1:D:1:MET:SD	2.90	0.42
1:D:113:LEU:O	1:D:117:LEU:HB2	2.19	0.42
1:D:142:ALA:O	1:D:146:LYS:HG3	2.18	0.42
1:D:869:PHE:CD2	1:D:870:ARG:HG2	2.55	0.42
1:A:832:ASP:N	1:A:833:PRO:HD2	2.34	0.42
1:A:879:LEU:HD12	1:A:882:LEU:HB2	2.00	0.42
1:A:1594:ALA:O	1:A:1597:MET:HB2	2.19	0.42
1:A:1596:GLN:HG2	1:A:1600:LEU:HG	2.01	0.42
2:B:70:LEU:C	2:B:73:PRO:HD2	2.45	0.42
3:C:579:LEU:HD12	3:C:580:SER:H	1.84	0.42
1:D:87:LEU:CD1	1:D:145:LYS:HG3	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:493:ILE:HD12	1:D:493:ILE:H	1.85	0.42
1:D:842:LYS:O	1:D:845:GLN:HG2	2.20	0.42
3:F:579:LEU:HD12	3:F:580:SER:H	1.84	0.42
1:A:9:ARG:HA	1:A:9:ARG:HD3	1.82	0.42
1:A:73:ASP:C	1:A:79:THR:HG23	2.45	0.42
1:A:113:LEU:O	1:A:117:LEU:HB2	2.19	0.42
1:A:262:TRP:CZ2	1:A:358:ARG:HB3	2.54	0.42
1:A:564:ASP:HA	1:A:624:THR:H	1.83	0.42
1:A:1259:GLU:N	1:A:1259:GLU:OE1	2.49	0.42
1:A:1574:LYS:HD2	1:A:1574:LYS:HA	1.82	0.42
2:B:68:ARG:N	2:B:69:PRO:HD3	2.34	0.42
1:D:238:ASP:HB2	1:D:295:SER:HA	2.02	0.42
1:D:906:LEU:HA	1:D:909:ILE:HG12	2.00	0.42
1:D:1016:VAL:HG23	1:D:1017:PHE:HD1	1.83	0.42
2:E:145:MET:O	2:E:149:ILE:HG23	2.18	0.42
3:F:677:MET:CB	3:F:682:THR:HG21	2.49	0.42
1:A:894:SER:O	1:A:897:PRO:HD2	2.20	0.42
2:B:55:LEU:HD21	2:B:169:PHE:HE1	1.83	0.42
1:D:1451:LEU:O	1:D:1455:ARG:HG3	2.19	0.42
1:A:166:ARG:O	1:A:171:ASN:ND2	2.53	0.42
1:A:493:ILE:HD12	1:A:493:ILE:H	1.85	0.42
1:A:694:PHE:HB2	1:A:757:LEU:HD13	2.02	0.42
1:D:896:LYS:HG3	1:D:897:PRO:HD3	2.02	0.42
1:D:1007:MET:HE3	1:D:1007:MET:HB3	1.69	0.42
1:A:414:GLN:HG3	1:A:416:ASN:N	2.35	0.42
1:A:787:PHE:O	1:A:791:ILE:HG12	2.20	0.42
1:A:842:LYS:O	1:A:845:GLN:HG2	2.20	0.42
1:A:869:PHE:CD2	1:A:870:ARG:HG2	2.55	0.42
1:A:997:ILE:HD12	1:A:997:ILE:HA	1.94	0.42
1:A:1261:ALA:HB2	1:A:1307:TYR:HB3	2.02	0.42
1:D:262:TRP:CH2	1:D:358:ARG:HB3	2.55	0.42
1:D:687:GLU:HA	1:D:754:PHE:HZ	1.84	0.42
1:D:857:LEU:HD13	1:D:905:LEU:HD11	2.01	0.42
1:D:1256:ASN:O	1:D:1259:GLU:N	2.52	0.42
1:D:1596:GLN:HG2	1:D:1600:LEU:HG	2.01	0.42
1:D:1607:HIS:NE2	1:D:1619:HIS:HB2	2.34	0.42
2:E:98:TYR:CE1	2:E:149:ILE:HG22	2.55	0.42
1:A:721:TYR:HB3	1:A:723:HIS:CD2	2.54	0.42
1:A:885:GLN:O	1:A:889:GLN:HG2	2.20	0.42
1:A:1451:LEU:O	1:A:1455:ARG:HG3	2.19	0.42
1:A:1614:GLN:NE2	2:B:74:GLN:OE1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:663:CYS:HA	3:C:666:THR:HG22	2.02	0.42
1:D:832:ASP:N	1:D:833:PRO:HD2	2.34	0.42
1:D:938:ARG:HG3	1:D:941:ILE:HD12	2.01	0.42
1:D:1054:LEU:HD21	1:D:1112:VAL:CG2	2.49	0.42
1:D:1261:ALA:HB2	1:D:1307:TYR:HB3	2.02	0.42
2:E:55:LEU:HD21	2:E:169:PHE:HE1	1.84	0.42
1:A:248:PRO:HB3	1:A:283:ASP:OD1	2.20	0.41
1:A:372:VAL:HG13	1:A:373:ILE:HG13	2.02	0.41
1:A:910:LEU:HD11	1:A:960:LEU:HB2	2.02	0.41
1:A:965:ASP:H	1:A:968:HIS:HB2	1.85	0.41
1:A:1113:THR:HG22	1:A:1168:TYR:HE2	1.86	0.41
2:B:84:LEU:HD22	2:B:137:ILE:O	2.20	0.41
1:D:683:MET:HA	1:D:737:LEU:HD21	2.02	0.41
1:D:694:PHE:HB2	1:D:757:LEU:HD13	2.02	0.41
1:A:707:ILE:O	1:A:710:GLN:HB3	2.20	0.41
1:A:1235:LYS:HE2	1:A:1235:LYS:HB2	1.83	0.41
1:A:1448:GLU:O	1:A:1449:GLN:C	2.63	0.41
1:A:1516:GLU:O	1:A:1520:GLU:OE1	2.37	0.41
2:B:137:ILE:HD12	2:B:137:ILE:H	1.85	0.41
1:D:721:TYR:HB3	1:D:723:HIS:CD2	2.54	0.41
1:D:910:LEU:HD11	1:D:960:LEU:HB2	2.02	0.41
1:D:929:MET:HE1	1:D:968:HIS:C	2.46	0.41
1:D:1086:ARG:HA	1:D:1089:ASP:OD2	2.21	0.41
1:D:1387:GLU:HG2	1:D:1388:TYR:N	2.34	0.41
1:A:17:TYR:CA	3:C:536:LEU:HD21	2.47	0.41
1:A:741:VAL:O	1:A:741:VAL:HG12	2.20	0.41
1:A:959:ALA:O	1:A:963:GLN:HG3	2.20	0.41
1:A:1557:PRO:HG3	1:A:1563:PHE:HE2	1.84	0.41
1:D:73:ASP:C	1:D:79:THR:HG23	2.45	0.41
1:D:741:VAL:O	1:D:741:VAL:HG12	2.20	0.41
1:D:1469:ARG:HD3	1:D:1469:ARG:HA	1.91	0.41
1:D:1574:LYS:HA	1:D:1574:LYS:HD2	1.82	0.41
2:E:6:CYS:HA	2:E:77:VAL:O	2.20	0.41
2:E:9:VAL:HB	2:E:97:TRP:CE3	2.56	0.41
1:A:32:GLY:C	3:C:697:ARG:HH21	2.29	0.41
1:A:691:PHE:HD1	1:A:692:LEU:HD23	1.84	0.41
1:A:697:LEU:HA	1:A:700:ILE:HD12	2.01	0.41
1:A:839:LEU:HB3	1:A:878:LEU:HD21	2.02	0.41
1:A:896:LYS:HG3	1:A:897:PRO:HD3	2.02	0.41
1:A:1129:PHE:HA	1:A:1132:MET:HG3	2.01	0.41
1:A:1165:ASP:O	1:A:1168:TYR:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1197:VAL:O	1:A:1201:LEU:HD23	2.20	0.41
2:B:98:TYR:O	2:B:102:ARG:HB3	2.21	0.41
1:D:787:PHE:O	1:D:791:ILE:HG12	2.20	0.41
1:D:885:GLN:O	1:D:889:GLN:HG2	2.20	0.41
1:D:1047:PHE:HD2	1:D:1101:PHE:HE2	1.68	0.41
1:D:1338:LEU:O	1:D:1342:LEU:HD23	2.21	0.41
2:E:87:PRO:HD2	2:E:134:LEU:HD13	2.02	0.41
1:A:70:THR:HG22	1:A:71:VAL:N	2.36	0.41
1:A:98:TRP:HA	1:A:101:ILE:HG22	2.02	0.41
1:A:1044:ASN:HA	1:A:1101:PHE:CZ	2.56	0.41
1:A:1554:ILE:HA	2:B:37:PHE:CD1	2.54	0.41
1:D:2:ALA:H	3:F:717:PRO:HG2	1.85	0.41
1:D:184:PHE:HD1	1:D:1009:MET:HE1	1.85	0.41
1:D:248:PRO:HB3	1:D:283:ASP:OD1	2.20	0.41
1:D:691:PHE:HD1	1:D:692:LEU:HD23	1.84	0.41
1:D:795:PHE:O	1:D:798:PHE:HB2	2.20	0.41
1:D:894:SER:O	1:D:897:PRO:HD2	2.20	0.41
1:D:965:ASP:H	1:D:968:HIS:HB2	1.86	0.41
1:D:1392:GLU:OE1	1:D:1392:GLU:N	2.54	0.41
1:A:38:LEU:HB3	3:C:724:TYR:HE2	1.86	0.41
1:A:87:LEU:CD1	1:A:145:LYS:HG3	2.48	0.41
1:A:438:LEU:O	1:A:630:LYS:NZ	2.50	0.41
1:A:929:MET:HE1	1:A:968:HIS:C	2.45	0.41
1:A:1086:ARG:HA	1:A:1089:ASP:OD2	2.21	0.41
1:A:1466:ARG:NH1	2:B:31:GLU:OE2	2.53	0.41
1:A:1607:HIS:NE2	1:A:1619:HIS:HB2	2.34	0.41
1:D:17:TYR:HB2	3:F:536:LEU:HD11	2.02	0.41
1:D:1250:LEU:HD23	1:D:1250:LEU:HA	1.94	0.41
1:D:1353:ILE:HD13	1:D:1353:ILE:HA	1.91	0.41
1:D:1399:LEU:HD12	3:F:607:LYS:HD3	2.00	0.41
1:D:1557:PRO:HG3	1:D:1563:PHE:HE2	1.85	0.41
2:E:126:ILE:O	2:E:130:LYS:HG2	2.21	0.41
3:F:590:ASP:HB2	3:F:604:LEU:HD12	2.02	0.41
1:A:14:VAL:HG13	3:C:700:ASP:HB3	2.03	0.41
1:A:255:SER:C	1:A:256:GLU:HG2	2.46	0.41
1:A:948:PRO:C	1:A:950:ILE:H	2.29	0.41
1:A:994:LYS:CA	1:A:1049:LEU:HD13	2.51	0.41
3:C:575:TRP:HA	3:C:591:LEU:HB2	2.03	0.41
1:D:707:ILE:O	1:D:710:GLN:HB3	2.20	0.41
1:D:948:PRO:C	1:D:950:ILE:H	2.29	0.41
1:D:1129:PHE:HA	1:D:1132:MET:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1612:THR:H	1:D:1615:LEU:HB2	1.86	0.41
2:E:108:THR:HG22	2:E:109:PRO:O	2.20	0.41
2:B:7:VAL:HG12	2:B:9:VAL:HG13	2.03	0.41
2:B:126:ILE:O	2:B:130:LYS:HG2	2.21	0.41
1:D:237:GLU:HB2	1:D:497:LYS:HB3	2.03	0.41
1:D:749:LYS:HA	1:D:753:LEU:HD23	2.03	0.41
1:D:947:SER:N	1:D:948:PRO:HD2	2.36	0.41
2:E:7:VAL:HG12	2:E:9:VAL:HG13	2.03	0.41
1:A:124:LEU:HA	1:A:127:TRP:HE3	1.85	0.41
1:A:230:ASN:HA	1:A:342:LYS:O	2.21	0.41
1:A:238:ASP:HB2	1:A:295:SER:HA	2.02	0.41
1:A:277:LEU:HD12	1:A:373:ILE:HG12	2.02	0.41
1:A:795:PHE:O	1:A:798:PHE:HB2	2.20	0.41
1:A:914:ASP:HB2	1:A:963:GLN:NE2	2.36	0.41
1:A:1047:PHE:HD2	1:A:1101:PHE:HE2	1.68	0.41
1:A:1517:ASN:O	1:A:1521:THR:HG23	2.21	0.41
1:A:1545:HIS:CE1	1:A:1549:MET:HG2	2.56	0.41
1:A:1615:LEU:HD23	1:A:1615:LEU:HA	1.93	0.41
2:B:98:TYR:CE1	2:B:149:ILE:HG22	2.55	0.41
2:B:108:THR:HG22	2:B:109:PRO:O	2.21	0.41
1:D:62:THR:OG1	3:F:711:PRO:HB3	2.21	0.41
1:D:166:ARG:O	1:D:171:ASN:ND2	2.53	0.41
1:D:758:LYS:HG3	1:D:759:ALA:N	2.36	0.41
1:D:851:GLN:O	1:D:851:GLN:HG3	2.20	0.41
1:D:1113:THR:HG22	1:D:1168:TYR:HE2	1.86	0.41
1:D:1197:VAL:O	1:D:1201:LEU:HD23	2.20	0.41
1:D:1235:LYS:HE2	1:D:1235:LYS:HB2	1.83	0.41
1:D:1399:LEU:HD11	1:D:1407:LYS:NZ	2.36	0.41
1:D:1401:GLN:O	1:D:1401:GLN:HG3	2.21	0.41
3:F:575:TRP:HA	3:F:591:LEU:HB2	2.03	0.41
3:F:663:CYS:HA	3:F:666:THR:HG22	2.02	0.41
1:A:88:VAL:O	1:A:92:THR:HG23	2.21	0.41
1:A:233:CYS:SG	1:A:299:GLN:NE2	2.83	0.41
1:A:683:MET:HA	1:A:737:LEU:HD21	2.02	0.41
1:A:766:PHE:CE2	1:A:828:LYS:HA	2.55	0.41
1:A:1079:MET:HB3	1:A:1079:MET:HE2	1.59	0.41
1:A:1322:LYS:HA	1:A:1345:ARG:NH2	2.36	0.41
1:A:1452:ASN:OD1	1:A:1452:ASN:C	2.64	0.41
1:A:1595:LEU:C	1:A:1598:PRO:HD2	2.46	0.41
1:A:1612:THR:H	1:A:1615:LEU:HB2	1.86	0.41
3:C:590:ASP:HB2	3:C:604:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:TRP:O	3:F:723:VAL:HB	2.20	0.41
1:D:163:LEU:HD21	1:D:194:ILE:HD12	2.04	0.41
1:D:450:LEU:HB2	1:D:510:TYR:CD1	2.56	0.41
1:D:938:ARG:HA	1:D:941:ILE:HD12	2.03	0.41
1:D:1305:ILE:CD1	1:D:1320:LEU:HB2	2.47	0.41
3:F:622:CYS:HB3	3:F:624:HIS:ND1	2.36	0.41
1:A:1399:LEU:HD11	1:A:1407:LYS:NZ	2.36	0.40
2:B:6:CYS:HA	2:B:77:VAL:O	2.20	0.40
2:B:9:VAL:HB	2:B:97:TRP:CE3	2.56	0.40
2:B:87:PRO:HD2	2:B:134:LEU:HD13	2.02	0.40
3:C:588:TYR:CE1	3:C:608:LEU:HB2	2.56	0.40
1:D:124:LEU:HA	1:D:127:TRP:HE3	1.85	0.40
1:D:372:VAL:HG13	1:D:373:ILE:HG13	2.02	0.40
1:D:404:LYS:C	1:D:407:PRO:HD2	2.46	0.40
1:D:766:PHE:CE2	1:D:828:LYS:HA	2.55	0.40
1:D:852:LEU:HD23	1:D:889:GLN:HE22	1.87	0.40
1:D:959:ALA:O	1:D:963:GLN:HG3	2.20	0.40
1:D:994:LYS:CA	1:D:1049:LEU:HD13	2.51	0.40
1:D:1065:SER:OG	1:D:1068:LYS:N	2.55	0.40
1:D:1095:GLY:HA3	1:D:1096:PRO:HD3	1.95	0.40
1:D:1404:ASN:HD21	1:D:1424:GLN:CD	2.30	0.40
2:E:98:TYR:O	2:E:102:ARG:HB3	2.21	0.40
2:E:137:ILE:HD12	2:E:137:ILE:H	1.85	0.40
3:F:588:TYR:CE1	3:F:608:LEU:HB2	2.56	0.40
3:F:616:VAL:HG13	3:F:643:SER:C	2.47	0.40
1:A:18:ASN:CG	3:C:536:LEU:HG	2.46	0.40
1:A:30:GLN:N	1:A:33:ASP:OD2	2.55	0.40
1:A:404:LYS:C	1:A:407:PRO:HD2	2.46	0.40
1:A:1135:GLU:OE1	1:A:1144:PHE:HA	2.21	0.40
1:A:1338:LEU:O	1:A:1342:LEU:HD23	2.21	0.40
1:A:1401:GLN:O	1:A:1401:GLN:HG3	2.21	0.40
2:B:81:CYS:HA	2:B:113:VAL:HG22	2.04	0.40
3:C:610:VAL:HG12	3:C:613:ILE:HG13	2.04	0.40
3:C:708:ASP:OD1	3:C:709:ALA:N	2.54	0.40
1:D:255:SER:C	1:D:256:GLU:HG2	2.46	0.40
1:D:1165:ASP:O	1:D:1168:TYR:HB3	2.21	0.40
1:A:758:LYS:HG3	1:A:759:ALA:N	2.36	0.40
1:A:853:VAL:C	1:A:854:ARG:HG3	2.47	0.40
1:D:914:ASP:HB2	1:D:963:GLN:NE2	2.36	0.40
1:D:1127:ILE:H	1:D:1127:ILE:HG13	1.71	0.40
1:D:1322:LYS:HA	1:D:1345:ARG:NH2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1448:GLU:O	1:D:1449:GLN:C	2.63	0.40
3:F:708:ASP:OD1	3:F:709:ALA:N	2.54	0.40
1:A:184:PHE:HD1	1:A:1009:MET:HE1	1.85	0.40
1:A:450:LEU:HB2	1:A:510:TYR:CD1	2.56	0.40
1:A:506:GLN:N	1:A:507:PRO:HD2	2.37	0.40
1:A:519:ILE:HA	1:A:522:VAL:HG12	2.04	0.40
1:A:766:PHE:O	1:A:770:SER:HB3	2.22	0.40
1:A:843:PHE:CE2	1:A:878:LEU:HA	2.57	0.40
1:A:1175:LEU:HD12	1:A:1179:HIS:CE1	2.57	0.40
1:A:1467:PRO:HG3	2:B:33:ILE:CG1	2.49	0.40
1:A:1474:ASP:HB2	1:A:1475:PRO:HD2	2.04	0.40
1:D:30:GLN:N	1:D:33:ASP:OD2	2.55	0.40
1:D:101:ILE:HD13	1:D:101:ILE:HG21	1.89	0.40
1:D:183:LEU:HD13	1:D:1012:THR:HG21	2.04	0.40
1:D:277:LEU:HD12	1:D:373:ILE:HG12	2.02	0.40
1:D:506:GLN:N	1:D:507:PRO:HD2	2.37	0.40
1:D:637:LEU:HD12	1:D:638:LEU:HD12	2.04	0.40
1:D:798:PHE:O	1:D:802:MET:HB2	2.21	0.40
1:D:1165:ASP:H	1:D:1168:TYR:HB3	1.86	0.40
2:E:36:VAL:HG23	2:E:37:PHE:CD2	2.57	0.40
3:F:541:GLN:O	3:F:544:ILE:HG22	2.20	0.40
1:A:163:LEU:HD21	1:A:194:ILE:HD12	2.04	0.40
1:A:264:SER:HB3	1:A:303:VAL:HB	2.03	0.40
1:A:658:MET:HE2	1:A:658:MET:HB2	2.01	0.40
1:A:767:ILE:HG13	1:A:768:ILE:HG13	2.02	0.40
1:A:938:ARG:O	1:A:941:ILE:HB	2.21	0.40
3:C:541:GLN:O	3:C:544:ILE:HG22	2.20	0.40
3:C:659:LYS:NZ	3:C:680:ASP:OD2	2.40	0.40
1:D:414:GLN:HG3	1:D:416:ASN:N	2.35	0.40
1:D:763:LEU:HG	1:D:827:VAL:HG21	2.04	0.40
1:D:845:GLN:HG3	1:D:846:SER:N	2.37	0.40
1:D:1175:LEU:HD12	1:D:1179:HIS:CE1	2.57	0.40
1:D:1452:ASN:OD1	1:D:1452:ASN:C	2.64	0.40
1:D:1474:ASP:HB2	1:D:1475:PRO:HD2	2.04	0.40
1:D:1536:HIS:HE1	1:D:1610:LYS:HG3	1.86	0.40
1:D:1545:HIS:CE1	1:D:1549:MET:HG2	2.56	0.40
2:E:1:MET:HE3	2:E:1:MET:HB3	1.95	0.40
2:E:23:TYR:HB2	2:E:165:LEU:HD21	2.04	0.40
3:F:573:LYS:HE2	3:F:573:LYS:HB3	1.95	0.40
3:F:689:LEU:HA	3:F:689:LEU:HD23	1.87	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	1640/1648 (100%)	1434 (87%)	206 (13%)	0	100	100
1	D	1640/1648 (100%)	1437 (88%)	203 (12%)	0	100	100
2	B	175/184 (95%)	158 (90%)	17 (10%)	0	100	100
2	E	175/184 (95%)	157 (90%)	18 (10%)	0	100	100
3	C	196/733 (27%)	170 (87%)	26 (13%)	0	100	100
3	F	196/733 (27%)	170 (87%)	26 (13%)	0	100	100
All	All	4022/5130 (78%)	3526 (88%)	496 (12%)	0	100	100

There are no Ramachandran outliers to report.

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	1495/1497 (100%)	1495 (100%)	0	100	100
1	D	1495/1497 (100%)	1495 (100%)	0	100	100
2	B	153/157 (98%)	153 (100%)	0	100	100
2	E	153/157 (98%)	153 (100%)	0	100	100
3	C	183/664 (28%)	183 (100%)	0	100	100
3	F	183/664 (28%)	183 (100%)	0	100	100
All	All	3662/4636 (79%)	3662 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	206	GLN
1	A	275	ASN
1	A	371	HIS
1	A	394	HIS
1	A	563	GLN
1	A	713	ASN
1	A	738	ASN
1	A	780	GLN
1	A	799	ASN
1	A	825	ASN
1	A	889	GLN
1	A	937	ASN
1	A	1093	ASN
1	A	1157	GLN
1	A	1281	HIS
1	A	1302	GLN
1	A	1370	GLN
1	A	1477	ASN
1	A	1517	ASN
1	A	1531	ASN
1	A	1583	GLN
1	A	1596	GLN
3	C	554	ASN
3	C	566	ASN
3	C	571	GLN
1	D	51	GLN
1	D	206	GLN
1	D	250	GLN
1	D	275	ASN
1	D	371	HIS
1	D	394	HIS
1	D	563	GLN
1	D	713	ASN
1	D	738	ASN
1	D	799	ASN
1	D	825	ASN
1	D	937	ASN
1	D	1093	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	1097	HIS
1	D	1157	GLN
1	D	1281	HIS
1	D	1302	GLN
1	D	1370	GLN
1	D	1404	ASN
1	D	1517	ASN
1	D	1531	ASN
1	D	1545	HIS
1	D	1583	GLN
1	D	1596	GLN
2	E	92	ASN
3	F	554	ASN
3	F	566	ASN
3	F	571	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

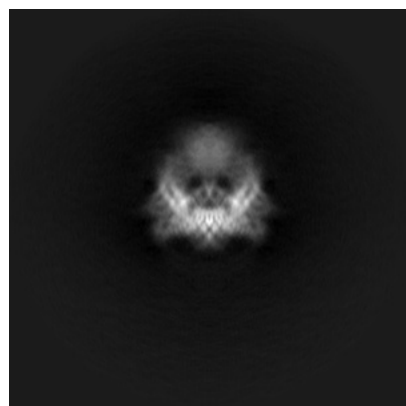
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30802. These allow visual inspection of the internal detail of the map and identification of artifacts.

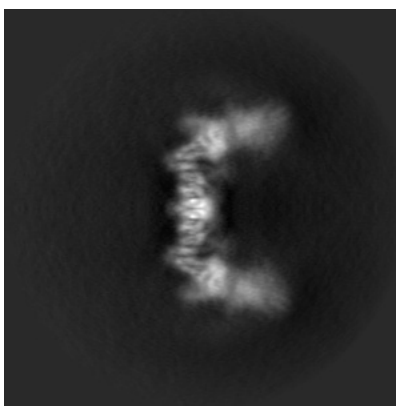
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

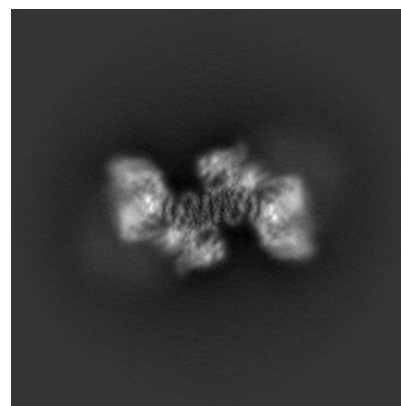
6.1.1 Primary map



X

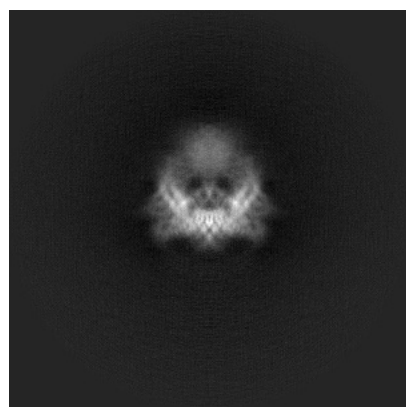


Y

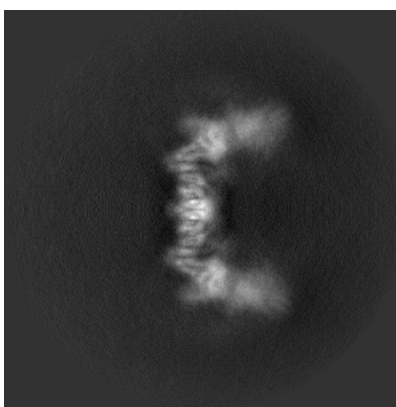


Z

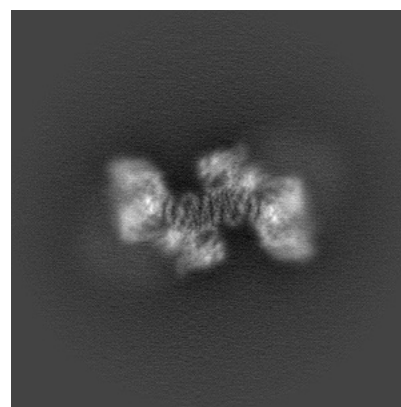
6.1.2 Raw map



X



Y

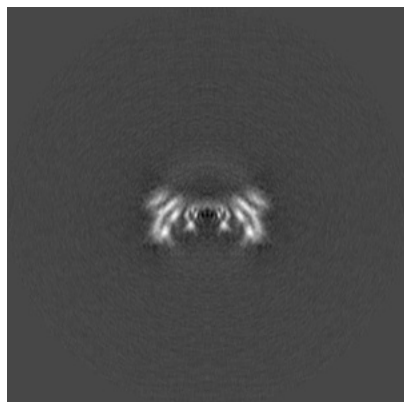


Z

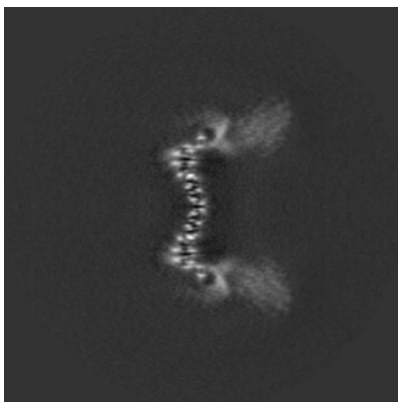
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

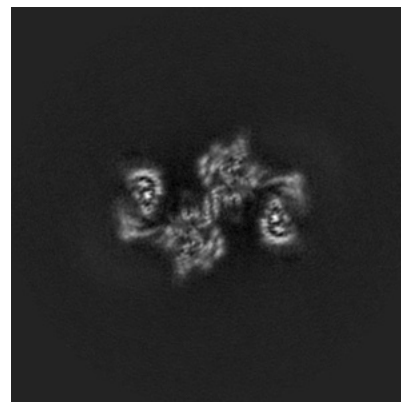
6.2.1 Primary map



X Index: 260

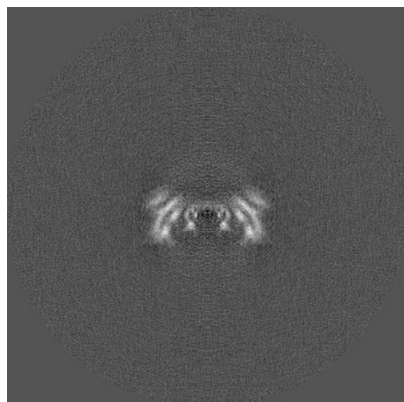


Y Index: 260

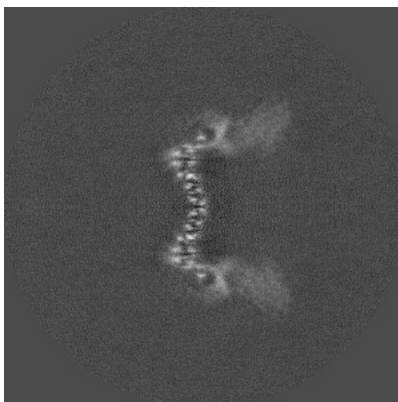


Z Index: 260

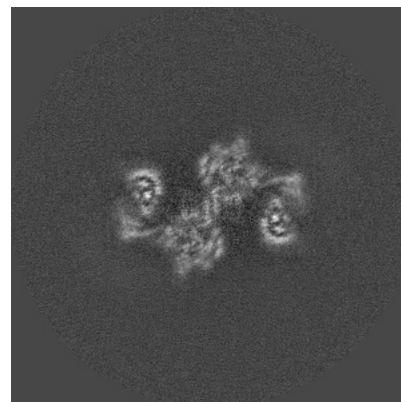
6.2.2 Raw map



X Index: 260



Y Index: 260

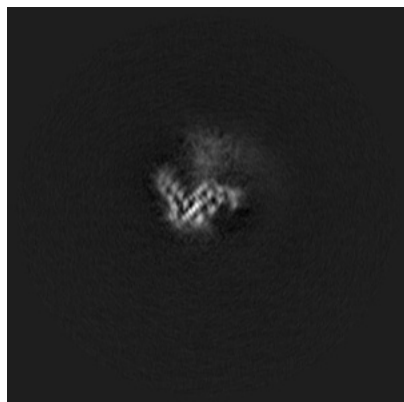


Z Index: 260

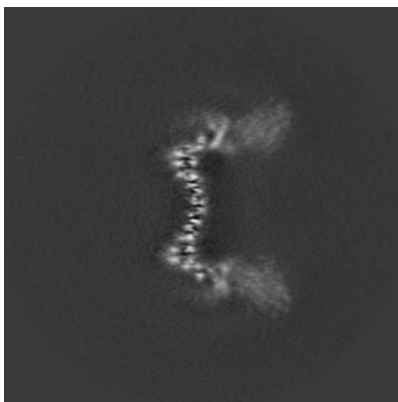
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

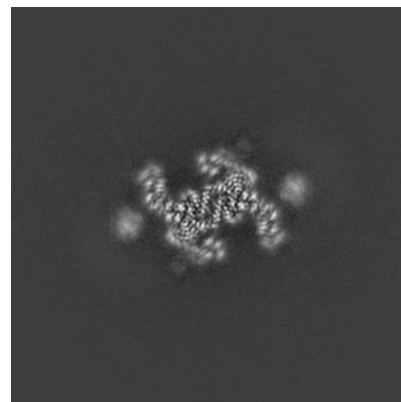
6.3.1 Primary map



X Index: 343

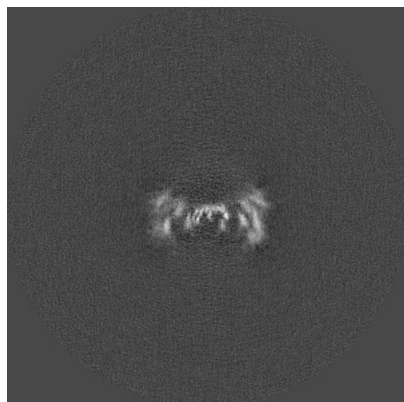


Y Index: 262

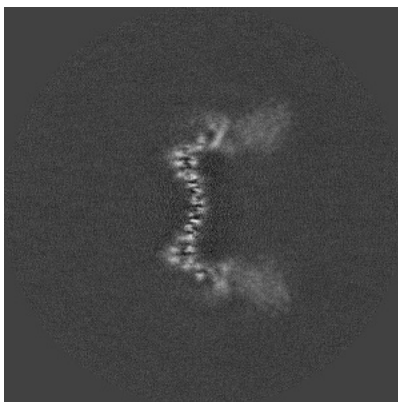


Z Index: 244

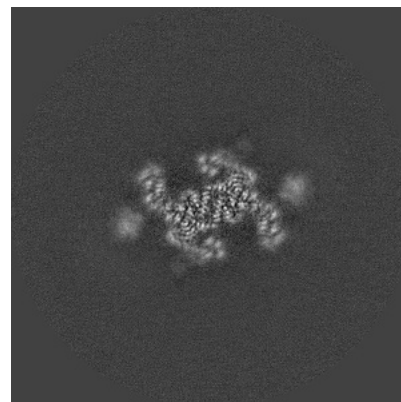
6.3.2 Raw map



X Index: 264



Y Index: 262



Z Index: 245

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

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

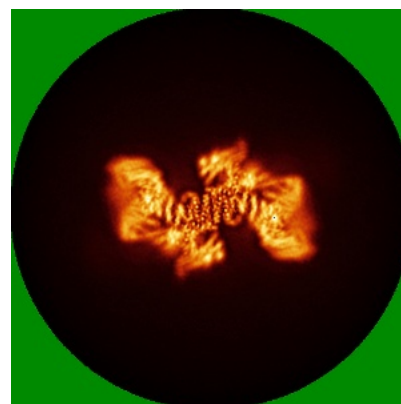
6.4.1 Primary map



X

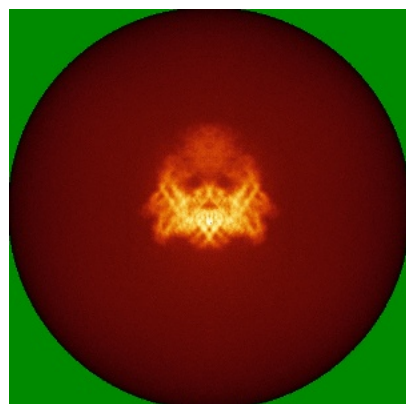


Y

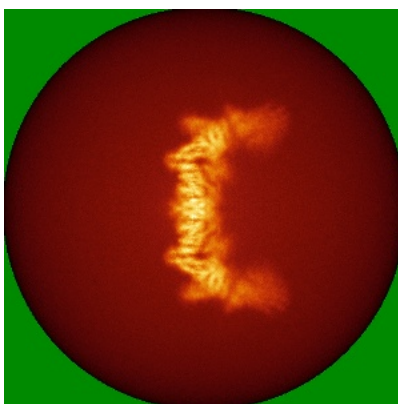


Z

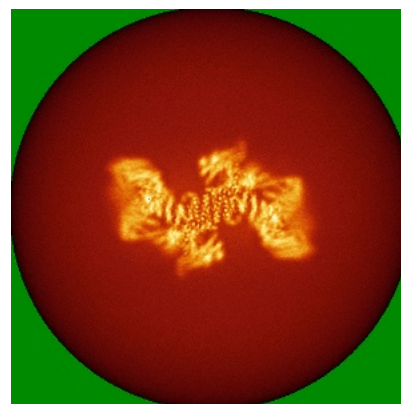
6.4.2 Raw map



X



Y

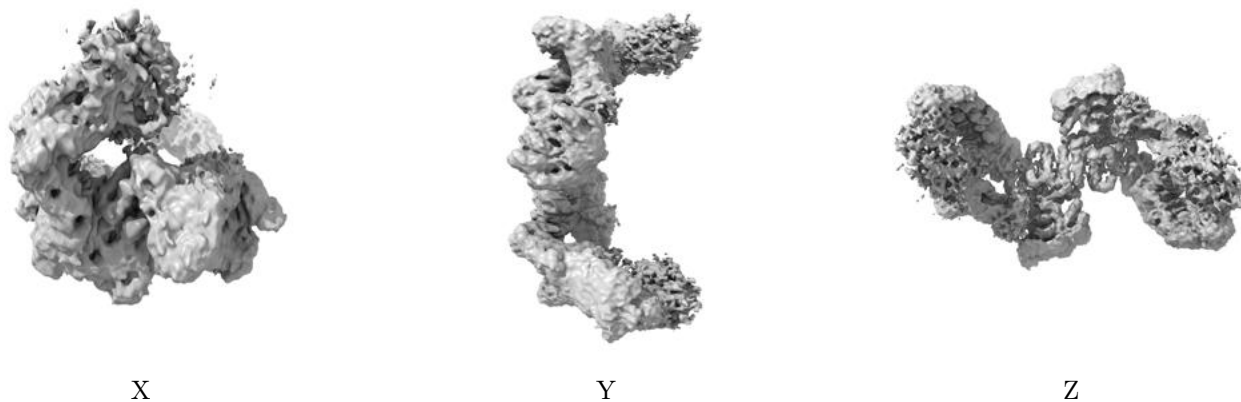


Z

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.

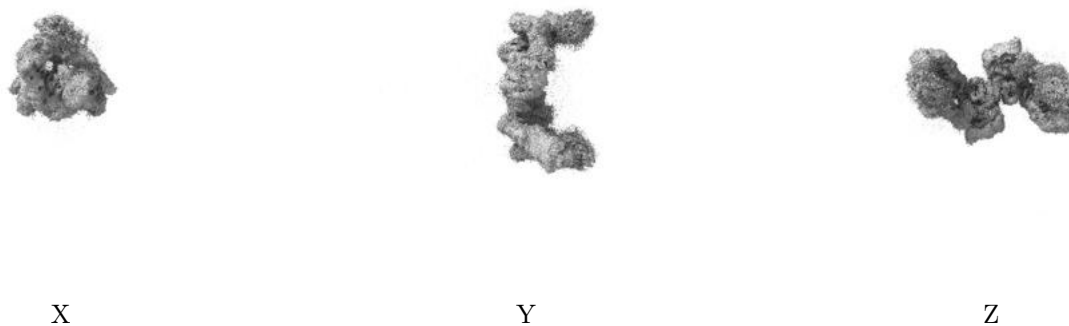
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.004. 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.

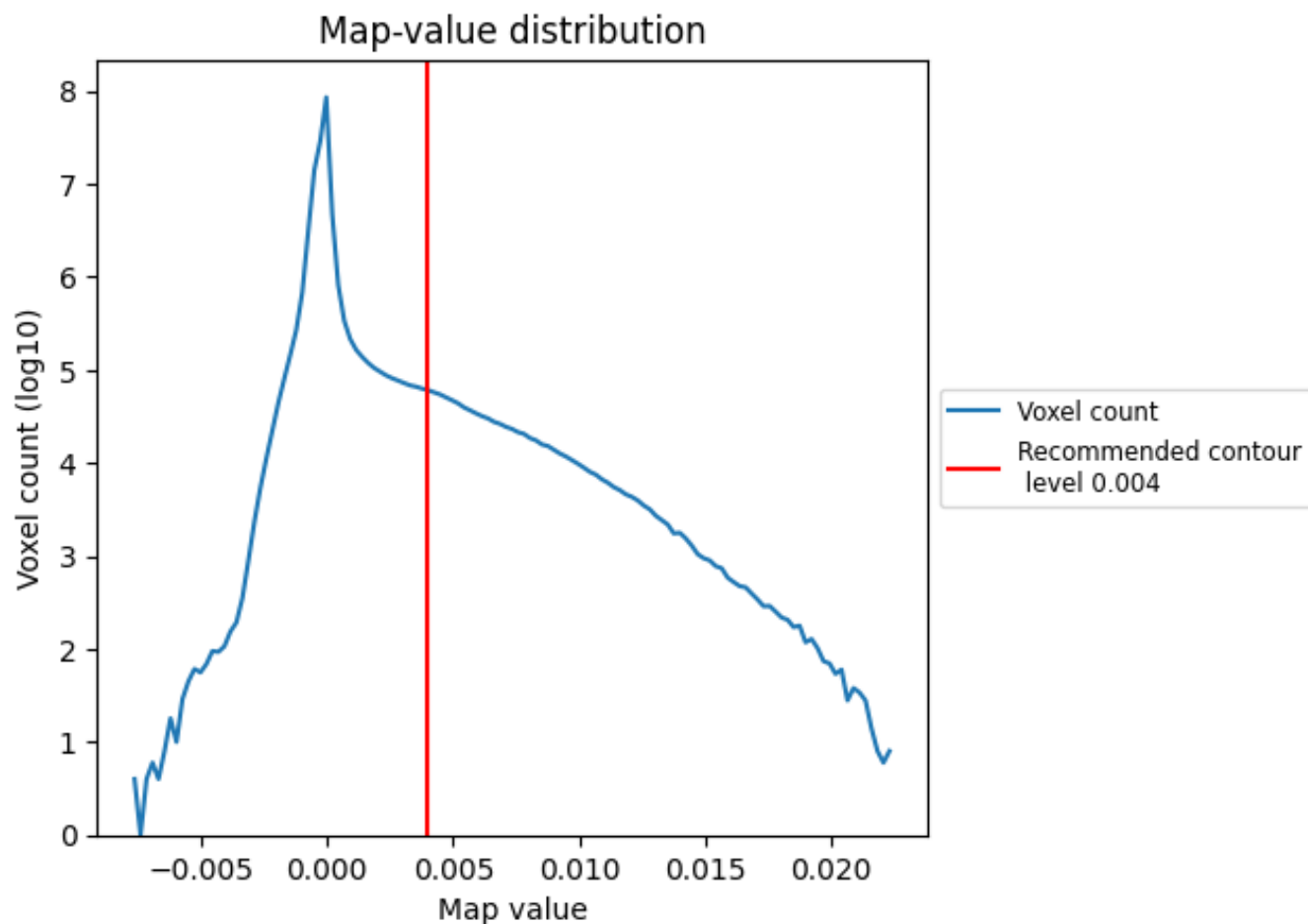
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

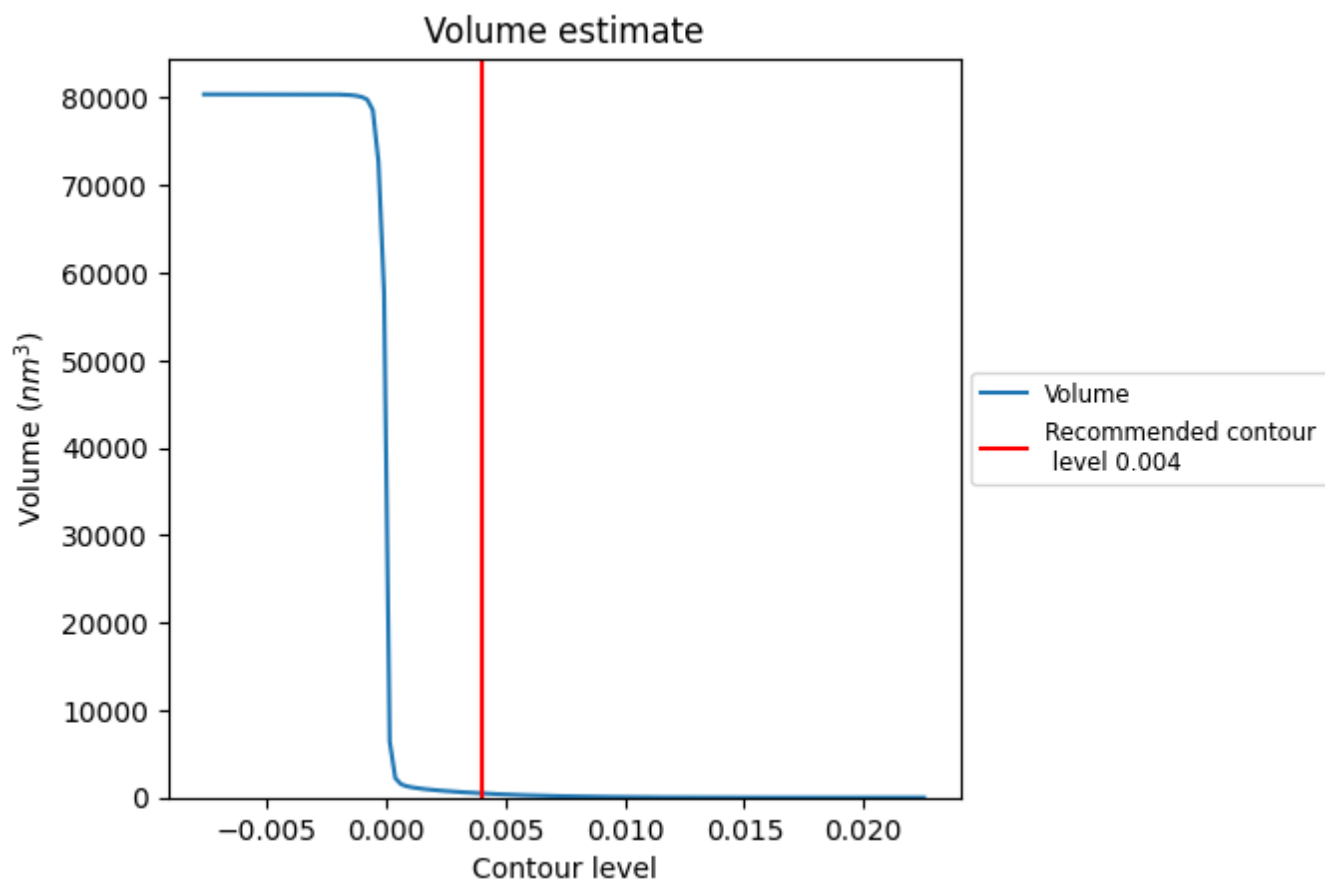
This section contains the results of statistical analysis of the map.

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.

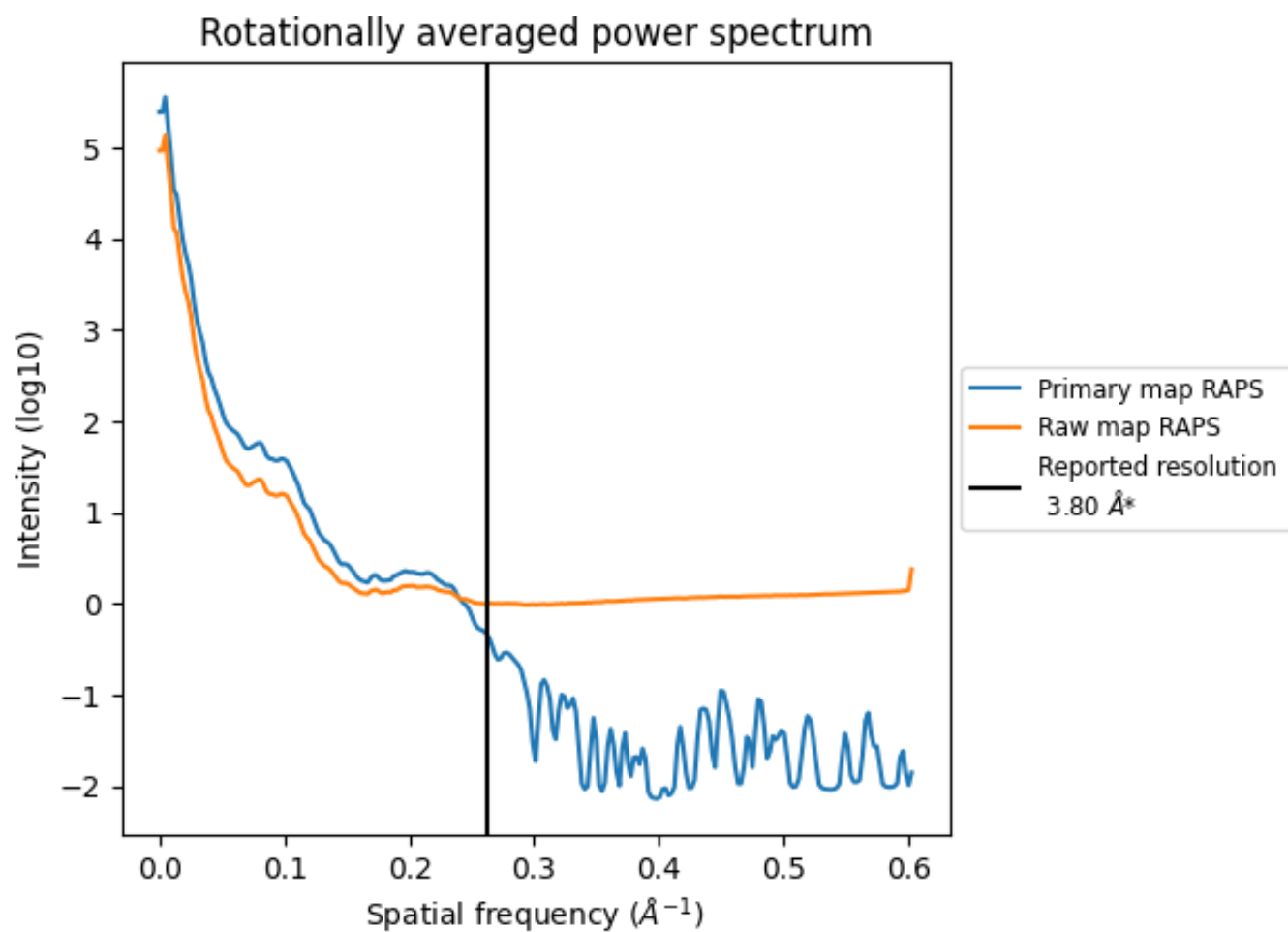
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 485 nm^3 ; this corresponds to an approximate mass of 439 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 ⓘ

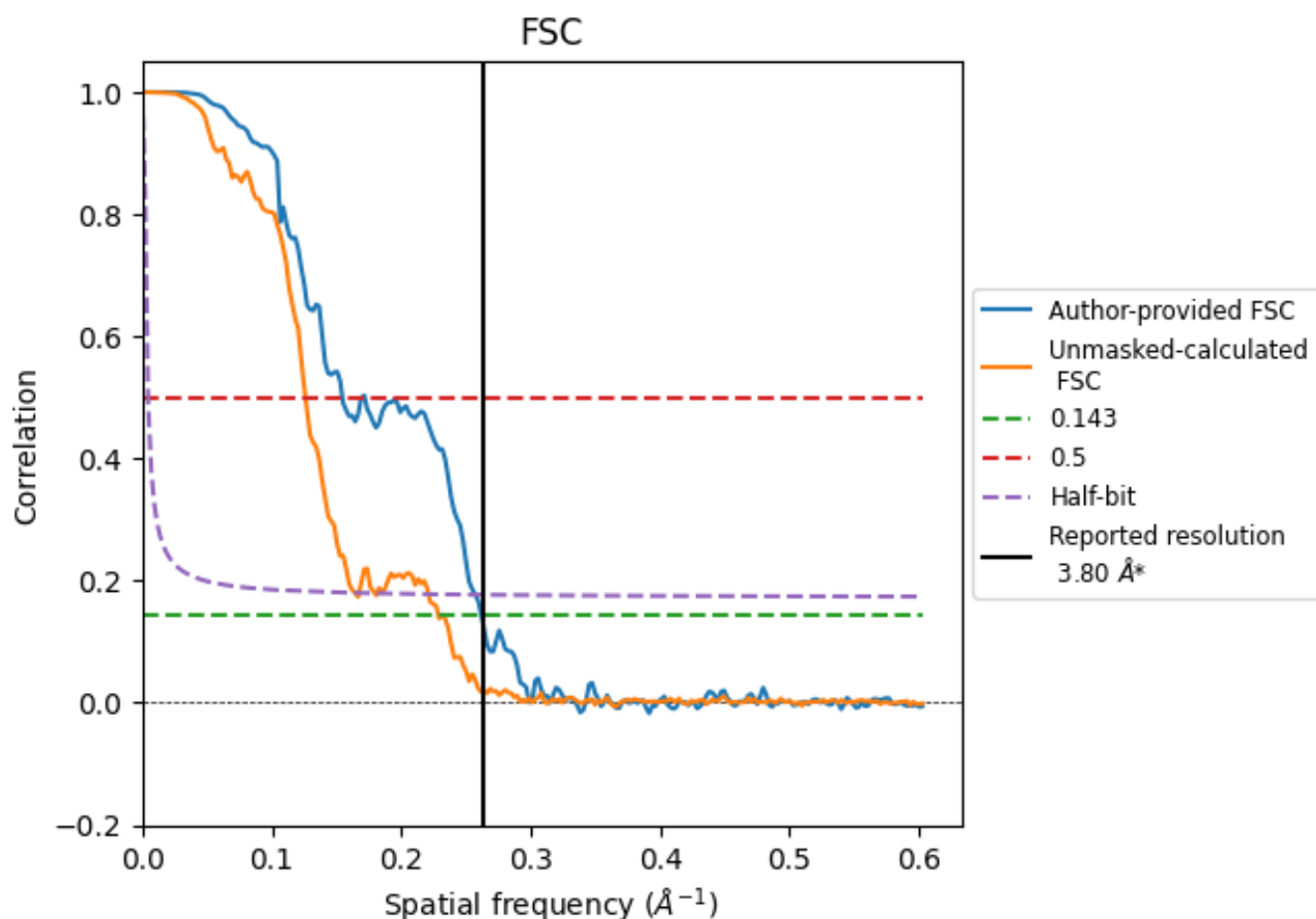


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 0.263 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

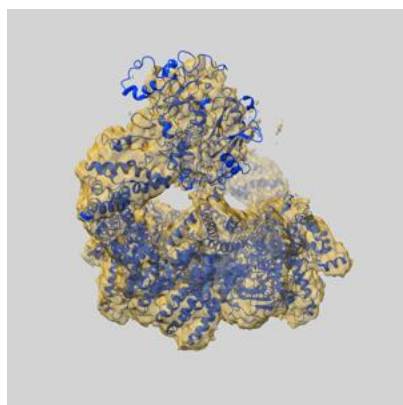
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.82	6.47	3.89
Unmasked-calculated*	4.37	7.93	6.08

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.37 differs from the reported value 3.8 by more than 10 %

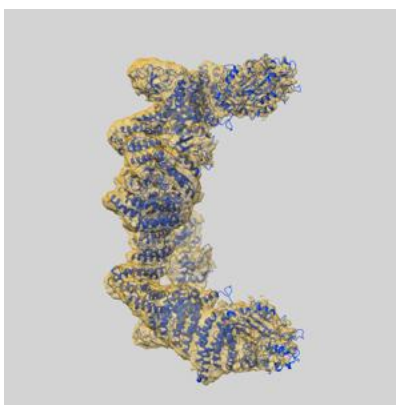
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30802 and PDB model 7DPA. Per-residue inclusion information can be found in section [3](#) on page [6](#).

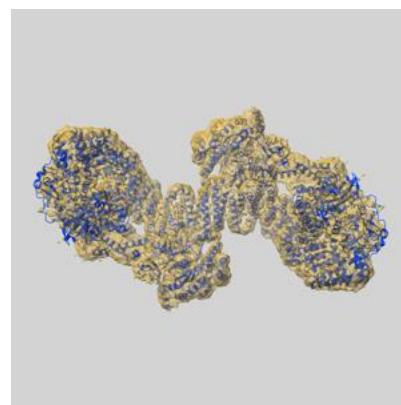
9.1 Map-model overlay [i](#)



X



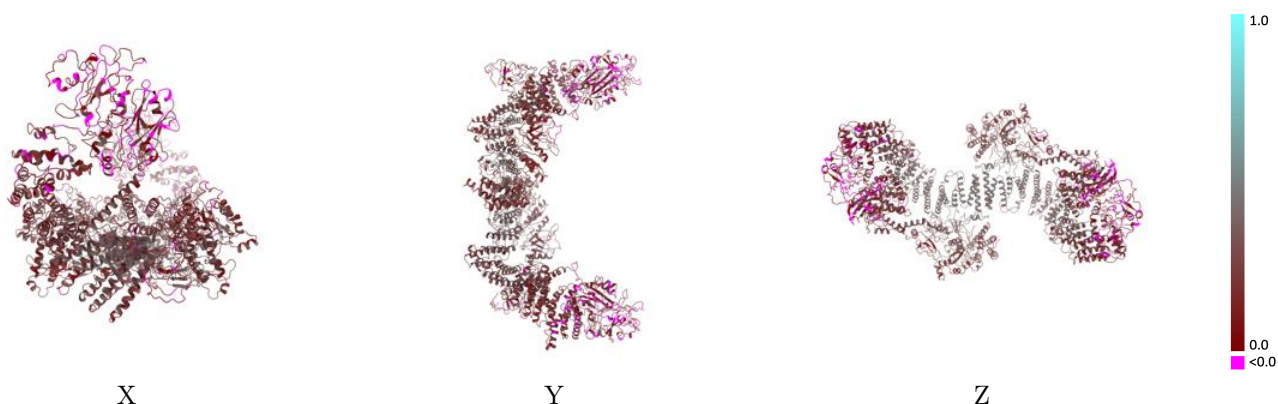
Y



Z

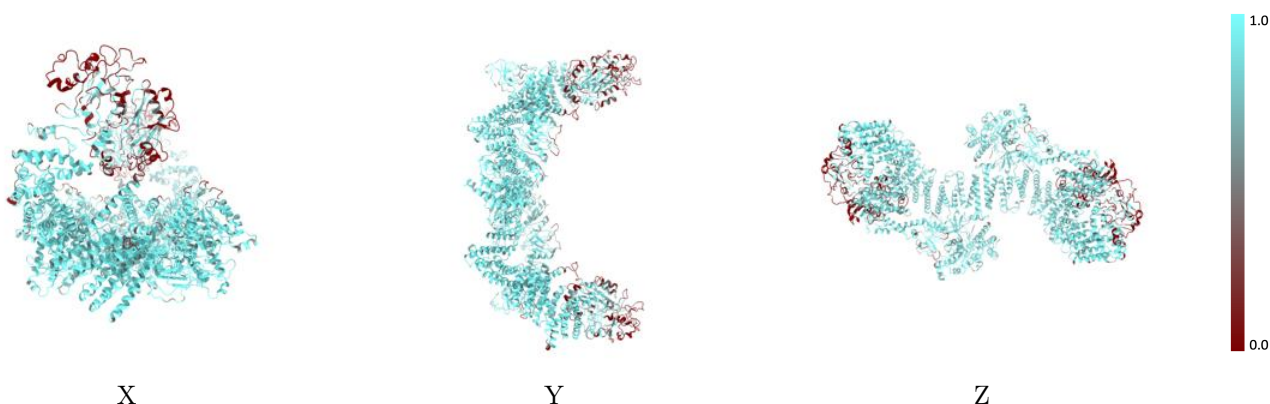
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



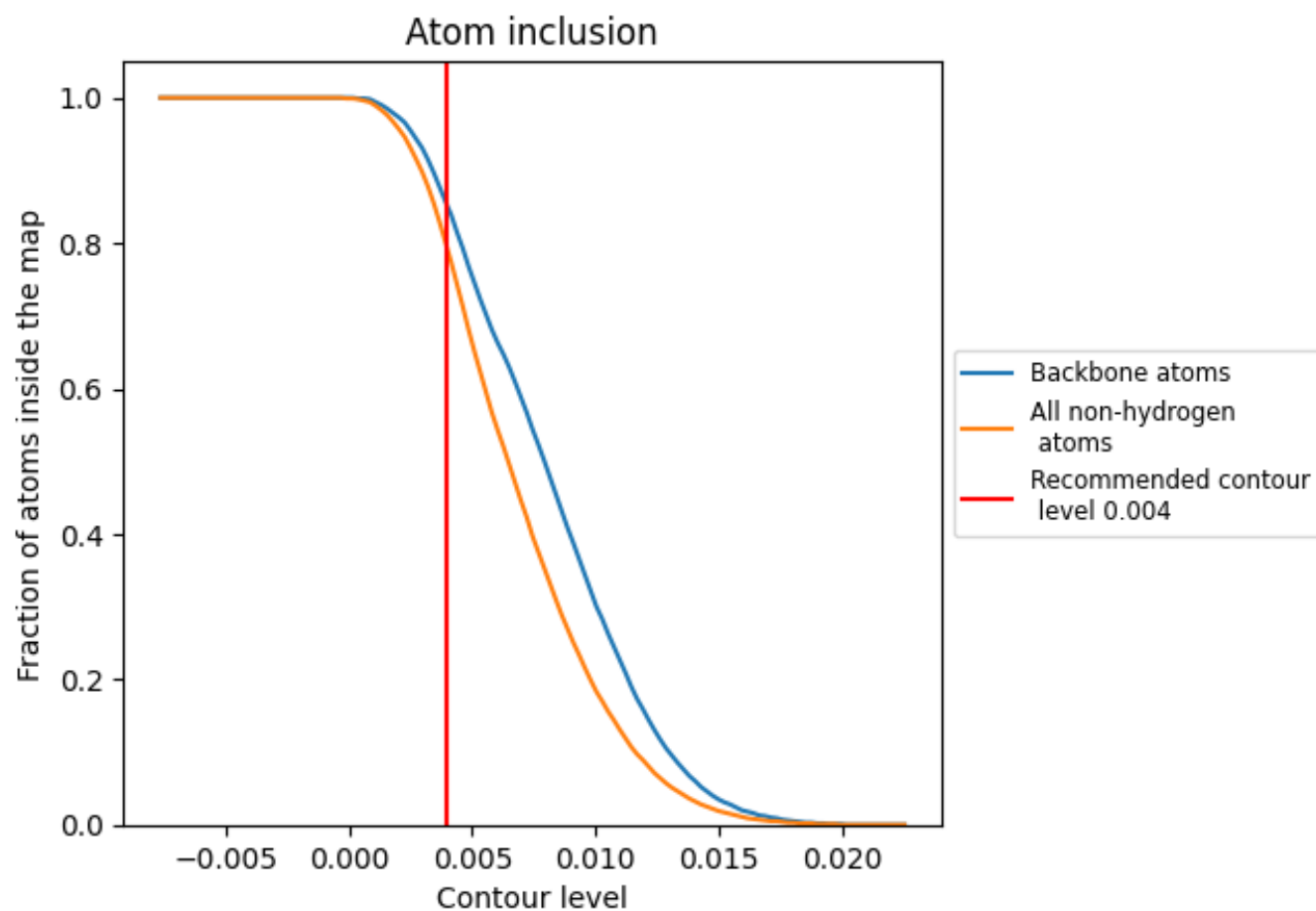
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.004).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 79% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7920	0.2390
A	0.7810	0.2390
B	0.8410	0.2650
C	0.8440	0.2220
D	0.7810	0.2380
E	0.8440	0.2710
F	0.8430	0.2230

1.0

0.0

<0.0