



Full wwPDB EM Validation Report ⓘ

Oct 14, 2024 – 05:31 PM JST

PDB ID : 7F56
EMDB ID : EMD-31459
Title : DNQX-bound GluK2-1xNeto2 complex, with asymmetric LBD
Authors : He, L.L.; Gao, Y.W.; Li, B.; Zhao, Y.
Deposited on : 2021-06-21
Resolution : 4.10 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.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

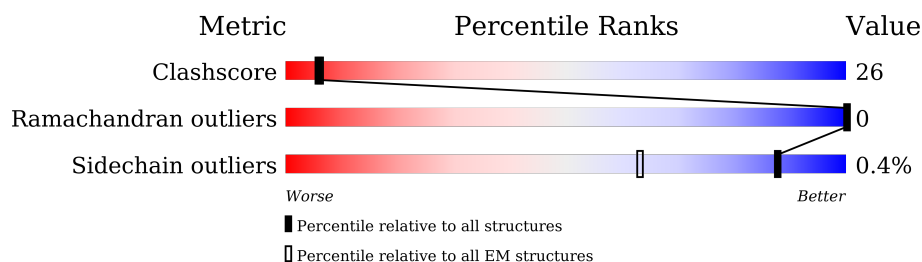
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 Å.

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




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	908	<div> <div>5%</div> <div>46%</div> <div>45%</div> <div>8%</div> </div>
1	B	908	<div> <div>7%</div> <div>50%</div> <div>42%</div> <div>8%</div> </div>
1	C	908	<div> <div>7%</div> <div>46%</div> <div>45%</div> <div>8%</div> </div>
1	D	908	<div> <div>6%</div> <div>49%</div> <div>41%</div> <div>10%</div> </div>
2	E	525	<div> <div>7%</div> <div>15%</div> <div>14%</div> <div>71%</div> </div>
3	F	3	<div> <div>33%</div> <div>67%</div> </div>
3	G	3	<div> <div>67%</div> <div>33%</div> </div>
3	H	3	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
3	I	3	 <div>33% 67%</div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	G	1	-	-	X	-
3	NAG	H	1	X	-	-	-
4	NAG	B	1004	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 27834 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 Glutamate receptor ionotropic, kainate 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	831	Total	C	N	O	S	0	0
			6578	4218	1095	1227	38		
1	B	831	Total	C	N	O	S	0	0
			6575	4216	1095	1227	37		
1	C	835	Total	C	N	O	S	0	0
			6604	4231	1102	1232	39		
1	D	818	Total	C	N	O	S	0	0
			6471	4152	1077	1207	35		

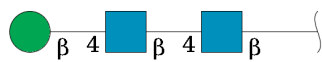
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	107	LEU	PHE	engineered mutation	UNP P42260
A	567	VAL	ILE	variant	UNP P42260
A	571	CYS	TYR	variant	UNP P42260
B	107	LEU	PHE	engineered mutation	UNP P42260
B	567	VAL	ILE	variant	UNP P42260
B	571	CYS	TYR	variant	UNP P42260
C	107	LEU	PHE	engineered mutation	UNP P42260
C	567	VAL	ILE	variant	UNP P42260
C	571	CYS	TYR	variant	UNP P42260
D	107	LEU	PHE	engineered mutation	UNP P42260
D	567	VAL	ILE	variant	UNP P42260
D	571	CYS	TYR	variant	UNP P42260

- Molecule 2 is a protein called Neuropilin and tolloid-like protein 2.

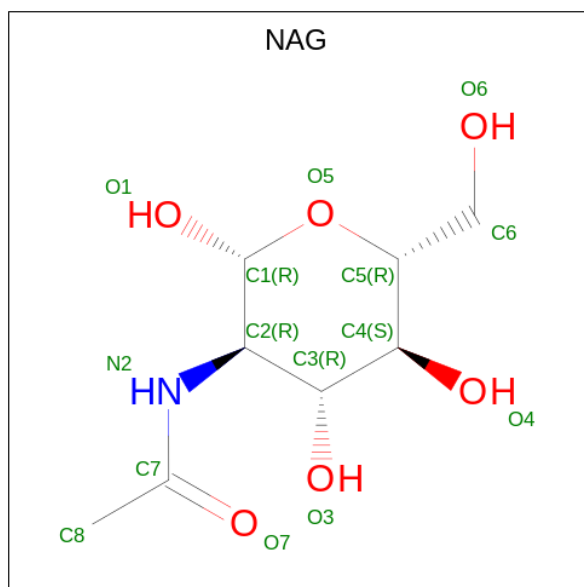
Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	153	Total	C	N	O	S	0	0
			1226	793	208	217	8		

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
3	H	3	Total	C	N	O	0	0
			39	22	2	15		
3	F	3	Total	C	N	O	0	0
			39	22	2	15		
3	G	3	Total	C	N	O	0	0
			39	22	2	15		
3	I	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	

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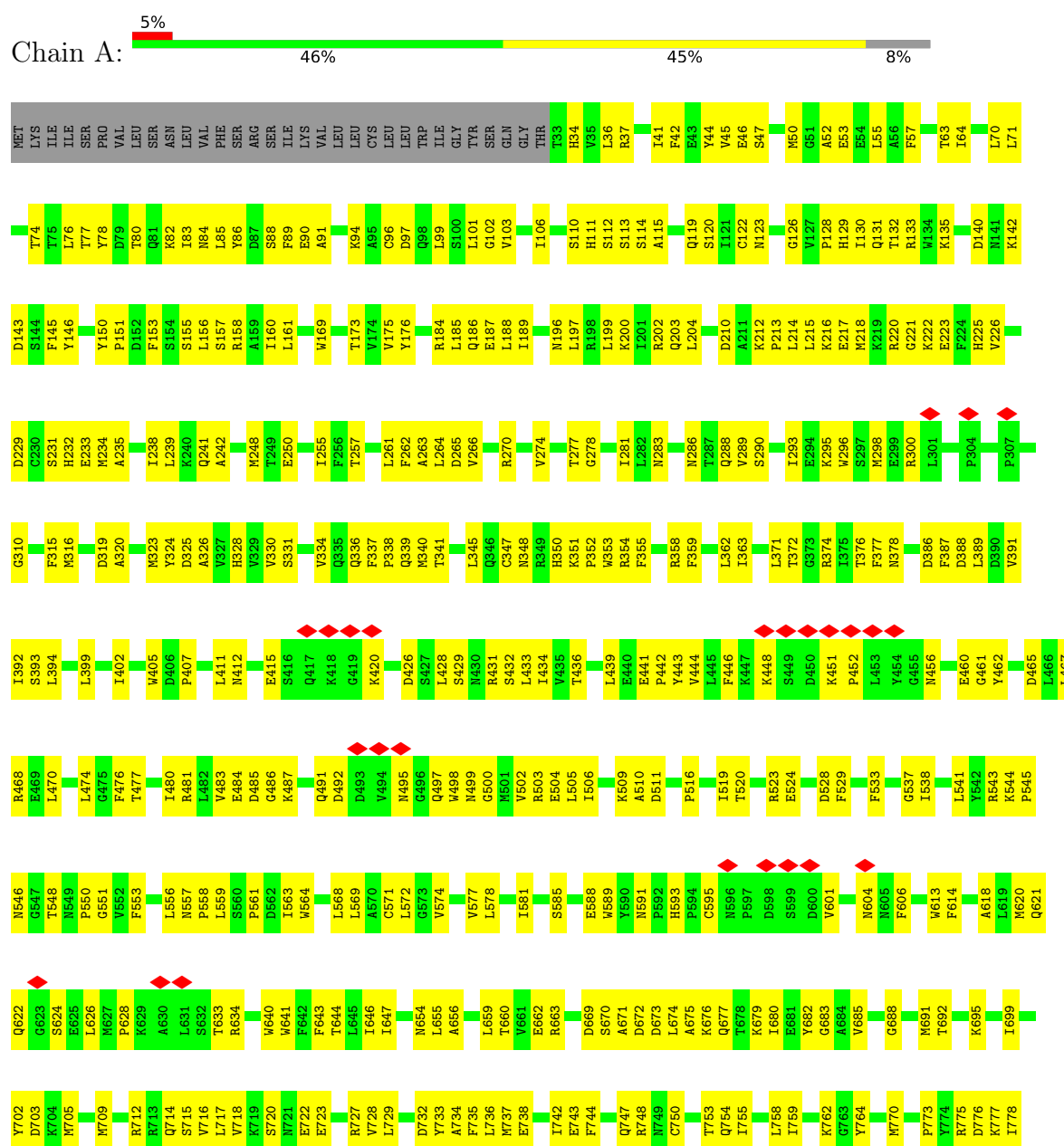
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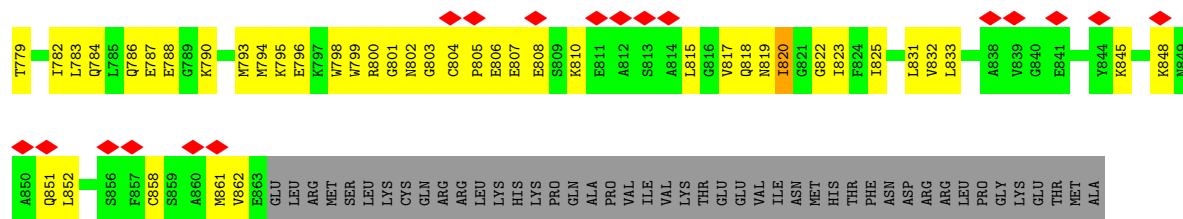
Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots

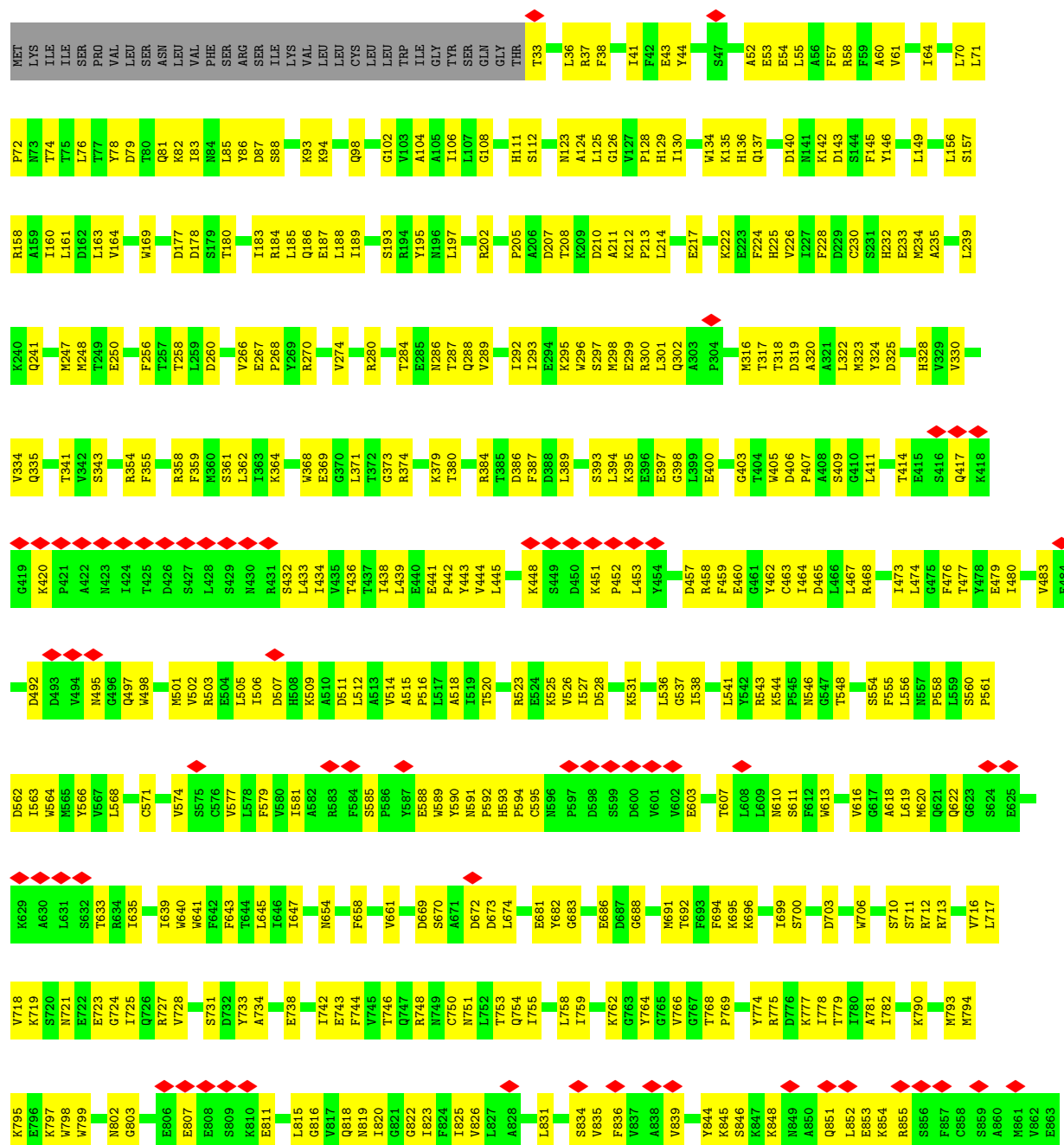
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Glutamate receptor ionotropic, kainate 2





- Molecule 1: Glutamate receptor ionotropic, kainate 2



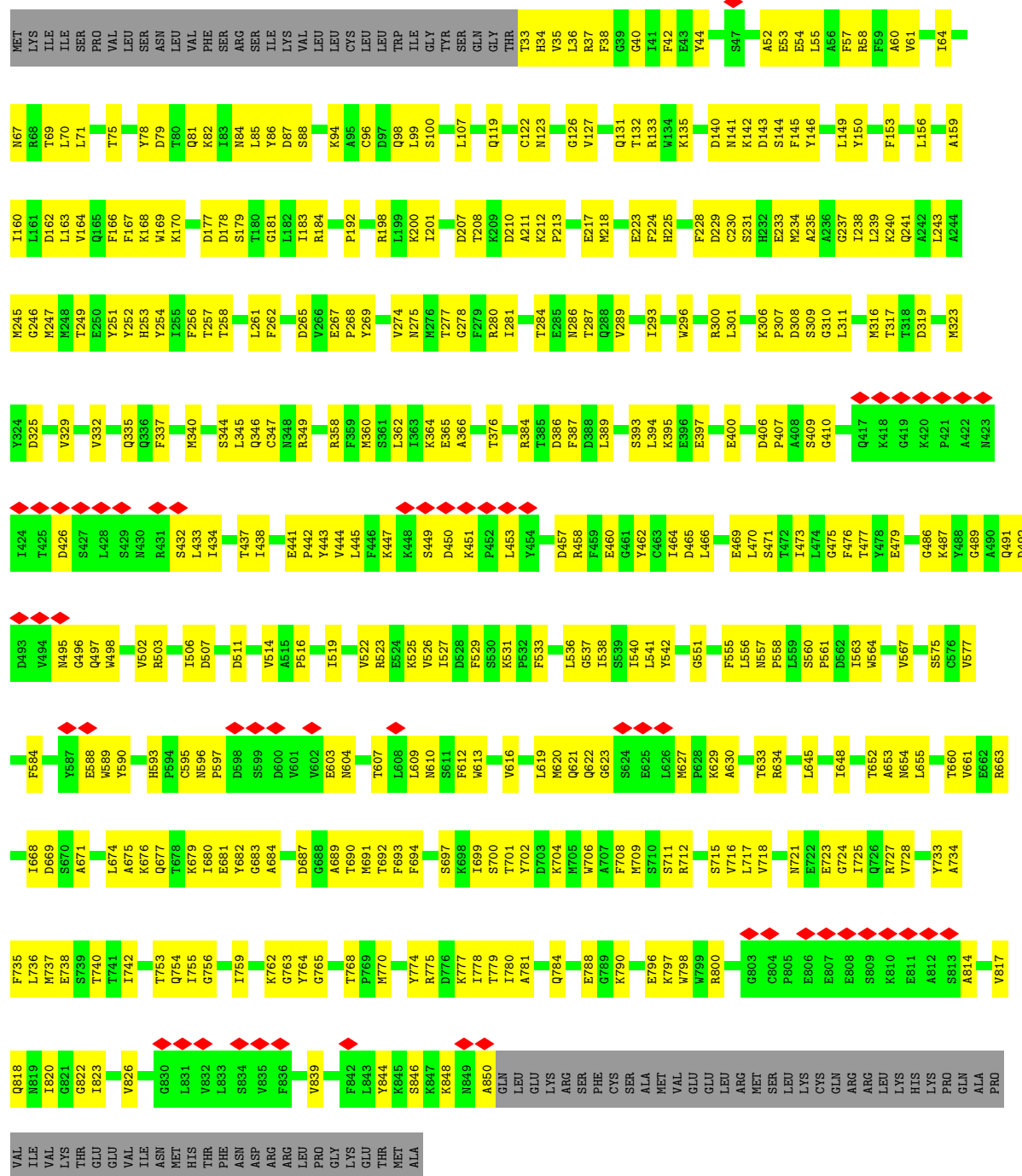
GLU	LEU	ARG	ILE	MET	SER	LEU	LYS	CYS	GLN	ARG	ARG	LEU	LYS	HIS	PRO	LYS	PRO	GLN	ALA	LYS	PRO	VAL	ILE	VAL	LYS	THR	GLU	GLY	VAL	ILE	ASN	MET	GLY	HIS	THR	PHE	ASN	ASP	ASP	ARG	ARG	LEU	PRO	GLY	LYS	GLU	THR	MET	ALA
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• Molecule 1: Glutamate receptor ionotropic, kainate 2

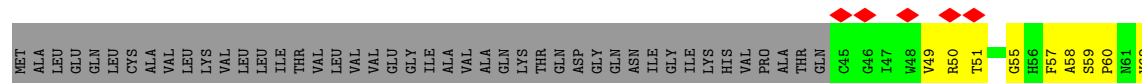


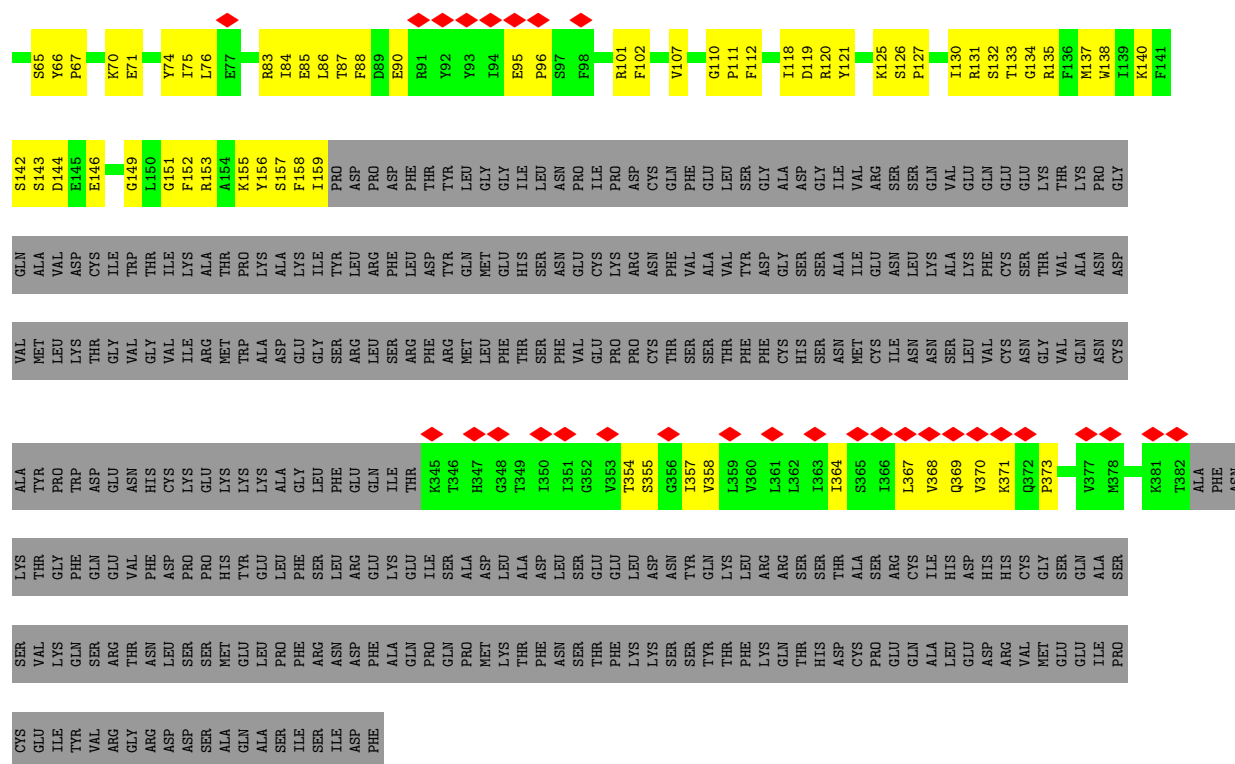
Met	Lys	Ile	Ile	Ser	Pro	Val	Leu	Ser	Leu	Asn	Arg	Leu	Val	Phe	Ser	Arg	Ser	Ile	Lys	Val	Leu	Leu	Cys	Leu	Leu	Thr	Gly	Gly	Thr	T33	H34	V35	L36	R37	F38	G39	G40	I41	F42	Q43	E44	E45	L55	R58	V61	I64	N65	R68	I69	L70	L71																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
P72	N73	T74	T75	L76	T77	Y78	Q81	K82	I83	N84	V85	L86	L88	Y86	C96	D97	Q98	L99	S100	V103	A104	L105	L107	G108	P109	S110	H111	Q119	C122	N123	A124	L125	G126	V127	H129	I130	F141	Q131	T132	R133	W134	K135	H136	D140	N141	K142	D143	I144	F145	Y146	L149	L158																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
A159	D162	F167	K168	W169	K170	T171	T172	T173	N174	V174	W175	Y176	D177	D178	G181	Q182	L182	I183	R184	L185	Q186	I189	P192	R198	L199	K200	Q203	L204	A211	L215	K216	F224	H225	E233	M234	A235	T238	L239	K240	M248	T249	E250	Y251	H252	Y254	L255	F256																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
L259	D260	L261	L264	D265	V266	R270	V274	N275	M276	T277	L282	N283	T284	E285	N286	T287	Q288	V289	S290	I293	W296	R296	R300	A303	P304	D308	M316	T317	T318	D319	H225	A320	M323	A326	V327	H328	V329	W330	S331	V332	F337	L345	Q346	C347	N348	R349																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
H350	K351	P352	W353	R354	F355	G356	T357	R358	M360	S361	L362	I363	K364	E365	W368	E369	G370	T371	T372	G373	R374	I375	T376	D386	F387	D388	L392	S393	L394	K395	E396	E397	Q398	L399	D406	M409	S410	L411	S416	Q417	K418	G419	K420	P421	A422	N423	I424	T425	D426	S427																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
L428	S429	N430	R431	S432	L433	I434	V435	T436	L439	E440	Y443	V444	K447	K448	S449	D450	K451	P452	L453	Y454	G455	N456	D457	R458	F459	G460	G461	Y462	C463	I464	D465	L466	L467	R468	E469	L470	S471	T472	I473	L474	Y478	E479	I480	R481	L482	V483	E484	D485	A490	Q491	D492	D493	V494	N495																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
G496	Q497	W498	N499	G500	M501	V502	R503	E504	L505	L506	K509	A510	D511	L512	A513	P516	Y521	V522	K525	V526	I527	D528	F529	S530	K531	P532	F533	M534	T535	L536	G537	I538	S539	L540	R543	N546	G547	T548	N549	P550	G551	V552	P558	L559	S560	M561	D562	I563	M564	M565	Y566	V567																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
L568	L569	A570	C571	V574	S575	C576	V577	L578	F579	V580	R583	F584	E588	W589	N591	P592	H593	P594	C595	N596	P597	D598	S599	E600	V601	V602	E603	N604	M605	G606	N610	S611	F612	W613	F614	G615	V616	G617	A618	L619	M620	Q621	E625	L626	M627	P628	V629	A630	L631	S632	T633	I635																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
V636	T639	W640	W641	T646	S647	S648	S649	L655	A656	A657	T660	R663	R664	T668	D673	L674	N678	C679	A680	N681	W682	G683	E686	M691	T692	P693	F694	K695	K696	S697	T701	Y702	T703	K704	M705	W706	M709	S710	S711	R712	E787	E788	G789	K790	L791	H792	V718																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
K719	S720	N721	E722	E723	G724	I725	V728	L729	Y733	A734	F735	L736	S739	V745	T746	Q747	R748	N749	C750	W751	L752	T753	K754	I755	L758	L759	D760	S761	K762	G763	Y764	P769	Y774	R775	D776	K777	I778	T779	I780	A781	I782	L783	Q784	L785	S846	K847	K848	N849	A850	Q851	L852	S859	A860	N861	W862	E863																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
K795	E796	L797	W798	W799	R800	G801	N802	G803	C804	P805	E806	E807	E808	S809	K810	E811	A812	G816	R817	Q818	N819	I820	L823	F824	I825	R826	L827	L828	A829	G830	W831	R832	L833	S834	R835	F836	W839	G840	E841	F842	L843	Y844	K845	R846	K847	K848	N849	A850	Q851	L852	S859	A860	N861	W862	E863																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
E864	L865	R866	S867	Ser	Leu	Leu	Lys	Cys	Gln	Arg	Arg	Leu	Lys	His	Lys	Pro	Gln	Ala	Pro	Pro	Val	Ile	Val	Val	Lys	Thr	Thr	Thr	Thr	Thr	Thr	Thr	Thr	Thr	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met	Met</

• Molecule 1: Glutamate receptor ionotropic, kainate 2



• Molecule 2: Neuropilin and tolloid-like protein 2







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90580	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.109	Depositor
Minimum map value	-0.620	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.085	Depositor
Recommended contour level	0.455	Depositor
Map size (\AA)	348.16, 348.16, 348.16	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.36, 1.36, 1.36	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.41	0/6727	0.58	0/9110
1	B	0.44	0/6724	0.57	0/9107
1	C	0.46	0/6752	0.59	0/9142
1	D	0.48	0/6619	0.59	0/8968
2	E	0.41	0/1258	0.55	0/1699
All	All	0.45	0/28080	0.58	0/38026

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	6578	0	6556	394	0
1	B	6575	0	6546	345	0
1	C	6604	0	6578	390	0
1	D	6471	0	6442	327	0
2	E	1226	0	1220	79	0
3	F	39	0	34	0	0
3	G	39	0	34	11	0
3	H	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	39	0	34	1	0
4	A	42	0	39	6	0
4	B	56	0	52	8	0
4	C	70	0	65	1	0
4	D	56	0	52	5	0
All	All	27834	0	27686	1460	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 26.

All (1460) 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:275:ASN:ND2	4:D:1003:NAG:C1	1.70	1.52
1:A:378:ASN:CG	3:G:1:NAG:C8	1.83	1.46
1:A:412:ASN:HD21	4:A:1003:NAG:C1	1.29	1.44
1:C:216:LYS:HE3	2:E:102:PHE:CE2	1.56	1.41
1:A:412:ASN:ND2	4:A:1003:NAG:C1	1.81	1.39
1:A:378:ASN:CG	3:G:1:NAG:H82	1.44	1.23
1:A:378:ASN:OD1	3:G:1:NAG:H83	1.09	1.20
1:A:432:SER:HA	1:A:477:THR:CG2	1.69	1.20
1:C:420:LYS:HD2	1:C:421:PRO:HD2	1.18	1.16
1:C:709:MET:SD	1:C:717:LEU:HD21	1.85	1.16
1:A:378:ASN:CG	3:G:1:NAG:H83	1.56	1.11
1:A:378:ASN:OD1	3:G:1:NAG:C8	1.93	1.09
1:A:378:ASN:ND2	3:G:1:NAG:H82	1.70	1.06
1:A:432:SER:HA	1:A:477:THR:HG22	1.36	1.05
1:B:417:GLN:HG3	4:B:1004:NAG:O6	1.57	1.03
1:A:432:SER:CA	1:A:477:THR:CG2	2.39	1.00
1:C:713:ARG:O	1:C:714:GLN:HG2	1.62	0.98
1:D:296:TRP:HE1	1:D:300:ARG:HH11	0.99	0.98
2:E:90:GLU:HB2	2:E:126:SER:HB2	1.46	0.97
1:A:432:SER:CB	1:A:477:THR:CG2	2.45	0.94
1:A:140:ASP:HB2	1:B:86:TYR:CZ	2.02	0.94
1:C:216:LYS:CE	2:E:102:PHE:CE2	2.51	0.93
1:C:136:HIS:HD2	1:C:183:ILE:HD13	1.33	0.92
1:C:216:LYS:HE3	2:E:102:PHE:HE2	1.30	0.91
1:A:378:ASN:CB	3:G:1:NAG:C8	2.49	0.91
1:A:432:SER:HA	1:A:477:THR:HG23	1.53	0.90
1:A:36:LEU:HB3	1:A:76:LEU:HD22	1.54	0.90
1:C:136:HIS:CD2	1:C:183:ILE:HD13	2.06	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:ASN:CB	3:G:1:NAG:H82	2.04	0.88
1:C:71:LEU:HB3	1:C:74:THR:HB	1.57	0.86
1:A:412:ASN:CG	4:A:1003:NAG:C1	2.42	0.86
1:B:434:ILE:H	1:B:511:ASP:HB2	1.40	0.86
1:A:533:PHE:HB3	1:A:782:ILE:HD11	1.55	0.85
1:D:817:VAL:HA	1:D:820:ILE:HG22	1.59	0.85
1:C:718:VAL:HG12	1:C:720:SER:H	1.40	0.85
1:A:432:SER:OG	1:A:477:THR:HG23	1.76	0.85
1:C:551:GLY:HA2	1:C:820:ILE:HA	1.59	0.84
1:C:568:LEU:O	1:C:571:CYS:SG	2.36	0.83
1:A:432:SER:CB	1:A:477:THR:HG21	2.08	0.83
1:C:107:LEU:HD23	1:C:130:ILE:HB	1.61	0.83
1:D:360:MET:HG3	1:D:364:LYS:HE3	1.60	0.82
1:A:432:SER:HB2	1:A:477:THR:HG21	1.62	0.82
1:C:483:VAL:HG11	1:C:500:GLY:HA2	1.62	0.81
1:A:520:THR:HG23	1:A:523:ARG:H	1.46	0.80
1:C:502:VAL:HG13	1:C:527:ILE:HD11	1.63	0.80
1:A:391:VAL:HG13	1:A:402:ILE:HG13	1.64	0.80
1:C:470:LEU:HD22	1:C:778:ILE:HD11	1.63	0.80
1:A:296:TRP:HE1	1:A:300:ARG:HH11	1.27	0.80
1:C:435:VAL:HG21	1:C:467:LEU:HD11	1.63	0.80
1:D:296:TRP:HE1	1:D:300:ARG:NH1	1.78	0.79
1:B:845:LYS:HA	1:B:848:LYS:HE2	1.65	0.79
1:A:606:PHE:CE1	1:A:626:LEU:HB3	2.17	0.79
1:A:548:THR:HG23	1:A:548:THR:O	1.81	0.79
2:E:112:PHE:HB2	2:E:138:TRP:HB3	1.64	0.79
1:A:432:SER:CB	1:A:477:THR:HG23	2.13	0.78
1:A:677:GLN:HE21	1:A:679:LYS:HB2	1.48	0.78
1:C:395:LYS:HG3	1:C:400:GLU:HB2	1.64	0.78
1:C:591:ASN:HB3	1:C:596:ASN:HD22	1.48	0.78
1:C:561:PRO:HA	1:C:564:TRP:HD1	1.49	0.77
1:B:498:TRP:H	1:B:503:ARG:HD3	1.48	0.77
1:C:420:LYS:CD	1:C:421:PRO:HD2	2.08	0.77
1:A:432:SER:CA	1:A:477:THR:HG23	2.11	0.77
1:C:216:LYS:HE3	2:E:102:PHE:CD2	2.17	0.77
1:C:808:GLU:HG2	1:C:809:SER:H	1.51	0.76
1:D:486:GLY:O	1:D:487:LYS:HG2	1.85	0.76
1:B:433:LEU:HD13	1:B:476:PHE:HB2	1.68	0.76
1:C:808:GLU:HG2	1:C:809:SER:N	2.01	0.76
1:D:486:GLY:O	1:D:487:LYS:HD3	1.86	0.76
1:C:61:VAL:HA	1:C:64:ILE:HD12	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:ARG:NH2	1:A:484:GLU:OE2	2.20	0.75
1:C:172:VAL:HG13	1:C:199:LEU:HD13	1.65	0.75
1:C:198:ARG:HG2	1:D:198:ARG:HH22	1.50	0.75
2:E:107:VAL:HG12	2:E:118:ILE:HD12	1.66	0.75
2:E:70:LYS:H	2:E:143:SER:HB2	1.52	0.74
1:B:85:LEU:HG	1:B:86:TYR:CD2	2.22	0.74
1:B:728:VAL:HA	1:B:733:TYR:HB3	1.68	0.74
1:D:486:GLY:O	1:D:487:LYS:CG	2.35	0.74
1:B:710:SER:HA	1:B:713:ARG:HE	1.51	0.74
1:D:607:THR:H	1:D:610:ASN:HB2	1.51	0.74
1:A:161:LEU:HD21	1:A:188:LEU:HA	1.70	0.74
1:A:845:LYS:HA	1:A:848:LYS:HE2	1.70	0.74
1:A:52:ALA:HA	1:A:55:LEU:HD12	1.69	0.74
1:D:486:GLY:O	1:D:487:LYS:CD	2.36	0.74
1:A:37:ARG:NH1	1:A:102:GLY:O	2.21	0.74
1:C:456:ASN:HA	1:C:480:ILE:HG22	1.69	0.74
1:C:434:ILE:HG23	1:C:479:GLU:HB3	1.70	0.73
1:D:35:VAL:HG22	1:D:75:THR:HB	1.70	0.73
1:B:300:ARG:NH1	1:B:316:MET:SD	2.62	0.73
1:C:823:ILE:HG13	1:C:826:VAL:HG13	1.70	0.73
1:A:99:LEU:HD11	1:A:345:LEU:HB2	1.70	0.73
1:C:596:ASN:O	1:D:593:HIS:NE2	2.20	0.73
1:C:34:HIS:HB3	1:C:74:THR:HG23	1.71	0.72
1:D:699:ILE:HG21	1:D:702:TYR:HD2	1.54	0.72
1:C:540:ILE:HG22	1:C:736:LEU:HG	1.71	0.72
1:B:543:ARG:NH1	1:B:544:LYS:O	2.21	0.72
1:A:683:GLY:O	1:A:736:LEU:N	2.22	0.72
1:A:718:VAL:HG13	1:A:723:GLU:HG3	1.71	0.72
1:B:744:PHE:O	1:B:748:ARG:NH1	2.23	0.71
1:C:774:TYR:HA	1:C:777:LYS:HD2	1.72	0.71
1:D:58:ARG:NH1	1:D:78:TYR:OH	2.23	0.71
1:A:436:THR:HG22	1:A:481:ARG:HH11	1.53	0.71
1:B:52:ALA:HA	1:B:55:LEU:HD12	1.73	0.71
1:B:140:ASP:O	1:B:142:LYS:NZ	2.21	0.71
1:D:309:SER:HB2	1:D:311:LEU:HD13	1.72	0.71
1:A:319:ASP:OD1	1:A:320:ALA:N	2.23	0.71
1:A:497:GLN:NE2	1:A:498:TRP:O	2.24	0.71
1:A:569:LEU:HA	1:A:572:LEU:HD12	1.72	0.71
1:D:233:GLU:OE1	1:D:233:GLU:N	2.17	0.71
1:D:700:SER:O	1:D:704:LYS:NZ	2.23	0.71
1:B:445:LEU:O	1:B:460:GLU:N	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:654:ASN:ND2	1:C:817:VAL:HG21	2.06	0.71
1:D:306:LYS:HD2	1:D:307:PRO:HD2	1.72	0.71
1:D:433:LEU:HD13	1:D:477:THR:H	1.56	0.71
1:B:299:GLU:O	1:B:302:GLN:NE2	2.24	0.71
1:D:87:ASP:OD1	1:D:88:SER:N	2.24	0.71
1:A:358:ARG:HH11	1:A:362:LEU:HD11	1.56	0.70
1:C:39:GLY:HA3	1:C:106:ILE:HD13	1.73	0.70
1:C:465:ASP:OD2	1:C:798:TRP:NE1	2.22	0.70
1:C:713:ARG:O	1:C:714:GLN:CG	2.37	0.70
1:A:44:TYR:CE1	1:A:82:LYS:HB3	2.25	0.70
1:C:686:GLU:HA	1:C:691:MET:HG2	1.73	0.70
1:A:350:HIS:CD2	1:B:93:LYS:HZ3	2.09	0.70
1:D:79:ASP:OD2	1:D:81:GLN:NE2	2.24	0.69
2:E:87:THR:O	2:E:155:LYS:N	2.24	0.69
1:C:37:ARG:O	1:C:104:ALA:N	2.25	0.69
1:C:589:TRP:HE3	1:C:603:GLU:HA	1.57	0.69
2:E:50:ARG:HG2	2:E:51:THR:HG23	1.74	0.69
1:B:531:LYS:NZ	1:C:530:SER:O	2.25	0.69
1:B:661:VAL:HB	1:C:663:ARG:HH11	1.57	0.69
1:B:445:LEU:N	1:B:460:GLU:O	2.26	0.69
1:B:561:PRO:HA	1:B:564:TRP:HD1	1.56	0.69
1:D:275:ASN:OD1	4:D:1003:NAG:C7	2.41	0.69
1:D:492:ASP:N	1:D:497:GLN:O	2.21	0.69
1:A:393:SER:HB2	1:A:402:ILE:HD13	1.75	0.69
1:B:135:LYS:HZ1	1:B:137:GLN:HA	1.57	0.69
1:D:33:THR:HG22	1:D:33:THR:O	1.92	0.68
1:D:275:ASN:CG	4:D:1003:NAG:C1	2.58	0.68
1:B:233:GLU:OE1	1:B:233:GLU:N	2.24	0.68
1:D:64:ILE:HG23	1:D:70:LEU:HD23	1.74	0.68
1:C:107:LEU:CD2	1:C:130:ILE:HB	2.23	0.68
2:E:354:THR:HG22	2:E:357:ILE:HG13	1.75	0.68
1:B:202:ARG:NH1	1:B:217:GLU:OE1	2.27	0.68
1:D:489:GLY:O	1:D:523:ARG:NH1	2.26	0.68
2:E:83:ARG:HB2	2:E:159:ILE:HG13	1.74	0.68
1:A:822:GLY:HA2	1:A:825:ILE:HD13	1.76	0.68
1:A:217:GLU:O	1:A:221:GLY:N	2.23	0.68
1:A:331:SER:HA	1:A:334:VAL:HG12	1.75	0.68
1:C:433:LEU:HD21	1:C:512:LEU:HD22	1.76	0.68
1:A:817:VAL:HG12	1:A:820:ILE:HG12	1.77	0.67
1:C:250:GLU:N	1:C:250:GLU:OE1	2.26	0.67
1:C:360:MET:HA	1:C:363:ILE:HD12	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:809:SER:HB2	1:C:811:GLU:HG3	1.75	0.67
1:D:526:VAL:HG13	1:D:527:ILE:HG13	1.77	0.67
1:A:663:ARG:HH12	1:A:815:LEU:HD13	1.60	0.67
1:D:708:PHE:HB3	1:D:712:ARG:HH12	1.59	0.67
1:A:389:LEU:O	1:A:405:TRP:N	2.26	0.67
1:B:743:GLU:OE1	1:B:743:GLU:N	2.27	0.67
1:D:486:GLY:C	1:D:487:LYS:HG2	2.15	0.67
1:B:212:LYS:NZ	1:B:241:GLN:OE1	2.22	0.67
1:C:714:GLN:HA	1:C:717:LEU:HB2	1.75	0.67
1:D:122:CYS:SG	1:D:123:ASN:N	2.67	0.67
1:A:563:ILE:HG21	1:B:820:ILE:HD11	1.76	0.67
1:B:38:PHE:O	1:B:79:ASP:N	2.26	0.67
1:C:158:ARG:NH1	1:C:162:ASP:OD2	2.28	0.67
1:A:151:PRO:HB2	1:A:156:LEU:HD11	1.76	0.67
1:C:677:GLN:HE22	1:C:679:LYS:HB2	1.60	0.67
2:E:155:LYS:NZ	2:E:156:TYR:O	2.24	0.66
1:A:622:GLN:NE2	1:D:623:GLY:HA3	2.09	0.66
1:C:616:VAL:O	1:C:620:MET:HB2	1.95	0.66
1:A:509:LYS:O	1:A:509:LYS:NZ	2.25	0.66
1:D:81:GLN:HG2	1:D:98:GLN:HE21	1.60	0.66
1:D:99:LEU:HD11	1:D:127:VAL:HG21	1.76	0.66
1:B:177:ASP:OD1	1:B:178:ASP:N	2.27	0.66
1:D:489:GLY:HA3	1:D:502:VAL:HG23	1.77	0.66
2:E:85:GLU:HB2	2:E:157:SER:HB2	1.78	0.66
1:B:123:ASN:ND2	1:B:143:ASP:OD1	2.28	0.66
1:B:135:LYS:NZ	1:B:136:HIS:O	2.29	0.66
1:A:263:ALA:HB2	1:A:315:PHE:HD2	1.61	0.66
1:B:364:LYS:HD3	1:B:379:LYS:HA	1.76	0.66
1:C:694:PHE:HB3	1:C:706:TRP:HB2	1.76	0.66
1:B:585:SER:HB2	1:B:588:GLU:HG2	1.77	0.65
1:B:444:VAL:HG12	1:B:464:ILE:HG12	1.78	0.65
1:C:817:VAL:HG12	1:C:817:VAL:O	1.96	0.65
1:D:432:SER:HA	1:D:477:THR:HB	1.78	0.65
1:A:545:PRO:HA	4:A:1002:NAG:H82	1.78	0.65
1:B:87:ASP:OD1	1:B:88:SER:N	2.30	0.65
1:C:286:ASN:HB3	1:C:289:VAL:HG23	1.78	0.65
1:A:432:SER:OG	1:A:477:THR:CG2	2.43	0.65
1:C:785:LEU:O	1:C:789:GLY:N	2.28	0.65
2:E:86:LEU:O	2:E:131:ARG:NH2	2.29	0.65
1:A:790:LYS:HA	1:A:793:MET:HG2	1.77	0.65
1:C:551:GLY:HA3	1:C:819:ASN:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:677:GLN:HE22	1:A:680:ILE:H	1.42	0.65
1:B:541:LEU:HD13	1:B:742:ILE:HG23	1.79	0.65
2:E:96:PRO:HD2	2:E:125:LYS:HE3	1.78	0.65
1:B:53:GLU:HG2	1:B:54:GLU:N	2.11	0.65
1:C:211:ALA:O	1:C:215:LEU:N	2.21	0.65
1:D:52:ALA:HA	1:D:55:LEU:HD12	1.79	0.65
1:C:531:LYS:HB2	1:C:782:ILE:HD11	1.78	0.65
1:B:807:GLU:OE1	1:B:807:GLU:N	2.30	0.65
1:C:483:VAL:HG12	1:C:485:ASP:H	1.62	0.65
1:D:393:SER:OG	1:D:394:LEU:N	2.30	0.65
1:D:275:ASN:OD1	4:D:1003:NAG:O7	2.14	0.65
1:D:465:ASP:OD2	1:D:797:LYS:NZ	2.29	0.65
1:D:445:LEU:O	1:D:460:GLU:N	2.30	0.64
1:D:774:TYR:HA	1:D:777:LYS:HE3	1.79	0.64
1:D:784:GLN:HG2	2:E:135:ARG:HH21	1.61	0.64
1:A:374:ARG:NH2	1:A:388:ASP:OD1	2.25	0.64
1:C:248:MET:HE1	1:C:274:VAL:HG11	1.80	0.64
2:E:101:ARG:HA	2:E:120:ARG:HH22	1.63	0.64
1:A:677:GLN:NE2	1:A:680:ILE:H	1.95	0.64
1:D:149:LEU:O	1:D:384:ARG:HD3	1.98	0.64
1:A:392:ILE:HD12	1:A:399:LEU:HD23	1.79	0.64
1:A:654:ASN:OD1	1:A:655:LEU:N	2.32	0.63
1:C:533:PHE:CD1	1:C:534:MET:HG2	2.33	0.63
1:C:526:VAL:HG23	1:C:527:ILE:HD12	1.81	0.63
1:D:471:SER:O	1:D:475:GLY:N	2.23	0.63
1:B:433:LEU:HD13	1:B:476:PHE:CB	2.28	0.63
1:B:536:LEU:N	1:B:762:LYS:O	2.24	0.63
1:B:766:VAL:HG21	1:B:778:ILE:HD13	1.80	0.63
1:C:174:VAL:HG23	1:C:199:LEU:HD11	1.79	0.63
1:C:374:ARG:NE	1:C:388:ASP:OD2	2.21	0.63
1:A:405:TRP:HD1	1:A:411:LEU:HG	1.62	0.63
1:A:498:TRP:HB3	1:A:502:VAL:HB	1.80	0.63
1:D:281:ILE:HD13	1:D:389:LEU:HD23	1.81	0.63
1:B:79:ASP:OD2	1:B:98:GLN:NE2	2.32	0.63
1:C:58:ARG:NH1	1:C:78:TYR:OH	2.31	0.63
1:C:319:ASP:OD1	1:C:320:ALA:N	2.31	0.63
1:A:563:ILE:HD11	1:B:816:GLY:HA2	1.80	0.62
1:C:177:ASP:OD1	1:C:178:ASP:N	2.32	0.62
2:E:76:LEU:HB2	2:E:137:MET:HB2	1.80	0.62
1:C:286:ASN:HD21	1:C:288:GLN:HB2	1.64	0.62
1:C:550:PRO:HB2	1:C:552:VAL:HG22	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:GLN:HB3	1:D:94:LYS:NZ	2.14	0.62
1:D:441:GLU:HB3	1:D:442:PRO:HD3	1.82	0.62
1:D:53:GLU:HB3	1:D:323:MET:HE1	1.82	0.62
1:D:126:GLY:HA2	1:D:145:PHE:CE2	2.35	0.62
1:B:256:PHE:HB3	1:B:258:THR:HG22	1.82	0.62
1:A:378:ASN:ND2	3:G:1:NAG:C8	2.42	0.62
1:A:659:LEU:O	1:A:662:GLU:HG3	2.00	0.62
1:D:177:ASP:OD1	1:D:178:ASP:N	2.33	0.62
1:B:33:THR:HG22	1:B:33:THR:O	2.00	0.62
1:B:661:VAL:HG21	1:C:663:ARG:HB3	1.82	0.62
1:B:692:THR:HA	1:B:695:LYS:HZ2	1.64	0.62
1:D:387:PHE:O	1:D:407:PRO:HD3	2.00	0.62
1:C:349:ARG:HH11	1:C:351:LYS:HB3	1.65	0.62
1:A:266:VAL:HG12	1:A:266:VAL:O	2.00	0.62
1:B:853:GLU:OE2	1:B:855:ARG:NH1	2.33	0.61
1:D:590:TYR:N	1:D:603:GLU:O	2.27	0.61
1:B:38:PHE:H	1:B:78:TYR:HA	1.63	0.61
1:B:571:CYS:HA	1:B:574:VAL:HG12	1.82	0.61
1:D:337:PHE:CD2	1:D:340:MET:HB3	2.35	0.61
1:B:186:GLN:HA	1:B:189:ILE:HD12	1.81	0.61
1:D:300:ARG:CZ	1:D:316:MET:HA	2.30	0.61
2:E:84:ILE:HG23	2:E:158:PHE:HE1	1.65	0.61
1:B:43:GLU:OE1	1:B:111:HIS:HE1	1.83	0.61
1:A:441:GLU:HB2	1:A:442:PRO:HD3	1.83	0.61
1:D:668:ILE:HB	1:D:671:ALA:HB2	1.81	0.61
2:E:88:PHE:CD2	2:E:127:PRO:HD2	2.36	0.61
1:B:536:LEU:HD11	1:B:764:TYR:CE1	2.36	0.61
1:A:716:VAL:HB	1:A:733:TYR:HE1	1.66	0.61
1:D:498:TRP:H	1:D:503:ARG:HD3	1.66	0.61
1:D:536:LEU:HB3	1:D:762:LYS:H	1.66	0.61
1:A:36:LEU:HD23	1:A:76:LEU:HD13	1.83	0.61
1:C:70:LEU:HD21	1:C:331:SER:HB3	1.82	0.61
1:A:44:TYR:CE2	1:A:46:GLU:HA	2.35	0.61
1:B:156:LEU:O	1:B:160:ILE:HG12	2.01	0.61
1:B:374:ARG:NH2	1:B:386:ASP:OD1	2.31	0.61
1:C:183:ILE:HD11	1:D:183:ILE:CD1	2.31	0.61
1:C:405:TRP:HD1	1:C:411:LEU:HA	1.66	0.61
1:A:173:THR:HB	1:A:226:VAL:HG22	1.81	0.60
1:B:718:VAL:HB	1:B:723:GLU:HB3	1.83	0.60
1:C:808:GLU:CG	1:C:809:SER:H	2.13	0.60
1:A:796:GLU:HA	1:A:800:ARG:H	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:ASN:ND2	1:C:143:ASP:OD1	2.33	0.60
1:D:502:VAL:HG13	1:D:527:ILE:HD11	1.82	0.60
1:C:536:LEU:O	1:C:762:LYS:N	2.35	0.60
1:C:795:LYS:O	1:C:799:TRP:HB2	2.00	0.60
1:C:266:VAL:HG11	1:C:394:LEU:HD13	1.82	0.60
1:C:172:VAL:HA	1:C:225:HIS:HB2	1.83	0.60
1:C:613:TRP:HA	1:C:616:VAL:HB	1.84	0.60
1:D:561:PRO:HA	1:D:564:TRP:HB2	1.83	0.60
1:B:531:LYS:H	1:B:779:THR:HG22	1.66	0.60
1:C:34:HIS:N	1:C:74:THR:HA	2.17	0.60
1:C:41:ILE:HD11	1:C:83:ILE:HG12	1.84	0.60
1:C:540:ILE:HG13	1:C:755:ILE:HB	1.84	0.60
1:D:447:LYS:N	1:D:458:ARG:O	2.26	0.60
1:A:270:ARG:HA	1:A:394:LEU:HD21	1.83	0.59
1:A:718:VAL:HG12	1:A:720:SER:H	1.66	0.59
1:B:319:ASP:OD1	1:B:320:ALA:N	2.35	0.59
1:B:451:LYS:HB2	1:B:452:PRO:HD3	1.83	0.59
1:C:171:THR:OG1	1:C:198:ARG:NH2	2.35	0.59
1:A:439:LEU:HA	1:A:444:VAL:HB	1.83	0.59
1:C:224:PHE:HA	1:C:252:TYR:CD2	2.37	0.59
1:C:579:PHE:HD2	1:C:611:SER:HG	1.50	0.59
1:A:618:ALA:HB3	1:A:640:TRP:HE1	1.67	0.59
1:A:628:PRO:HB3	1:A:633:THR:HG23	1.82	0.59
1:A:699:ILE:O	1:A:703:ASP:N	2.28	0.59
1:B:85:LEU:HG	1:B:86:TYR:HD2	1.64	0.59
1:D:590:TYR:HB3	1:D:603:GLU:HB3	1.84	0.59
1:A:202:ARG:NH2	1:A:223:GLU:OE2	2.25	0.59
1:B:518:ALA:HB1	1:B:520:THR:HG23	1.84	0.59
1:C:842:PHE:HA	1:C:845:LYS:NZ	2.17	0.59
1:A:255:ILE:HG12	1:A:277:THR:HB	1.84	0.59
1:A:428:LEU:HD13	1:A:431:ARG:HH21	1.67	0.59
1:B:654:ASN:ND2	1:C:817:VAL:CG2	2.66	0.59
1:C:677:GLN:NE2	1:C:680:ILE:H	2.01	0.59
1:A:663:ARG:HG2	1:D:661:VAL:HG21	1.83	0.59
1:C:39:GLY:HA3	1:C:106:ILE:HA	1.83	0.59
1:C:282:LEU:HA	1:C:372:THR:HG22	1.84	0.59
2:E:87:THR:N	2:E:155:LYS:O	2.20	0.59
1:A:470:LEU:HD13	1:A:778:ILE:HD11	1.85	0.59
1:B:158:ARG:NH1	1:B:407:PRO:O	2.34	0.59
1:D:682:TYR:OH	1:D:708:PHE:HB2	2.01	0.59
1:A:460:GLU:OE2	1:A:461:GLY:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:566:TYR:HB3	1:C:824:PHE:HE2	1.67	0.59
1:A:83:ILE:HG22	1:A:94:LYS:HG3	1.84	0.59
1:B:44:TYR:HB3	1:B:82:LYS:HD3	1.84	0.59
1:B:691:MET:SD	1:B:695:LYS:NZ	2.74	0.59
1:A:543:ARG:HD3	1:A:729:LEU:HD13	1.84	0.59
1:B:681:GLU:HG2	1:B:733:TYR:HA	1.84	0.59
1:C:454:TYR:HA	1:C:458:ARG:HD2	1.84	0.58
1:C:616:VAL:O	1:C:620:MET:CB	2.51	0.58
1:B:692:THR:HA	1:B:695:LYS:HG2	1.85	0.58
1:C:122:CYS:SG	1:C:129:HIS:HB2	2.43	0.58
1:A:497:GLN:HE21	1:A:503:ARG:HD2	1.68	0.58
1:C:439:LEU:HD23	1:C:444:VAL:HG12	1.85	0.58
1:B:661:VAL:HG11	1:C:663:ARG:HG2	1.85	0.58
1:C:543:ARG:NH1	1:C:728:VAL:O	2.35	0.58
1:C:657:ALA:HA	1:D:660:THR:HG22	1.85	0.58
1:D:141:ASN:ND2	1:D:143:ASP:OD2	2.36	0.58
1:B:81:GLN:HB3	1:B:94:LYS:NZ	2.18	0.58
1:B:325:ASP:OD1	1:B:371:LEU:HG	2.04	0.58
1:D:768:THR:HG21	1:D:775:ARG:HB2	1.85	0.58
2:E:87:THR:HB	2:E:155:LYS:HB3	1.85	0.58
1:A:123:ASN:ND2	1:A:143:ASP:HA	2.19	0.58
1:A:796:GLU:O	1:A:801:GLY:N	2.26	0.58
1:D:319:ASP:OD1	1:D:319:ASP:N	2.35	0.58
1:A:156:LEU:O	1:A:160:ILE:HG12	2.04	0.58
1:A:503:ARG:HA	1:A:506:ILE:HG22	1.85	0.58
1:B:123:ASN:HD22	1:B:143:ASP:CG	2.07	0.58
1:D:275:ASN:ND2	4:D:1003:NAG:O5	2.32	0.58
2:E:49:VAL:HB	2:E:156:TYR:CZ	2.39	0.58
1:B:300:ARG:HH22	1:B:317:THR:H	1.51	0.58
1:C:722:GLU:OE1	1:C:722:GLU:N	2.25	0.58
1:A:88:SER:OG	1:A:89:PHE:N	2.35	0.57
1:A:123:ASN:HD22	1:A:143:ASP:HA	1.69	0.57
1:C:434:ILE:HB	1:C:510:ALA:HB2	1.85	0.57
2:E:75:ILE:HG12	2:E:138:TRP:CE3	2.39	0.57
1:D:589:TRP:CZ3	1:D:604:ASN:HB3	2.38	0.57
1:A:793:MET:O	1:A:796:GLU:HG2	2.05	0.57
1:A:795:LYS:O	1:A:799:TRP:N	2.31	0.57
1:B:157:SER:OG	1:B:188:LEU:N	2.37	0.57
1:B:536:LEU:HB2	1:B:762:LYS:HB2	1.85	0.57
1:C:270:ARG:NH1	1:C:396:GLU:O	2.32	0.57
1:A:45:VAL:HG12	1:A:47:SER:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:VAL:HG11	1:B:831:LEU:HD11	1.87	0.57
1:B:417:GLN:HG3	4:B:1004:NAG:C6	2.34	0.57
1:B:686:GLU:HG2	1:B:717:LEU:HB3	1.85	0.57
1:B:795:LYS:HD2	1:B:799:TRP:CD1	2.40	0.57
1:C:718:VAL:HG12	1:C:719:LYS:N	2.18	0.57
1:D:207:ASP:OD1	1:D:208:THR:N	2.38	0.57
1:A:176:TYR:OH	1:A:203:GLN:HB2	2.05	0.57
1:A:487:LYS:HD3	1:A:499:ASN:OD1	2.05	0.57
1:A:286:ASN:ND2	1:A:288:GLN:HB2	2.19	0.57
1:B:417:GLN:HG3	4:B:1004:NAG:HO6	1.67	0.57
1:D:536:LEU:HD22	1:D:762:LYS:HB2	1.85	0.57
1:A:348:ASN:HA	1:A:350:HIS:CE1	2.40	0.57
1:A:537:GLY:HA3	1:A:758:LEU:HG	1.87	0.57
1:A:818:GLN:HG3	1:A:819:ASN:N	2.20	0.57
1:C:356:GLY:HA2	1:C:359:PHE:HB3	1.86	0.57
1:B:669:ASP:OD1	1:B:670:SER:N	2.37	0.57
1:B:683:GLY:N	1:B:734:ALA:O	2.37	0.57
1:C:521:TYR:CZ	1:C:525:LYS:HE3	2.40	0.57
1:D:491:GLN:HB2	1:D:498:TRP:CE2	2.40	0.57
1:A:428:LEU:HB3	1:A:431:ARG:HD3	1.86	0.57
1:C:85:LEU:HD11	1:C:111:HIS:CE1	2.39	0.57
1:B:248:MET:HG3	1:B:274:VAL:HG21	1.85	0.57
1:B:457:ASP:OD2	1:B:458:ARG:NH2	2.37	0.57
1:C:583:ARG:NH1	1:C:604:ASN:HB2	2.19	0.57
2:E:60:PRO:O	2:E:67:PRO:HD3	2.05	0.57
1:A:677:GLN:HE22	1:A:680:ILE:HG23	1.70	0.56
1:C:460:GLU:C	1:C:464:ILE:HD13	2.25	0.56
1:A:290:SER:O	1:A:293:ILE:N	2.39	0.56
1:B:374:ARG:O	1:B:384:ARG:NH2	2.37	0.56
1:A:34:HIS:HB3	1:A:74:THR:HG23	1.86	0.56
1:A:42:PHE:CE2	1:A:80:THR:HB	2.40	0.56
1:A:265:ASP:HB2	1:A:310:GLY:O	2.06	0.56
1:A:443:TYR:O	1:A:462:TYR:N	2.38	0.56
1:A:556:LEU:HD23	1:A:556:LEU:H	1.70	0.56
1:A:669:ASP:HA	1:A:673:ASP:HB2	1.87	0.56
1:B:355:PHE:O	1:B:359:PHE:N	2.24	0.56
1:B:721:ASN:O	1:B:725:ILE:HG12	2.05	0.56
1:C:183:ILE:HD11	1:D:183:ILE:HD11	1.87	0.56
1:C:189:ILE:O	1:C:192:PRO:HD2	2.05	0.56
1:D:300:ARG:HH22	1:D:317:THR:H	1.50	0.56
1:A:233:GLU:OE1	1:A:233:GLU:N	2.29	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:ASP:OD2	1:C:318:THR:N	2.20	0.56
1:D:224:PHE:CE1	1:D:251:TYR:HB3	2.40	0.56
1:D:449:SER:OG	1:D:450:ASP:N	2.36	0.56
1:A:585:SER:HB3	1:A:588:GLU:HG2	1.86	0.56
1:B:85:LEU:HD12	1:B:111:HIS:CE1	2.41	0.56
1:B:746:THR:OG1	1:B:753:THR:HA	2.06	0.56
1:C:84:ASN:OD1	1:C:85:LEU:N	2.35	0.56
1:C:167:PHE:HE2	1:C:253:HIS:NE2	2.03	0.56
1:C:171:THR:HG1	1:C:198:ARG:HH21	1.51	0.56
1:C:695:LYS:HG2	1:C:706:TRP:CZ2	2.41	0.56
1:D:715:SER:HB2	1:D:727:ARG:NH2	2.20	0.56
1:A:250:GLU:OE1	1:A:250:GLU:N	2.34	0.56
1:A:326:ALA:O	1:A:330:VAL:HG23	2.04	0.56
1:A:546:ASN:H	4:A:1002:NAG:H82	1.70	0.56
1:B:126:GLY:HA2	1:B:145:PHE:CE2	2.41	0.56
1:D:228:PHE:HE2	1:D:254:TYR:HD2	1.54	0.56
1:D:267:GLU:HB2	1:D:268:PRO:HD3	1.87	0.56
1:C:619:LEU:HB2	1:C:640:TRP:CZ2	2.40	0.56
1:C:709:MET:SD	1:C:717:LEU:CD2	2.77	0.56
1:D:34:HIS:O	1:D:75:THR:N	2.39	0.56
1:A:277:THR:HG23	1:A:402:ILE:HD11	1.87	0.56
1:C:149:LEU:HD12	1:C:149:LEU:H	1.71	0.56
1:A:266:VAL:HG11	1:A:394:LEU:HD13	1.86	0.55
1:B:37:ARG:HD3	1:B:79:ASP:HB2	1.87	0.55
1:D:630:ALA:O	1:D:633:THR:OG1	2.21	0.55
2:E:369:GLN:O	2:E:373:PRO:HD3	2.06	0.55
1:C:473:ILE:HG23	1:C:474:LEU:HG	1.88	0.55
1:C:591:ASN:HB3	1:C:596:ASN:ND2	2.20	0.55
1:D:519:ILE:HG12	1:D:763:GLY:O	2.06	0.55
2:E:75:ILE:HG12	2:E:138:TRP:CZ3	2.40	0.55
1:B:300:ARG:NH1	1:B:316:MET:HA	2.21	0.55
1:C:252:TYR:O	1:C:274:VAL:HG23	2.06	0.55
2:E:85:GLU:O	2:E:157:SER:N	2.34	0.55
1:B:497:GLN:OE1	1:B:503:ARG:NE	2.39	0.55
1:C:211:ALA:HB3	1:C:238:ILE:HD11	1.89	0.55
1:C:677:GLN:HE22	1:C:680:ILE:H	1.54	0.55
1:D:131:GLN:HE22	1:D:135:LYS:HE2	1.70	0.55
1:D:519:ILE:HD12	1:D:529:PHE:HB3	1.87	0.55
1:A:286:ASN:HD21	1:A:288:GLN:HB2	1.70	0.55
1:A:359:PHE:HA	1:A:362:LEU:HD12	1.88	0.55
1:B:681:GLU:O	1:B:734:ALA:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:802:ASN:OD1	1:B:803:GLY:N	2.39	0.55
1:C:177:ASP:HB3	1:C:204:LEU:HD12	1.87	0.55
1:C:551:GLY:CA	1:C:820:ILE:HA	2.35	0.55
1:D:551:GLY:HA3	1:D:818:GLN:O	2.07	0.55
1:A:263:ALA:HB2	1:A:315:PHE:CD2	2.42	0.55
1:A:456:ASN:HB2	1:A:480:ILE:HD12	1.89	0.55
1:C:123:ASN:HD22	1:C:143:ASP:CG	2.09	0.55
1:D:60:ALA:O	1:D:64:ILE:HG12	2.07	0.55
1:A:85:LEU:HG	1:A:86:TYR:CD2	2.42	0.55
1:A:432:SER:CA	1:A:477:THR:HG22	2.21	0.55
1:B:296:TRP:O	1:B:300:ARG:HB2	2.06	0.55
1:D:536:LEU:HD13	1:D:762:LYS:HB2	1.89	0.55
1:D:588:GLU:OE2	1:D:630:ALA:N	2.38	0.55
1:C:284:THR:HA	1:C:289:VAL:HG11	1.88	0.55
1:A:184:ARG:NH1	1:A:229:ASP:OD1	2.40	0.54
1:B:448:LYS:NZ	1:B:460:GLU:OE2	2.40	0.54
1:C:353:TRP:CH2	1:C:355:PHE:HB2	2.43	0.54
1:D:269:TYR:CD1	1:D:269:TYR:N	2.73	0.54
1:D:179:SER:O	1:D:181:GLY:N	2.40	0.54
1:D:434:ILE:HA	1:D:479:GLU:HB3	1.89	0.54
2:E:84:ILE:HD13	2:E:137:MET:HG2	1.89	0.54
1:A:210:ASP:O	1:A:213:PRO:HD2	2.08	0.54
1:B:444:VAL:HG13	1:B:463:CYS:HB3	1.89	0.54
1:C:492:ASP:OD1	1:C:499:ASN:ND2	2.41	0.54
1:C:610:ASN:HB3	1:C:626:LEU:HD22	1.90	0.54
1:C:630:ALA:HB3	1:C:633:THR:HG22	1.89	0.54
1:A:129:HIS:O	1:A:146:TYR:HA	2.07	0.54
1:C:185:LEU:O	1:C:189:ILE:HG13	2.06	0.54
1:C:725:ILE:O	1:C:729:LEU:HG	2.07	0.54
1:A:483:VAL:HG13	1:A:486:GLY:H	1.73	0.54
1:B:205:PRO:HD3	1:B:214:LEU:HD11	1.89	0.54
1:A:795:LYS:HG3	1:A:799:TRP:CE3	2.43	0.54
1:D:716:VAL:HG23	1:D:717:LEU:HD12	1.90	0.54
1:B:459:PHE:HD2	1:B:480:ILE:HD12	1.72	0.54
1:B:846:SER:HB3	1:B:854:LYS:HE2	1.90	0.54
1:C:290:SER:O	1:C:293:ILE:HB	2.08	0.54
1:C:533:PHE:HD1	1:C:534:MET:HG2	1.72	0.54
1:C:583:ARG:HH11	1:C:604:ASN:HB2	1.72	0.54
1:D:453:LEU:HD23	1:D:457:ASP:HB3	1.89	0.54
1:A:218:MET:O	1:A:222:LYS:N	2.40	0.54
1:C:326:ALA:O	1:C:329:VAL:HG12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:663:ARG:HH22	1:D:814:ALA:HA	1.72	0.54
1:A:250:GLU:HG3	1:A:773:PRO:HG3	1.90	0.53
1:A:262:PHE:HA	1:A:399:LEU:HD22	1.89	0.53
1:C:395:LYS:N	1:C:398:GLY:O	2.40	0.53
1:D:140:ASP:O	1:D:142:LYS:NZ	2.36	0.53
1:D:445:LEU:N	1:D:460:GLU:O	2.23	0.53
1:B:393:SER:OG	1:B:394:LEU:N	2.41	0.53
1:B:593:HIS:NE2	1:B:595:CYS:HB2	2.23	0.53
1:D:470:LEU:HD13	1:D:778:ILE:HD11	1.89	0.53
1:A:41:ILE:HG13	1:A:106:ILE:HD11	1.89	0.53
1:A:674:LEU:O	1:A:682:TYR:OH	2.25	0.53
1:B:439:LEU:HD13	1:B:459:PHE:HE1	1.74	0.53
1:C:290:SER:HA	1:C:293:ILE:HD12	1.91	0.53
1:D:84:ASN:OD1	1:D:85:LEU:HG	2.09	0.53
1:A:64:ILE:HA	1:A:70:LEU:HD11	1.89	0.53
1:A:641:TRP:HB3	1:B:620:MET:HE2	1.91	0.53
1:B:248:MET:SD	1:B:274:VAL:HG21	2.47	0.53
1:B:683:GLY:HA3	1:B:733:TYR:CZ	2.44	0.53
1:C:492:ASP:N	1:C:497:GLN:O	2.23	0.53
1:C:748:ARG:HD2	1:C:802:ASN:CG	2.28	0.53
1:D:376:THR:CG2	1:D:386:ASP:HB3	2.38	0.53
1:A:185:LEU:O	1:A:188:LEU:HB3	2.08	0.53
1:A:744:PHE:CZ	1:A:748:ARG:HD3	2.44	0.53
1:B:436:THR:HG22	1:B:501:MET:HE1	1.89	0.53
1:C:34:HIS:H	1:C:74:THR:HA	1.74	0.53
1:C:53:GLU:OE2	1:C:110:SER:OG	2.21	0.53
1:C:776:ASP:O	1:C:779:THR:OG1	2.23	0.53
1:D:689:ALA:O	1:D:692:THR:OG1	2.25	0.53
1:A:528:ASP:OD2	1:A:775:ARG:HG3	2.07	0.53
1:B:492:ASP:HB2	1:B:497:GLN:HB3	1.90	0.53
1:C:289:VAL:O	1:C:293:ILE:HG13	2.09	0.53
1:A:621:GLN:HG3	1:D:621:GLN:HG2	1.90	0.53
1:B:672:ASP:OD1	1:B:673:ASP:N	2.41	0.53
1:C:565:MET:SD	1:C:565:MET:N	2.81	0.53
1:A:628:PRO:O	1:A:634:ARG:NE	2.42	0.53
1:A:831:LEU:HD11	1:D:577:VAL:HG11	1.91	0.53
1:C:440:GLU:HB2	1:C:443:TYR:HB2	1.89	0.53
1:D:708:PHE:HB3	1:D:712:ARG:NH1	2.23	0.53
1:A:213:PRO:O	1:A:216:LYS:HB3	2.08	0.53
1:A:465:ASP:O	1:A:468:ARG:N	2.42	0.53
1:A:748:ARG:HH11	1:A:802:ASN:HB3	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:VAL:HG11	1:B:228:PHE:CZ	2.44	0.53
1:D:788:GLU:OE1	1:D:790:LYS:N	2.42	0.53
2:E:364:ILE:O	2:E:368:VAL:HG22	2.09	0.53
1:A:444:VAL:HA	1:A:461:GLY:HA3	1.90	0.53
1:C:119:GLN:HE22	1:C:141:ASN:HD21	1.55	0.53
1:C:300:ARG:NH1	1:C:303:ALA:HB3	2.24	0.53
1:D:677:GLN:NE2	1:D:679:LYS:HB3	2.23	0.53
1:A:155:SER:HA	1:A:158:ARG:NH1	2.23	0.52
1:A:200:LYS:HD3	1:B:193:SER:HA	1.91	0.52
1:A:699:ILE:HA	1:D:708:PHE:HE1	1.74	0.52
1:D:207:ASP:HB3	1:D:210:ASP:OD2	2.09	0.52
1:D:230:CYS:SG	1:D:234:MET:HB3	2.49	0.52
1:D:536:LEU:HD23	1:D:537:GLY:N	2.24	0.52
1:D:728:VAL:HG22	1:D:733:TYR:O	2.08	0.52
1:A:175:VAL:HG22	1:A:202:ARG:HB2	1.90	0.52
1:A:674:LEU:HB3	1:A:682:TYR:HE1	1.74	0.52
1:A:714:GLN:HA	1:A:717:LEU:HB2	1.91	0.52
1:B:654:ASN:HD21	1:C:817:VAL:CG2	2.23	0.52
1:C:37:ARG:HB3	1:C:103:VAL:HG12	1.92	0.52
1:C:216:LYS:HG3	2:E:102:PHE:CZ	2.45	0.52
1:C:539:SER:OG	1:C:754:GLN:OE1	2.25	0.52
1:C:615:GLY:HA2	1:C:640:TRP:HE1	1.75	0.52
1:C:792:HIS:O	1:C:796:GLU:HG2	2.08	0.52
1:D:300:ARG:NH1	1:D:316:MET:HA	2.24	0.52
1:D:450:ASP:OD1	1:D:451:LYS:N	2.42	0.52
1:D:538:ILE:HG13	1:D:759:ILE:HB	1.91	0.52
1:D:699:ILE:HG21	1:D:702:TYR:CD2	2.40	0.52
2:E:354:THR:CG2	2:E:357:ILE:HG13	2.38	0.52
1:C:123:ASN:OD1	1:C:145:PHE:CD2	2.62	0.52
2:E:76:LEU:HD12	2:E:137:MET:HB2	1.90	0.52
1:A:42:PHE:HE2	1:A:80:THR:HB	1.73	0.52
1:A:42:PHE:HD2	1:A:82:LYS:HG2	1.74	0.52
1:A:796:GLU:HB2	1:A:800:ARG:HB3	1.90	0.52
1:B:595:CYS:HB3	1:C:593:HIS:CE1	2.45	0.52
1:D:239:LEU:HD21	1:D:256:PHE:HZ	1.74	0.52
1:D:555:PHE:CZ	1:D:820:ILE:HD12	2.45	0.52
1:B:556:LEU:HD23	1:B:556:LEU:H	1.73	0.52
1:B:566:TYR:HB3	1:C:824:PHE:CE2	2.44	0.52
2:E:370:VAL:O	2:E:373:PRO:HD2	2.10	0.52
1:B:528:ASP:HB3	1:B:768:THR:HG23	1.91	0.52
1:B:744:PHE:HB2	1:B:799:TRP:CE3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:GLY:HA2	1:C:145:PHE:CE2	2.44	0.52
1:C:200:LYS:HE2	1:D:192:PRO:O	2.09	0.52
1:C:358:ARG:HD2	1:C:362:LEU:HG	1.91	0.52
1:C:635:ILE:O	1:C:639:ILE:HG12	2.10	0.52
1:D:126:GLY:HA2	1:D:145:PHE:CD2	2.44	0.52
1:D:329:VAL:O	1:D:332:VAL:HG12	2.09	0.52
1:D:337:PHE:HD2	1:D:340:MET:HB3	1.75	0.52
1:A:78:TYR:HD2	1:A:80:THR:HG23	1.75	0.52
1:A:266:VAL:O	1:A:266:VAL:CG1	2.57	0.52
1:B:403:GLY:HA2	1:B:414:THR:HG23	1.90	0.52
1:B:727:ARG:HB3	1:B:733:TYR:CD2	2.45	0.52
1:C:531:LYS:HG2	1:C:779:THR:HG22	1.91	0.52
1:A:212:LYS:HB2	1:A:213:PRO:HD3	1.92	0.52
1:B:498:TRP:N	1:B:503:ARG:HD3	2.21	0.52
1:B:790:LYS:O	1:B:794:MET:HG3	2.09	0.52
1:B:797:LYS:HD2	1:B:798:TRP:CZ3	2.44	0.52
1:C:668:ILE:HG13	1:C:673:ASP:OD2	2.10	0.52
1:D:239:LEU:HB3	1:D:269:TYR:CE2	2.44	0.52
1:D:560:SER:HB3	1:D:563:ILE:CD1	2.40	0.52
1:A:412:ASN:OD1	4:A:1003:NAG:C1	2.57	0.52
1:A:628:PRO:HB2	1:A:634:ARG:HG3	1.92	0.52
1:A:776:ASP:OD1	1:A:777:LYS:N	2.43	0.52
1:B:505:LEU:O	1:B:769:PRO:HG3	2.09	0.52
1:C:728:VAL:HG22	1:C:733:TYR:HB3	1.91	0.52
1:D:84:ASN:OD1	1:D:85:LEU:N	2.42	0.52
1:D:159:ALA:HA	1:D:162:ASP:OD2	2.09	0.52
1:A:571:CYS:HA	1:A:574:VAL:HG12	1.92	0.52
1:B:358:ARG:O	1:B:361:SER:HB3	2.09	0.52
1:C:775:ARG:O	1:C:779:THR:HG23	2.10	0.52
1:D:132:THR:OG1	1:D:133:ARG:N	2.42	0.52
1:D:486:GLY:C	1:D:487:LYS:CG	2.79	0.52
1:A:446:PHE:O	1:A:448:LYS:NZ	2.43	0.51
1:A:656:ALA:O	1:A:660:THR:OG1	2.21	0.51
1:B:548:THR:HB	1:B:818:GLN:NE2	2.24	0.51
1:C:349:ARG:HD3	1:C:351:LYS:HB3	1.93	0.51
1:C:641:TRP:HB3	1:D:620:MET:HG2	1.91	0.51
1:C:649:SER:OG	1:D:652:THR:OG1	2.20	0.51
1:C:702:TYR:CZ	1:C:759:ILE:HG23	2.45	0.51
1:D:495:ASN:O	1:D:497:GLN:NE2	2.42	0.51
1:D:778:ILE:HD12	1:D:781:ALA:HB3	1.92	0.51
1:D:796:GLU:O	1:D:800:ARG:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:CYS:CB	1:A:347:CYS:HG	2.13	0.51
1:A:491:GLN:OE1	1:A:492:ASP:N	2.42	0.51
1:B:58:ARG:NH1	1:B:78:TYR:OH	2.43	0.51
1:B:134:TRP:NE1	1:B:135:LYS:O	2.44	0.51
1:B:498:TRP:C	1:B:503:ARG:HB2	2.31	0.51
1:C:675:ALA:HB2	1:C:705:MET:SD	2.50	0.51
1:C:729:LEU:HD21	1:C:752:LEU:HD11	1.92	0.51
1:D:44:TYR:CE1	1:D:82:LYS:HB3	2.44	0.51
1:D:218:MET:HG3	1:D:223:GLU:OE1	2.10	0.51
1:D:240:LYS:NZ	1:D:308:ASP:O	2.43	0.51
1:D:406:ASP:OD1	1:D:410:GLY:N	2.34	0.51
1:D:542:TYR:O	1:D:753:THR:HB	2.10	0.51
1:A:386:ASP:HA	1:A:407:PRO:HG2	1.91	0.51
1:A:589:TRP:CZ3	1:A:604:ASN:HA	2.46	0.51
1:A:682:TYR:OH	1:A:705:MET:SD	2.63	0.51
1:A:801:GLY:HA2	1:A:804:CYS:SG	2.50	0.51
1:C:186:GLN:O	1:C:189:ILE:N	2.42	0.51
1:C:546:ASN:OD1	1:C:548:THR:HG23	2.10	0.51
1:D:677:GLN:NE2	1:D:680:ILE:HG12	2.25	0.51
1:A:330:VAL:HA	1:A:363:ILE:HD11	1.92	0.51
1:A:806:GLU:HB2	1:A:808:GLU:HG3	1.93	0.51
1:B:61:VAL:HG11	1:B:78:TYR:HD1	1.76	0.51
1:B:267:GLU:HB3	1:B:268:PRO:HD3	1.92	0.51
1:B:560:SER:O	1:B:562:ASP:N	2.43	0.51
1:A:426:ASP:HB3	1:A:429:SER:HB3	1.92	0.51
1:B:81:GLN:HB3	1:B:94:LYS:HZ2	1.76	0.51
1:B:207:ASP:OD1	1:B:208:THR:N	2.39	0.51
1:C:417:GLN:HG3	1:C:421:PRO:HA	1.93	0.51
1:A:720:SER:OG	1:A:723:GLU:HG2	2.11	0.51
1:B:210:ASP:O	1:B:213:PRO:HD2	2.11	0.51
1:B:222:LYS:HB3	1:B:224:PHE:CE2	2.46	0.51
1:B:324:TYR:HH	1:B:328:HIS:HE2	1.57	0.51
1:B:439:LEU:HD11	1:B:445:LEU:HA	1.93	0.51
1:B:822:GLY:HA2	1:B:825:ILE:HD13	1.92	0.51
1:C:233:GLU:OE1	1:C:233:GLU:N	2.30	0.51
1:D:184:ARG:NH1	1:D:229:ASP:OD1	2.42	0.51
1:B:38:PHE:HE1	1:B:104:ALA:HB3	1.76	0.51
1:B:280:ARG:NH1	1:B:284:THR:OG1	2.43	0.51
1:C:559:LEU:HB3	1:C:564:TRP:CZ2	2.46	0.51
1:C:847:LYS:HD3	1:C:848:LYS:HZ2	1.76	0.51
1:D:677:GLN:HE22	1:D:679:LYS:HB3	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:LEU:HD13	1:D:86:TYR:HD2	1.76	0.51
1:D:438:ILE:HD13	1:D:486:GLY:HA2	1.93	0.51
1:D:737:MET:SD	1:D:738:GLU:N	2.84	0.51
2:E:102:PHE:O	2:E:144:ASP:HB3	2.11	0.51
1:A:161:LEU:HD11	1:A:187:GLU:HG3	1.91	0.51
1:A:196:ASN:O	1:A:197:LEU:HD12	2.10	0.51
1:C:256:PHE:HE1	1:C:276:MET:HG3	1.76	0.51
1:C:277:THR:HG23	1:C:392:ILE:O	2.10	0.51
1:C:747:GLN:HB3	1:C:803:GLY:HA3	1.92	0.51
1:D:261:LEU:HD23	1:D:278:GLY:HA3	1.93	0.51
2:E:62:TYR:CE1	2:E:153:ARG:HB2	2.46	0.51
1:A:589:TRP:HZ3	1:A:604:ASN:HA	1.77	0.50
1:A:750:CYS:HB2	1:A:807:GLU:HB3	1.92	0.50
1:B:53:GLU:HG2	1:B:54:GLU:H	1.75	0.50
1:C:64:ILE:HD13	1:C:76:LEU:HD12	1.93	0.50
1:C:97:ASP:O	1:C:100:SER:HB3	2.12	0.50
1:C:693:PHE:O	1:C:697:SER:N	2.44	0.50
1:D:519:ILE:HD11	1:D:765:GLY:H	1.75	0.50
1:A:528:ASP:OD1	1:A:775:ARG:NH1	2.43	0.50
1:A:614:PHE:HD1	1:A:624:SER:HB3	1.75	0.50
1:A:784:GLN:HA	1:A:787:GLU:CD	2.31	0.50
1:B:495:ASN:HD21	1:B:497:GLN:HB2	1.77	0.50
1:A:36:LEU:O	1:A:77:THR:N	2.44	0.50
1:B:330:VAL:O	1:B:334:VAL:HG23	2.11	0.50
1:B:443:TYR:O	1:B:463:CYS:N	2.43	0.50
1:D:132:THR:O	1:D:150:TYR:HB2	2.11	0.50
1:D:694:PHE:HB3	1:D:706:TRP:HB2	1.93	0.50
1:B:561:PRO:HA	1:B:564:TRP:CD1	2.42	0.50
1:C:96:CYS:CB	1:C:347:CYS:SG	2.98	0.50
1:D:123:ASN:ND2	1:D:143:ASP:HA	2.27	0.50
1:A:339:GLN:CD	1:A:339:GLN:H	2.14	0.50
1:A:443:TYR:HA	1:A:462:TYR:HB3	1.93	0.50
1:C:296:TRP:CD1	1:C:316:MET:SD	3.05	0.50
1:C:286:ASN:OD1	1:C:287:THR:N	2.45	0.50
1:C:337:PHE:CZ	1:C:355:PHE:HB3	2.47	0.50
1:D:53:GLU:HB3	1:D:323:MET:CE	2.41	0.50
1:A:248:MET:HB3	1:A:274:VAL:HG11	1.94	0.50
1:A:300:ARG:NH1	1:A:316:MET:HA	2.26	0.50
1:A:563:ILE:HD12	1:A:563:ILE:H	1.75	0.50
1:C:216:LYS:CE	2:E:102:PHE:CD2	2.87	0.50
1:C:253:HIS:CE1	1:C:275:ASN:HB2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:353:TRP:CG	1:C:354:ARG:N	2.80	0.50
1:A:36:LEU:CB	1:A:76:LEU:HD22	2.35	0.50
1:A:817:VAL:HG23	1:D:654:ASN:ND2	2.27	0.50
1:C:565:MET:HA	1:C:568:LEU:HD12	1.93	0.50
1:C:634:ARG:HD3	1:D:613:TRP:CD2	2.47	0.50
2:E:121:TYR:CE1	2:E:127:PRO:HB3	2.47	0.50
1:B:325:ASP:CG	1:B:371:LEU:H	2.16	0.50
1:C:558:PRO:HG3	1:C:655:LEU:HD13	1.94	0.50
2:E:88:PHE:CZ	2:E:152:PHE:HB2	2.46	0.50
1:A:120:SER:OG	1:B:87:ASP:OD1	2.29	0.49
1:C:41:ILE:HD11	1:C:83:ILE:HG23	1.93	0.49
1:A:53:GLU:O	1:A:323:MET:HE1	2.12	0.49
1:A:732:ASP:N	1:A:732:ASP:OD1	2.43	0.49
1:C:528:ASP:OD1	1:C:775:ARG:NH1	2.46	0.49
1:D:301:LEU:HD23	1:D:301:LEU:H	1.76	0.49
1:A:538:ILE:O	1:A:759:ILE:HG12	2.13	0.49
1:A:775:ARG:O	1:A:778:ILE:HG22	2.12	0.49
1:C:240:LYS:NZ	1:C:308:ASP:O	2.46	0.49
1:A:528:ASP:HB2	1:A:770:MET:HA	1.93	0.49
1:B:797:LYS:HD2	1:B:798:TRP:CE3	2.48	0.49
1:C:739:SER:HB2	1:C:758:LEU:HD11	1.94	0.49
1:C:846:SER:HA	1:C:850:ALA:HB3	1.95	0.49
1:A:235:ALA:O	1:A:239:LEU:HG	2.13	0.49
1:B:443:TYR:CE2	1:B:516:PRO:HG3	2.47	0.49
1:B:453:LEU:O	1:B:458:ARG:HG3	2.11	0.49
1:C:683:GLY:HA3	1:C:733:TYR:CE2	2.47	0.49
1:D:444:VAL:HG22	1:D:464:ILE:HG23	1.93	0.49
2:E:101:ARG:HE	2:E:120:ARG:NH2	2.11	0.49
2:E:132:SER:HB3	2:E:137:MET:HE1	1.94	0.49
1:A:374:ARG:NE	1:A:388:ASP:OD2	2.44	0.49
1:B:61:VAL:HG11	1:B:78:TYR:CD1	2.47	0.49
1:C:211:ALA:CB	1:C:238:ILE:HD11	2.43	0.49
1:A:817:VAL:HG23	1:D:654:ASN:HD22	1.76	0.49
1:B:71:LEU:HD21	1:B:74:THR:HB	1.94	0.49
1:B:195:TYR:HB2	1:B:197:LEU:HD13	1.95	0.49
1:B:593:HIS:CD2	1:B:595:CYS:HB2	2.47	0.49
1:C:129:HIS:CE1	1:C:131:GLN:HE21	2.30	0.49
1:C:516:PRO:HB3	1:C:764:TYR:CZ	2.48	0.49
1:D:325:ASP:O	1:D:329:VAL:HG23	2.13	0.49
2:E:119:ASP:OD1	2:E:120:ARG:N	2.46	0.49
1:A:262:PHE:HB3	1:A:315:PHE:CE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:GLN:HG2	4:B:1004:NAG:H61	1.94	0.49
1:B:738:GLU:O	1:B:742:ILE:HG13	2.13	0.49
1:B:136:HIS:CD2	1:B:183:ILE:HD13	2.47	0.49
1:B:618:ALA:HB3	1:B:640:TRP:NE1	2.28	0.49
1:C:576:CYS:SG	2:E:368:VAL:HG21	2.53	0.49
1:A:37:ARG:NH1	1:A:101:LEU:O	2.46	0.49
1:A:186:GLN:HA	1:A:189:ILE:HD12	1.93	0.49
1:A:516:PRO:HB3	1:A:764:TYR:CE2	2.48	0.49
1:D:306:LYS:HZ2	1:D:308:ASP:H	1.59	0.48
2:E:355:SER:O	2:E:358:VAL:N	2.46	0.48
1:C:536:LEU:HD12	1:C:739:SER:HB3	1.94	0.48
1:D:337:PHE:CE2	1:D:340:MET:HB3	2.48	0.48
1:D:531:LYS:H	1:D:779:THR:HG22	1.78	0.48
1:D:701:THR:HA	1:D:704:LYS:NZ	2.28	0.48
1:A:295:LYS:HA	1:A:298:MET:CE	2.43	0.48
1:A:378:ASN:HB2	3:G:1:NAG:H82	1.89	0.48
1:A:557:ASN:N	1:A:558:PRO:HD2	2.29	0.48
1:B:301:LEU:HD23	1:B:301:LEU:H	1.78	0.48
1:B:442:PRO:HD2	1:B:443:TYR:CD1	2.49	0.48
1:B:443:TYR:CZ	1:B:516:PRO:HG3	2.48	0.48
1:B:558:PRO:HA	1:B:658:PHE:CE2	2.48	0.48
1:C:198:ARG:HG2	1:D:198:ARG:NH2	2.25	0.48
1:A:551:GLY:HA2	1:A:819:ASN:C	2.33	0.48
1:A:568:LEU:O	1:A:572:LEU:HG	2.13	0.48
1:A:677:GLN:NE2	1:A:679:LYS:HB2	2.24	0.48
1:A:702:TYR:OH	1:A:759:ILE:HB	2.13	0.48
1:B:112:SER:OG	1:B:135:LYS:HB2	2.12	0.48
1:B:710:SER:HB2	1:B:713:ARG:HH21	1.78	0.48
1:B:811:GLU:N	1:B:811:GLU:OE2	2.46	0.48
1:C:498:TRP:CE3	1:C:502:VAL:HG11	2.49	0.48
1:C:618:ALA:HB3	1:C:640:TRP:NE1	2.29	0.48
1:C:748:ARG:HD2	1:C:802:ASN:ND2	2.29	0.48
1:D:432:SER:OG	1:D:479:GLU:HB2	2.13	0.48
2:E:130:ILE:O	2:E:131:ARG:NE	2.45	0.48
1:A:231:SER:OG	1:A:234:MET:HG2	2.13	0.48
1:A:622:GLN:HE22	1:D:623:GLY:CA	2.26	0.48
1:B:439:LEU:HD13	1:B:459:PHE:CE1	2.48	0.48
2:E:83:ARG:HG2	2:E:133:THR:HG22	1.96	0.48
1:A:126:GLY:HA2	1:A:145:PHE:HE2	1.78	0.48
1:A:175:VAL:CG1	1:A:204:LEU:HG	2.44	0.48
1:A:670:SER:OG	1:A:671:ALA:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:MET:CE	1:A:717:LEU:HG	2.44	0.48
1:B:232:HIS:O	1:B:235:ALA:N	2.46	0.48
1:C:122:CYS:HB3	1:C:127:VAL:O	2.13	0.48
1:C:443:TYR:HA	1:C:462:TYR:HB3	1.95	0.48
1:A:128:PRO:HA	1:A:145:PHE:HB3	1.96	0.48
1:A:460:GLU:HG3	1:A:798:TRP:HH2	1.79	0.48
1:A:622:GLN:NE2	1:D:623:GLY:CA	2.76	0.48
1:C:70:LEU:HG	1:C:71:LEU:HG	1.94	0.48
1:C:326:ALA:HA	1:C:329:VAL:HG12	1.96	0.48
2:E:83:ARG:N	2:E:159:ILE:O	2.38	0.48
1:B:60:ALA:O	1:B:64:ILE:HG12	2.14	0.48
1:B:83:ILE:HG22	1:B:94:LYS:HG3	1.96	0.48
1:B:439:LEU:HD12	1:B:444:VAL:HG23	1.94	0.48
1:B:595:CYS:SG	1:C:594:PRO:HD3	2.54	0.48
1:C:463:CYS:SG	1:C:516:PRO:HD3	2.54	0.48
1:C:704:LYS:HE3	1:D:700:SER:HB3	1.94	0.48
1:C:713:ARG:C	1:C:714:GLN:HG2	2.32	0.48
1:D:346:GLN:HB2	1:D:349:ARG:HG3	1.95	0.48
1:D:434:ILE:N	1:D:511:ASP:OD2	2.31	0.48
1:A:150:TYR:CD1	1:A:151:PRO:HD2	2.48	0.48
1:A:485:ASP:C	1:A:487:LYS:H	2.17	0.48
1:A:543:ARG:NE	1:A:728:VAL:O	2.30	0.48
1:C:85:LEU:HG	1:C:86:TYR:CD2	2.49	0.48
1:C:169:TRP:CZ2	1:C:253:HIS:HD2	2.32	0.48
1:C:361:SER:O	1:C:365:GLU:HG3	2.13	0.48
1:C:577:VAL:HA	1:C:580:VAL:HG12	1.96	0.48
1:D:160:ILE:O	1:D:164:VAL:HG23	2.14	0.48
1:D:691:MET:HG3	1:D:709:MET:SD	2.54	0.48
2:E:95:GLU:HA	2:E:125:LYS:HE3	1.96	0.48
1:A:634:ARG:HD3	1:B:613:TRP:CD2	2.49	0.48
1:B:681:GLU:OE2	1:B:731:SER:OG	2.32	0.48
1:D:286:ASN:OD1	1:D:287:THR:N	2.47	0.48
1:D:406:ASP:CG	1:D:409:SER:H	2.16	0.48
1:A:281:ILE:HG13	1:A:388:ASP:O	2.14	0.47
1:B:467:LEU:HD13	1:B:514:VAL:HG11	1.96	0.47
1:C:41:ILE:HG21	1:C:109:PRO:HD3	1.96	0.47
1:A:564:TRP:O	1:A:568:LEU:HD23	2.13	0.47
1:B:696:LYS:O	1:B:696:LYS:HG2	2.14	0.47
1:C:286:ASN:HB3	1:C:289:VAL:CG2	2.42	0.47
1:C:601:VAL:HG12	1:C:601:VAL:O	2.14	0.47
1:C:779:THR:O	1:C:783:LEU:HD23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:SER:HA	1:A:115:ALA:HB3	1.96	0.47
1:A:129:HIS:CE1	1:A:131:GLN:HE21	2.33	0.47
1:A:593:HIS:NE2	1:A:595:CYS:HB2	2.29	0.47
1:A:788:GLU:HB3	1:A:790:LYS:HE3	1.96	0.47
1:B:851:GLN:HG3	1:B:852:LEU:H	1.79	0.47
1:C:453:LEU:O	1:C:454:TYR:HD1	1.97	0.47
1:D:211:ALA:HB3	1:D:241:GLN:HG3	1.97	0.47
1:D:346:GLN:HG2	1:D:349:ARG:NH1	2.29	0.47
1:D:675:ALA:O	1:D:676:LYS:HG2	2.14	0.47
1:A:90:GLU:O	1:A:94:LYS:HG2	2.14	0.47
1:B:579:PHE:HB2	1:B:611:SER:OG	2.14	0.47
1:B:686:GLU:HA	1:B:717:LEU:HD22	1.96	0.47
1:C:433:LEU:HD11	1:C:512:LEU:HD13	1.96	0.47
1:C:782:ILE:HG13	1:C:783:LEU:N	2.28	0.47
1:D:469:GLU:O	1:D:473:ILE:HG12	2.14	0.47
1:D:687:ASP:H	1:D:691:MET:HE1	1.79	0.47
1:D:721:ASN:O	1:D:725:ILE:HG23	2.13	0.47
1:A:831:LEU:HD21	1:D:577:VAL:HG21	1.96	0.47
1:B:686:GLU:CG	1:B:717:LEU:HB3	2.45	0.47
1:A:591:ASN:HA	1:A:601:VAL:O	2.13	0.47
1:B:525:LYS:HE3	1:C:780:ILE:HD13	1.95	0.47
1:C:842:PHE:HA	1:C:845:LYS:HZ2	1.78	0.47
2:E:132:SER:HB3	2:E:137:MET:CE	2.44	0.47
1:A:286:ASN:O	1:A:289:VAL:HB	2.15	0.47
1:A:387:PHE:O	1:A:407:PRO:HD3	2.14	0.47
1:A:646:ILE:HD13	1:B:823:ILE:HG12	1.96	0.47
1:A:735:PHE:CE2	1:A:737:MET:HG2	2.50	0.47
1:A:779:THR:O	1:A:783:LEU:HD23	2.14	0.47
1:A:861:MET:O	1:D:584:PHE:HE1	1.98	0.47
1:B:178:ASP:OD1	1:B:180:THR:OG1	2.32	0.47
1:B:507:ASP:HB2	1:B:509:LYS:HD3	1.96	0.47
1:B:619:LEU:HB2	1:B:640:TRP:HZ2	1.78	0.47
1:B:775:ARG:O	1:B:779:THR:HG23	2.15	0.47
1:B:844:TYR:CZ	1:B:848:LYS:HD3	2.50	0.47
1:C:169:TRP:CZ3	1:C:225:HIS:HB3	2.50	0.47
1:C:718:VAL:CG1	1:C:719:LYS:N	2.78	0.47
1:D:57:PHE:O	1:D:61:VAL:HG23	2.15	0.47
1:D:309:SER:OG	1:D:311:LEU:HB2	2.14	0.47
1:D:376:THR:HG21	1:D:386:ASP:HB3	1.95	0.47
1:D:542:TYR:HB3	1:D:755:ILE:HG13	1.97	0.47
1:C:619:LEU:HB2	1:C:640:TRP:HZ2	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:THR:O	1:D:33:THR:CG2	2.61	0.47
1:D:235:ALA:HA	1:D:238:ILE:HG22	1.96	0.47
1:D:443:TYR:CD1	1:D:516:PRO:HG3	2.49	0.47
1:D:677:GLN:CD	1:D:680:ILE:HG12	2.34	0.47
2:E:354:THR:HG22	2:E:354:THR:O	2.15	0.47
1:A:541:LEU:HD21	1:A:742:ILE:HG23	1.96	0.47
1:B:134:TRP:HZ3	1:B:184:ARG:HH21	1.62	0.47
1:B:300:ARG:HH12	1:B:316:MET:HA	1.80	0.47
1:D:40:GLY:H	1:D:98:GLN:HE22	1.62	0.47
1:D:179:SER:C	1:D:181:GLY:N	2.67	0.47
2:E:101:ARG:HE	2:E:120:ARG:NH1	2.13	0.47
1:A:674:LEU:HB3	1:A:682:TYR:CE1	2.50	0.47
1:C:721:ASN:O	1:C:725:ILE:HG12	2.15	0.47
1:D:200:LYS:O	1:D:201:ILE:HG13	2.15	0.47
1:D:237:GLY:O	1:D:241:GLN:HG2	2.15	0.47
1:D:465:ASP:OD1	1:D:466:LEU:N	2.48	0.47
1:D:541:LEU:N	1:D:735:PHE:O	2.42	0.47
2:E:84:ILE:HD11	2:E:135:ARG:C	2.35	0.47
1:A:126:GLY:HA2	1:A:145:PHE:CE2	2.50	0.46
1:A:202:ARG:HB3	1:A:214:LEU:HD11	1.97	0.46
1:A:242:ALA:HB3	1:A:248:MET:HE2	1.96	0.46
1:A:561:PRO:HA	1:A:564:TRP:HD1	1.80	0.46
1:B:54:GLU:HA	1:B:57:PHE:HB3	1.97	0.46
1:B:432:SER:OG	1:B:479:GLU:HB2	2.15	0.46
1:B:574:VAL:HA	1:B:577:VAL:HG12	1.97	0.46
1:B:682:TYR:HA	1:B:734:ALA:HB3	1.97	0.46
1:B:699:ILE:HG13	1:B:700:SER:H	1.79	0.46
1:C:44:TYR:CD1	1:C:82:LYS:HB3	2.50	0.46
1:C:261:LEU:HD12	1:C:264:LEU:HD13	1.97	0.46
1:C:691:MET:SD	1:C:695:LYS:HE2	2.55	0.46
1:D:365:GLU:OE1	1:D:365:GLU:N	2.48	0.46
1:D:556:LEU:HG	1:D:564:TRP:CZ2	2.51	0.46
1:D:754:GLN:NE2	1:D:756:GLY:O	2.36	0.46
1:A:84:ASN:OD1	1:A:85:LEU:N	2.47	0.46
1:A:122:CYS:SG	1:A:129:HIS:HB2	2.55	0.46
1:A:820:ILE:O	1:A:823:ILE:HG12	2.16	0.46
1:B:136:HIS:CG	1:B:183:ILE:HD13	2.50	0.46
1:B:286:ASN:OD1	1:B:287:THR:N	2.48	0.46
1:C:817:VAL:O	1:C:817:VAL:CG1	2.62	0.46
1:D:44:TYR:CD1	1:D:82:LYS:HB3	2.50	0.46
1:D:100:SER:HB2	1:D:346:GLN:HE22	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:ASP:O	1:D:213:PRO:HD2	2.15	0.46
1:A:405:TRP:CH2	1:A:407:PRO:HA	2.50	0.46
1:A:606:PHE:HE1	1:A:626:LEU:HB3	1.75	0.46
1:A:699:ILE:HA	1:D:708:PHE:CE1	2.50	0.46
1:B:394:LEU:HD12	1:B:398:GLY:O	2.14	0.46
1:B:417:GLN:CG	4:B:1004:NAG:C6	2.93	0.46
1:B:443:TYR:HB3	1:B:463:CYS:HB2	1.98	0.46
1:B:502:VAL:O	1:B:506:ILE:HG23	2.15	0.46
1:C:538:ILE:HD12	1:C:760:ASP:HB2	1.97	0.46
1:D:846:SER:O	1:D:850:ALA:N	2.27	0.46
1:A:96:CYS:CB	1:A:347:CYS:SG	3.03	0.46
1:A:153:PHE:CG	1:A:184:ARG:HG3	2.51	0.46
1:A:220:ARG:O	1:A:222:LYS:HE3	2.16	0.46
1:A:232:HIS:NE2	1:A:233:GLU:OE2	2.49	0.46
1:A:283:ASN:O	1:A:289:VAL:HG11	2.14	0.46
1:A:491:GLN:HB2	1:A:498:TRP:CZ3	2.50	0.46
1:A:634:ARG:HD3	1:B:613:TRP:CE3	2.51	0.46
1:A:643:PHE:O	1:A:647:ILE:HG12	2.16	0.46
1:B:433:LEU:HD23	1:B:511:ASP:HB3	1.97	0.46
1:B:512:LEU:HD11	1:B:774:TYR:HB3	1.97	0.46
1:C:286:ASN:ND2	1:C:288:GLN:HB2	2.30	0.46
1:C:347:CYS:O	1:C:350:HIS:HD2	1.98	0.46
1:C:406:ASP:OD1	1:C:409:SER:N	2.41	0.46
1:C:618:ALA:HB3	1:C:640:TRP:HE1	1.79	0.46
1:D:541:LEU:O	1:D:735:PHE:N	2.36	0.46
1:D:822:GLY:O	1:D:826:VAL:HG23	2.15	0.46
1:A:286:ASN:HB3	1:A:289:VAL:HG23	1.97	0.46
1:A:578:LEU:HA	1:A:581:ILE:HG22	1.97	0.46
1:A:685:VAL:HG13	1:A:688:GLY:HA3	1.97	0.46
1:B:64:ILE:HG23	1:B:70:LEU:HD23	1.98	0.46
1:B:222:LYS:HB3	1:B:224:PHE:HE2	1.79	0.46
1:B:239:LEU:HA	1:B:239:LEU:HD23	1.64	0.46
1:C:42:PHE:CE2	1:C:54:GLU:HG3	2.51	0.46
1:C:584:PHE:HE2	1:D:839:VAL:HG12	1.81	0.46
3:I:1:NAG:H4	3:I:2:NAG:H2	1.81	0.46
1:A:431:ARG:HD2	1:A:431:ARG:N	2.31	0.46
1:A:559:LEU:HD23	1:A:559:LEU:HA	1.67	0.46
1:B:473:ILE:HD11	1:B:781:ALA:HB1	1.98	0.46
1:C:283:ASN:O	1:C:289:VAL:HG21	2.16	0.46
1:C:376:THR:HG21	1:C:386:ASP:HB3	1.97	0.46
1:D:437:THR:HG22	1:D:514:VAL:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ASP:HA	1:A:257:THR:HG22	1.96	0.46
1:A:709:MET:HE2	1:A:717:LEU:HG	1.98	0.46
1:A:804:CYS:HB2	1:A:805:PRO:HD3	1.97	0.46
1:B:169:TRP:CZ3	1:B:225:HIS:HB3	2.50	0.46
1:B:288:GLN:O	1:B:292:ILE:HG12	2.16	0.46
1:B:498:TRP:HB3	1:B:502:VAL:HG12	1.97	0.46
1:C:579:PHE:CE2	1:C:606:PHE:HB3	2.51	0.46
1:D:247:MET:HG3	1:D:252:TYR:CE2	2.51	0.46
1:D:693:PHE:O	1:D:697:SER:HB3	2.15	0.46
1:D:770:MET:SD	1:D:770:MET:N	2.88	0.46
1:A:36:LEU:HD22	1:A:340:MET:HE2	1.97	0.46
1:A:389:LEU:HB2	1:A:405:TRP:HB3	1.97	0.46
1:A:682:TYR:HA	1:A:734:ALA:HB3	1.98	0.46
1:A:743:GLU:O	1:A:747:GLN:HG2	2.14	0.46
1:C:140:ASP:HB3	1:C:142:LYS:NZ	2.30	0.46
1:C:566:TYR:HA	1:C:569:LEU:HG	1.96	0.46
1:D:709:MET:HA	1:D:716:VAL:HG21	1.98	0.46
1:D:844:TYR:CE2	1:D:848:LYS:HD2	2.51	0.46
2:E:88:PHE:CE2	2:E:127:PRO:HD2	2.51	0.46
1:A:672:ASP:O	1:A:676:LYS:HG2	2.16	0.46
1:A:691:MET:HE2	1:A:709:MET:HB3	1.97	0.46
1:B:694:PHE:HD2	1:B:706:TRP:HD1	1.64	0.46
1:C:374:ARG:HH21	1:C:388:ASP:CG	2.19	0.46
1:D:470:LEU:HD22	1:D:778:ILE:HD11	1.97	0.46
1:A:186:GLN:HG3	1:A:187:GLU:N	2.31	0.46
1:A:350:HIS:CD2	1:B:93:LYS:NZ	2.83	0.46
1:A:794:MET:O	1:A:798:TRP:HD1	1.99	0.46
1:B:293:ILE:HA	1:B:316:MET:HE2	1.97	0.46
1:B:318:THR:O	1:B:322:LEU:HD23	2.16	0.46
1:B:563:ILE:H	1:B:563:ILE:HD12	1.81	0.46
1:B:589:TRP:HE3	1:B:603:GLU:O	1.98	0.46
1:B:620:MET:O	1:B:622:GLN:N	2.45	0.46
1:B:754:GLN:NE2	1:B:755:ILE:O	2.49	0.46
1:C:534:MET:HE3	1:C:791:LEU:HB2	1.96	0.46
1:C:722:GLU:O	1:C:725:ILE:HB	2.16	0.46
1:D:706:TRP:HA	1:D:709:MET:HG2	1.97	0.46
2:E:66:TYR:HD2	2:E:151:GLY:HA2	1.80	0.46
1:A:42:PHE:O	1:A:44:TYR:HD1	1.98	0.45
1:A:669:ASP:N	1:A:673:ASP:OD2	2.49	0.45
1:B:248:MET:CG	1:B:274:VAL:HG21	2.47	0.45
1:B:432:SER:HA	1:B:477:THR:H	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:526:VAL:HG23	1:B:527:ILE:HG23	1.97	0.45
1:C:625:GLU:HG3	1:C:626:LEU:CD1	2.46	0.45
1:C:810:LYS:O	1:C:810:LYS:HG2	2.15	0.45
1:B:822:GLY:O	1:B:826:VAL:HG23	2.17	0.45
1:D:243:LEU:O	1:D:246:GLY:N	2.38	0.45
1:D:332:VAL:HG11	1:D:366:ALA:CB	2.45	0.45
1:D:462:TYR:HB2	1:D:798:TRP:CD1	2.51	0.45
1:D:491:GLN:HB2	1:D:498:TRP:CZ2	2.52	0.45
1:D:621:GLN:NE2	1:D:648:ILE:HG13	2.31	0.45
2:E:101:ARG:HE	2:E:120:ARG:CZ	2.29	0.45
1:A:132:THR:O	1:A:150:TYR:HB2	2.16	0.45
1:A:692:THR:HA	1:A:695:LYS:HG2	1.98	0.45
1:A:722:GLU:OE1	1:A:722:GLU:N	2.45	0.45
1:C:125:LEU:HD23	1:C:345:LEU:HB3	1.99	0.45
1:C:612:PHE:HD2	1:C:613:TRP:CD2	2.34	0.45
1:D:96:CYS:CB	1:D:347:CYS:SG	3.02	0.45
1:A:261:LEU:O	1:A:264:LEU:HD13	2.15	0.45
1:A:389:LEU:HD23	1:A:389:LEU:HA	1.80	0.45
1:A:779:THR:O	1:A:782:ILE:HG22	2.17	0.45
1:B:230:CYS:HB2	1:B:234:MET:HB3	1.97	0.45
1:B:296:TRP:HE1	1:B:300:ARG:NH1	2.15	0.45
1:C:68:ARG:HA	1:C:68:ARG:NE	2.31	0.45
1:C:591:ASN:HD21	1:C:599:SER:H	1.64	0.45
1:D:555:PHE:C	1:D:557:ASN:H	2.19	0.45
1:B:417:GLN:CG	4:B:1004:NAG:O6	2.47	0.45
1:B:641:TRP:HE3	1:C:620:MET:HG2	1.82	0.45
1:C:159:ALA:HB2	1:C:405:TRP:CH2	2.51	0.45
1:C:595:CYS:SG	1:D:595:CYS:HB2	2.56	0.45
1:C:646:ILE:HD11	1:D:555:PHE:CD1	2.51	0.45
1:D:358:ARG:NH2	1:D:362:LEU:HD11	2.32	0.45
1:A:86:TYR:HH	1:A:111:HIS:CE1	2.28	0.45
1:A:204:LEU:HD23	1:A:214:LEU:HD23	1.98	0.45
1:B:495:ASN:ND2	1:B:497:GLN:HB2	2.31	0.45
1:B:516:PRO:HB3	1:B:764:TYR:CZ	2.52	0.45
1:C:677:GLN:CD	1:C:680:ILE:H	2.19	0.45
1:C:787:GLU:OE1	1:C:788:GLU:HG3	2.17	0.45
1:D:289:VAL:O	1:D:293:ILE:HG13	2.17	0.45
1:A:71:LEU:HB3	1:A:74:THR:HB	1.97	0.45
1:A:113:SER:OG	1:A:114:SER:N	2.50	0.45
1:A:351:LYS:HA	1:A:352:PRO:HD3	1.87	0.45
1:A:548:THR:O	1:A:548:THR:CG2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:563:ILE:HG12	1:B:820:ILE:HD11	1.99	0.45
1:B:293:ILE:HA	1:B:316:MET:CE	2.47	0.45
1:B:585:SER:O	1:B:589:TRP:NE1	2.49	0.45
1:B:674:LEU:HD13	1:B:682:TYR:CE1	2.52	0.45
1:C:434:ILE:HG21	1:C:481:ARG:HE	1.82	0.45
1:D:57:PHE:CE1	1:D:107:LEU:HD12	2.52	0.45
1:D:71:LEU:HD13	1:D:335:GLN:HA	1.98	0.45
1:D:119:GLN:NE2	1:D:146:TYR:CD1	2.85	0.45
1:D:163:LEU:HD21	1:D:277:THR:HG21	1.98	0.45
1:D:684:ALA:HB2	1:D:736:LEU:HB3	1.99	0.45
1:A:88:SER:HA	1:A:114:SER:OG	2.17	0.45
1:A:428:LEU:HB3	1:A:431:ARG:HB2	1.98	0.45
1:A:675:ALA:HA	1:A:705:MET:SD	2.57	0.45
1:B:445:LEU:O	1:B:460:GLU:HG3	2.17	0.45
1:C:464:ILE:H	1:C:464:ILE:HD12	1.82	0.45
1:A:53:GLU:OE1	1:A:53:GLU:N	2.48	0.45
1:A:169:TRP:CE3	1:A:225:HIS:HB3	2.52	0.45
1:A:199:LEU:HD12	1:A:199:LEU:O	2.17	0.45
1:A:337:PHE:CE1	1:A:339:GLN:HB2	2.52	0.45
1:B:36:LEU:HB3	1:B:76:LEU:HD23	1.98	0.45
1:C:110:SER:HB3	1:C:133:ARG:HG3	1.99	0.45
1:C:444:VAL:HA	1:C:464:ILE:CD1	2.47	0.45
1:C:456:ASN:ND2	1:C:478:TYR:O	2.47	0.45
1:D:669:ASP:HB3	1:D:674:LEU:HD11	1.99	0.45
1:D:718:VAL:HG21	1:D:724:GLY:HA2	1.98	0.45
1:D:724:GLY:O	1:D:728:VAL:HG23	2.17	0.45
1:A:63:THR:HG21	1:A:324:TYR:OH	2.16	0.45
1:A:88:SER:O	1:A:91:ALA:N	2.50	0.45
1:A:215:LEU:HD11	1:A:238:ILE:HD11	1.99	0.45
1:A:295:LYS:HA	1:A:298:MET:HE3	1.99	0.45
1:A:500:GLY:O	1:A:504:GLU:HG2	2.16	0.45
1:C:368:TRP:CG	1:C:369:GLU:N	2.84	0.45
1:C:615:GLY:HA2	1:C:640:TRP:NE1	2.31	0.45
1:A:37:ARG:HB3	1:A:103:VAL:HG12	1.99	0.44
1:A:434:ILE:HG23	1:A:510:ALA:HA	2.00	0.44
1:A:620:MET:HA	1:D:645:LEU:HD11	1.98	0.44
1:B:41:ILE:CD1	1:B:81:GLN:HB2	2.47	0.44
1:B:160:ILE:O	1:B:164:VAL:HG23	2.16	0.44
1:B:531:LYS:HA	1:B:531:LYS:HD3	1.84	0.44
1:C:436:THR:OG1	1:C:483:VAL:HG23	2.17	0.44
1:C:439:LEU:HD21	1:C:459:PHE:HE1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:505:LEU:HD11	1:C:769:PRO:HD3	1.99	0.44
1:C:683:GLY:C	1:C:735:PHE:HA	2.38	0.44
1:C:825:ILE:O	1:C:825:ILE:HG22	2.16	0.44
1:C:828:ALA:O	1:C:831:LEU:HG	2.17	0.44
1:A:550:PRO:CB	1:A:553:PHE:HB2	2.46	0.44
1:A:685:VAL:HA	1:A:718:VAL:O	2.17	0.44
1:B:795:LYS:HD2	1:B:799:TRP:NE1	2.32	0.44
1:C:55:LEU:HD23	1:C:296:TRP:CH2	2.53	0.44
1:C:254:TYR:HB3	1:C:256:PHE:CE1	2.52	0.44
1:C:778:ILE:O	1:C:782:ILE:HG23	2.17	0.44
1:D:36:LEU:HD12	1:D:37:ARG:H	1.81	0.44
2:E:101:ARG:HH21	2:E:120:ARG:HH12	1.64	0.44
2:E:110:GLY:C	2:E:138:TRP:CD1	2.91	0.44
1:A:296:TRP:CD1	1:A:300:ARG:HB2	2.53	0.44
1:A:316:MET:SD	1:A:320:ALA:HB3	2.56	0.44
1:B:124:ALA:C	1:B:125:LEU:HD12	2.37	0.44
1:C:282:LEU:HD11	1:C:371:LEU:HB3	1.98	0.44
1:C:721:ASN:HA	1:C:735:PHE:CE2	2.52	0.44
1:A:50:MET:SD	1:A:55:LEU:HG	2.57	0.44
1:B:389:LEU:O	1:B:405:TRP:N	2.49	0.44
1:B:645:LEU:HD11	1:C:621:GLN:HB3	1.99	0.44
1:C:123:ASN:HA	1:C:145:PHE:HD2	1.82	0.44
1:C:745:VAL:O	1:C:749:ASN:HB2	2.18	0.44
2:E:367:LEU:O	2:E:371:LYS:HG3	2.17	0.44
1:A:261:LEU:HD22	1:A:278:GLY:HA3	2.00	0.44
1:A:712:ARG:O	1:A:715:SER:OG	2.27	0.44
1:B:128:PRO:HG2	1:B:359:PHE:CD2	2.53	0.44
1:B:538:ILE:HG22	1:B:759:ILE:HD12	1.98	0.44
1:C:447:LYS:HG3	1:C:459:PHE:C	2.38	0.44
1:C:561:PRO:HA	1:C:564:TRP:CD1	2.39	0.44
1:D:563:ILE:O	1:D:567:VAL:HG23	2.17	0.44
1:D:616:VAL:O	1:D:619:LEU:HB3	2.18	0.44
1:A:325:ASP:OD1	1:A:371:LEU:N	2.50	0.44
1:A:495:ASN:OD1	1:A:497:GLN:HB3	2.16	0.44
1:A:717:LEU:HD23	1:A:717:LEU:HA	1.90	0.44
1:B:417:GLN:CG	4:B:1004:NAG:H61	2.47	0.44
1:C:99:LEU:HD23	1:C:99:LEU:HA	1.71	0.44
1:C:420:LYS:HG3	1:C:422:ALA:H	1.82	0.44
1:D:471:SER:CB	1:D:476:PHE:HB2	2.47	0.44
1:A:699:ILE:HD13	1:A:702:TYR:HD2	1.82	0.44
1:B:129:HIS:O	1:B:146:TYR:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:LEU:HA	1:B:411:LEU:HD11	2.00	0.44
1:C:434:ILE:HG21	1:C:481:ARG:HH21	1.83	0.44
1:C:579:PHE:CE1	1:C:583:ARG:HG2	2.52	0.44
1:D:728:VAL:HA	1:D:733:TYR:HB3	1.99	0.44
1:A:462:TYR:HD1	1:A:794:MET:HB3	1.83	0.44
1:B:128:PRO:HG2	1:B:359:PHE:CE2	2.53	0.44
1:B:442:PRO:O	1:B:462:TYR:HB3	2.18	0.44
1:C:81:GLN:HG2	1:C:98:GLN:HE21	1.83	0.44
1:C:186:GLN:HA	1:C:189:ILE:HD12	2.00	0.44
1:C:847:LYS:HB3	1:C:848:LYS:HZ3	1.82	0.44
1:D:280:ARG:NH1	1:D:284:THR:OG1	2.50	0.44
1:D:462:TYR:HB2	1:D:798:TRP:CG	2.53	0.44
1:D:522:VAL:O	1:D:525:LYS:HG2	2.17	0.44
2:E:159:ILE:HG13	2:E:159:ILE:O	2.18	0.44
1:A:825:ILE:HD12	1:A:825:ILE:H	1.83	0.44
1:A:851:GLN:HG3	1:A:852:LEU:H	1.83	0.44
1:B:108:GLY:N	1:B:130:ILE:O	2.51	0.44
1:B:161:LEU:HD12	1:B:161:LEU:HA	1.83	0.44
1:B:607:THR:N	1:B:610:ASN:HB2	2.33	0.44
1:B:635:ILE:O	1:B:639:ILE:HG12	2.18	0.44
1:B:775:ARG:O	1:B:778:ILE:HG22	2.17	0.44
1:D:40:GLY:H	1:D:98:GLN:NE2	2.15	0.44
2:E:49:VAL:HB	2:E:156:TYR:OH	2.17	0.44
1:A:434:ILE:HD11	1:A:481:ARG:HD2	2.00	0.43
1:A:656:ALA:HA	1:D:653:ALA:HB1	2.00	0.43
1:A:832:VAL:HG23	1:A:833:LEU:HD22	1.98	0.43
1:B:71:LEU:HD11	1:B:74:THR:HB	1.99	0.43
1:B:369:GLU:HA	1:B:373:GLY:O	2.18	0.43
1:D:40:GLY:O	1:D:98:GLN:NE2	2.44	0.43
1:D:498:TRP:HB3	1:D:502:VAL:HB	1.99	0.43
2:E:58:ALA:HB2	2:E:153:ARG:HD2	2.00	0.43
1:B:505:LEU:HD21	1:B:768:THR:N	2.34	0.43
1:B:640:TRP:HZ3	1:B:643:PHE:HD2	1.65	0.43
1:B:710:SER:HB2	1:B:713:ARG:NH2	2.33	0.43
1:C:683:GLY:HA3	1:C:733:TYR:CZ	2.53	0.43
1:C:795:LYS:HD2	1:C:799:TRP:CZ3	2.53	0.43
1:D:395:LYS:HG3	1:D:400:GLU:OE1	2.18	0.43
1:A:290:SER:O	1:A:293:ILE:HB	2.18	0.43
1:A:296:TRP:CD1	1:A:316:MET:HB2	2.53	0.43
1:A:747:GLN:OE1	1:A:803:GLY:HA3	2.19	0.43
1:B:643:PHE:O	1:B:647:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:703:ASP:OD1	1:B:703:ASP:N	2.52	0.43
1:C:61:VAL:O	1:C:64:ILE:HB	2.18	0.43
1:C:129:HIS:O	1:C:146:TYR:HA	2.18	0.43
1:C:181:GLY:O	1:C:184:ARG:HG2	2.18	0.43
1:C:495:ASN:OD1	1:C:495:ASN:N	2.51	0.43
1:C:574:VAL:HG21	1:C:640:TRP:CE3	2.53	0.43
1:C:832:VAL:O	1:C:835:VAL:HG12	2.17	0.43
1:D:306:LYS:NZ	1:D:308:ASP:H	2.17	0.43
1:D:471:SER:HB2	1:D:476:PHE:HB2	1.99	0.43
1:A:341:THR:OG1	1:A:354:ARG:HD3	2.19	0.43
1:B:836:PHE:O	1:B:839:VAL:HG12	2.18	0.43
1:D:492:ASP:O	1:D:496:GLY:N	2.49	0.43
1:D:502:VAL:HG22	1:D:527:ILE:HD11	2.00	0.43
1:D:655:LEU:HD12	1:D:655:LEU:HA	1.80	0.43
1:D:682:TYR:HB3	1:D:734:ALA:HB3	2.00	0.43
1:D:690:THR:OG1	1:D:691:MET:N	2.52	0.43
2:E:125:LYS:HA	2:E:125:LYS:HE2	2.00	0.43
1:A:541:LEU:HD12	1:A:735:PHE:HD2	1.82	0.43
1:B:250:GLU:OE1	1:B:250:GLU:N	2.43	0.43
1:B:523:ARG:O	1:B:527:ILE:HG12	2.17	0.43
1:C:578:LEU:HD13	1:C:636:VAL:HB	2.00	0.43
1:C:716:VAL:HB	1:C:733:TYR:HE1	1.83	0.43
1:D:238:ILE:HG23	1:D:239:LEU:HD22	2.00	0.43
1:D:645:LEU:HD23	1:D:645:LEU:HA	1.90	0.43
1:D:844:TYR:OH	1:D:848:LYS:NZ	2.36	0.43
2:E:140:LYS:HZ2	2:E:142:SER:HB2	1.83	0.43
1:C:443:TYR:HB3	1:C:463:CYS:SG	2.59	0.43
1:C:538:ILE:HB	1:C:759:ILE:HB	1.99	0.43
1:C:634:ARG:NH1	1:D:609:LEU:HG	2.33	0.43
1:D:81:GLN:HB3	1:D:94:LYS:HZ2	1.81	0.43
1:D:228:PHE:CE1	1:D:238:ILE:HG12	2.54	0.43
1:D:231:SER:O	1:D:233:GLU:N	2.51	0.43
1:D:434:ILE:HG23	1:D:479:GLU:OE1	2.18	0.43
1:D:683:GLY:N	1:D:734:ALA:O	2.51	0.43
1:C:42:PHE:CD2	1:C:54:GLU:HG3	2.53	0.43
1:C:469:GLU:HA	1:C:472:THR:OG1	2.19	0.43
1:C:695:LYS:HA	1:C:706:TRP:CD1	2.53	0.43
1:C:701:THR:OG1	1:C:702:TYR:N	2.52	0.43
1:D:126:GLY:HA2	1:D:145:PHE:HE2	1.80	0.43
1:D:144:SER:O	1:D:364:LYS:NZ	2.51	0.43
1:D:489:GLY:HA3	1:D:502:VAL:CG2	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:GLU:HG2	1:A:529:PHE:HD2	1.83	0.43
1:B:284:THR:HA	1:B:289:VAL:HG11	2.00	0.43
1:B:358:ARG:CZ	1:B:362:LEU:HD21	2.48	0.43
1:C:216:LYS:HD3	2:E:146:GLU:OE2	2.19	0.43
1:D:541:LEU:HB2	1:D:742:ILE:HD12	2.01	0.43
2:E:67:PRO:HB2	2:E:70:LYS:HG3	2.00	0.43
1:A:110:SER:HB3	1:A:133:ARG:HG3	2.00	0.43
1:A:320:ALA:HA	1:A:323:MET:HG3	2.01	0.43
1:A:420:LYS:HD3	1:A:420:LYS:HA	1.83	0.43
1:A:712:ARG:HB3	1:A:715:SER:HB2	2.01	0.43
1:B:38:PHE:CE1	1:B:104:ALA:HB3	2.54	0.43
1:B:55:LEU:HB3	1:B:296:TRP:HH2	1.83	0.43
1:B:711:SER:OG	1:B:712:ARG:N	2.52	0.43
1:C:332:VAL:HG21	1:C:368:TRP:CE3	2.54	0.43
1:C:394:LEU:HA	1:C:399:LEU:HD23	2.00	0.43
1:C:724:GLY:O	1:C:728:VAL:HG23	2.19	0.43
1:A:348:ASN:HA	1:A:350:HIS:HE1	1.82	0.43
1:B:387:PHE:HE2	1:B:389:LEU:HD11	1.83	0.43
1:B:438:ILE:HG22	1:B:515:ALA:HB1	2.01	0.43
1:B:564:TRP:O	1:B:568:LEU:HD23	2.19	0.43
1:B:692:THR:HA	1:B:695:LYS:NZ	2.33	0.43
1:C:65:ASN:OD1	1:C:75:THR:HG23	2.19	0.43
1:D:386:ASP:OD1	1:D:387:PHE:N	2.52	0.43
1:D:540:ILE:O	1:D:755:ILE:HB	2.19	0.43
2:E:88:PHE:HZ	2:E:152:PHE:HB2	1.84	0.43
1:A:296:TRP:CD1	1:A:300:ARG:HD2	2.54	0.42
1:A:654:ASN:HD22	1:B:815:LEU:HD12	1.84	0.42
1:B:462:TYR:O	1:B:465:ASP:HB2	2.19	0.42
1:B:474:LEU:HD13	1:B:777:LYS:HE3	2.01	0.42
1:B:555:PHE:CE1	1:B:556:LEU:HD22	2.54	0.42
1:D:556:LEU:HA	1:D:564:TRP:CZ2	2.53	0.42
1:A:140:ASP:HB2	1:B:86:TYR:CE1	2.53	0.42
1:A:784:GLN:HA	1:A:787:GLU:OE2	2.18	0.42
1:B:185:LEU:O	1:B:189:ILE:HG13	2.19	0.42
1:B:595:CYS:HB3	1:C:593:HIS:ND1	2.34	0.42
1:C:38:PHE:CD1	1:C:104:ALA:HB3	2.54	0.42
1:C:266:VAL:HG21	1:C:399:LEU:HD11	2.01	0.42
1:C:560:SER:C	1:C:562:ASP:H	2.22	0.42
1:C:804:CYS:HB3	1:C:805:PRO:HD3	2.01	0.42
2:E:57:PHE:CE1	2:E:74:TYR:CG	3.07	0.42
1:A:669:ASP:O	1:A:755:ILE:HD12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:ASN:ND2	1:B:288:GLN:HB2	2.34	0.42
1:B:618:ALA:HB3	1:B:640:TRP:HE1	1.84	0.42
1:C:718:VAL:HG11	1:C:723:GLU:HB3	2.01	0.42
1:D:167:PHE:CE2	1:D:253:HIS:CE1	3.06	0.42
1:D:589:TRP:CE3	1:D:604:ASN:HB3	2.54	0.42
1:D:683:GLY:HA3	1:D:733:TYR:CE1	2.53	0.42
1:A:443:TYR:HD1	1:A:462:TYR:HD2	1.68	0.42
1:B:149:LEU:HB3	1:B:322:LEU:HD12	2.01	0.42
1:B:247:MET:O	1:B:247:MET:HG3	2.19	0.42
1:B:536:LEU:HD21	1:B:764:TYR:CE2	2.54	0.42
1:B:554:SER:HB3	1:B:819:ASN:O	2.19	0.42
1:C:248:MET:CE	1:C:274:VAL:HG11	2.47	0.42
1:D:169:TRP:CE2	1:D:225:HIS:ND1	2.88	0.42
1:A:94:LYS:HA	1:A:97:ASP:OD2	2.19	0.42
1:A:140:ASP:HB2	1:B:86:TYR:CE2	2.51	0.42
1:A:621:GLN:HG3	1:D:621:GLN:CG	2.49	0.42
1:A:692:THR:O	1:A:695:LYS:HG2	2.20	0.42
1:B:72:PRO:HD3	1:B:335:GLN:NE2	2.34	0.42
1:B:395:LYS:HB2	1:B:400:GLU:OE2	2.20	0.42
1:B:483:VAL:HB	1:B:501:MET:CE	2.49	0.42
1:B:618:ALA:HB1	1:B:641:TRP:CD1	2.54	0.42
1:B:681:GLU:H	1:B:681:GLU:CD	2.23	0.42
1:C:64:ILE:HD11	1:C:327:VAL:HG12	2.00	0.42
1:C:574:VAL:HG11	1:C:640:TRP:CD2	2.55	0.42
1:D:67:ASN:O	1:D:69:THR:N	2.53	0.42
1:D:166:PHE:O	1:D:168:LYS:HG3	2.19	0.42
1:D:397:GLU:OE1	1:D:397:GLU:N	2.36	0.42
1:A:99:LEU:HG	1:A:345:LEU:O	2.19	0.42
1:A:738:GLU:H	1:A:738:GLU:CD	2.23	0.42
1:B:368:TRP:NE1	1:B:369:GLU:O	2.53	0.42
1:B:451:LYS:H	1:B:451:LYS:HD2	1.84	0.42
1:D:230:CYS:O	1:D:258:THR:HB	2.20	0.42
1:D:249:THR:O	1:D:274:VAL:HG22	2.19	0.42
1:D:265:ASP:N	1:D:310:GLY:O	2.51	0.42
1:A:262:PHE:HA	1:A:399:LEU:CD2	2.49	0.42
1:A:325:ASP:CG	1:A:371:LEU:H	2.22	0.42
1:A:559:LEU:O	1:A:564:TRP:NE1	2.52	0.42
1:B:33:THR:O	1:B:33:THR:CG2	2.67	0.42
1:B:260:ASP:OD1	1:B:318:THR:OG1	2.34	0.42
1:B:710:SER:CB	1:B:713:ARG:HH21	2.32	0.42
1:B:743:GLU:HA	1:B:746:THR:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:HIS:ND1	1:C:275:ASN:HB2	2.34	0.42
1:C:270:ARG:NH1	1:C:397:GLU:HA	2.33	0.42
1:C:349:ARG:NH1	1:C:351:LYS:O	2.52	0.42
1:C:677:GLN:OE1	1:C:680:ILE:N	2.51	0.42
1:C:686:GLU:HG2	1:C:719:LYS:NZ	2.34	0.42
2:E:65:SER:HA	2:E:149:GLY:O	2.20	0.42
1:A:119:GLN:OE1	1:A:135:LYS:HE2	2.19	0.42
1:A:336:GLN:C	1:A:338:PRO:HD3	2.40	0.42
1:A:391:VAL:HG22	1:A:402:ILE:HD11	2.02	0.42
1:A:505:LEU:HD12	1:A:505:LEU:HA	1.88	0.42
1:A:585:SER:O	1:A:588:GLU:HG3	2.19	0.42
1:A:618:ALA:O	1:A:644:THR:HG21	2.20	0.42
1:B:106:ILE:HG23	1:B:129:HIS:HD2	1.85	0.42
1:B:266:VAL:HG11	1:B:394:LEU:HD21	2.02	0.42
1:B:300:ARG:HH22	1:B:317:THR:N	2.17	0.42
1:B:434:ILE:HG13	1:B:511:ASP:OD2	2.18	0.42
1:C:36:LEU:HB3	1:C:76:LEU:HD22	2.02	0.42
1:C:37:ARG:HB2	1:C:103:VAL:HA	2.02	0.42
1:C:411:LEU:HA	1:C:411:LEU:HD23	1.93	0.42
1:D:443:TYR:OH	1:D:740:THR:HG21	2.19	0.42
1:A:57:PHE:HE2	1:A:78:TYR:CD2	2.38	0.42
1:A:157:SER:OG	1:A:187:GLU:HB3	2.20	0.42
1:A:544:LYS:HG2	1:A:753:THR:HB	2.01	0.42
1:A:793:MET:HE2	1:A:793:MET:N	2.35	0.42
1:B:616:VAL:O	1:B:619:LEU:HB3	2.19	0.42
1:C:625:GLU:HG3	1:C:626:LEU:HD13	2.01	0.42
1:D:239:LEU:HD13	1:D:239:LEU:HA	1.84	0.42
1:D:558:PRO:HB2	1:D:654:ASN:HB3	2.02	0.42
1:A:281:ILE:HG12	1:A:372:THR:HB	2.01	0.42
1:B:467:LEU:HD12	1:B:467:LEU:HA	1.82	0.42
1:B:591:ASN:OD1	1:B:594:PRO:HG3	2.19	0.42
1:B:712:ARG:CZ	1:B:716:VAL:HG23	2.49	0.42
1:B:831:LEU:O	1:B:834:SER:OG	2.26	0.42
1:C:790:LYS:HD2	1:C:790:LYS:HA	1.77	0.42
1:C:866:ARG:HA	1:C:866:ARG:HD3	1.85	0.42
1:D:506:ILE:HG22	1:D:507:ASP:OD1	2.20	0.42
1:D:718:VAL:HG22	1:D:723:GLU:HG3	2.02	0.42
2:E:112:PHE:CZ	2:E:140:LYS:HB2	2.55	0.42
1:B:778:ILE:O	1:B:782:ILE:HG13	2.20	0.41
1:C:235:ALA:O	1:C:238:ILE:HG22	2.20	0.41
1:C:563:ILE:O	1:C:566:TYR:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:LEU:HD22	1:D:340:MET:HE3	2.01	0.41
1:D:38:PHE:H	1:D:78:TYR:HA	1.85	0.41
1:D:344:SER:O	1:D:345:LEU:HD23	2.20	0.41
1:D:681:GLU:HG2	1:D:716:VAL:HG12	2.02	0.41
2:E:59:SER:HB3	2:E:152:PHE:CD2	2.54	0.41
1:A:129:HIS:O	1:A:130:ILE:HD13	2.20	0.41
1:A:433:LEU:HD11	1:A:476:PHE:CG	2.55	0.41
1:A:810:LYS:HD3	1:A:810:LYS:HA	1.90	0.41
1:B:205:PRO:HD3	1:B:214:LEU:CD1	2.49	0.41
1:B:695:LYS:HB3	1:B:706:TRP:CE2	2.55	0.41
1:D:629:LYS:HA	1:D:634:ARG:HH21	1.85	0.41
1:A:238:ILE:HD12	1:A:241:GLN:HG3	2.02	0.41
1:A:762:LYS:HB3	1:A:762:LYS:HE2	1.80	0.41
1:B:126:GLY:HA2	1:B:145:PHE:HE2	1.85	0.41
1:B:270:ARG:NH1	1:B:397:GLU:HA	2.35	0.41
1:B:688:GLY:O	1:B:692:THR:HG23	2.20	0.41
1:C:296:TRP:O	1:C:300:ARG:CB	2.68	0.41
1:C:490:ALA:H	1:C:499:ASN:HB2	1.85	0.41
1:C:504:GLU:OE1	1:C:509:LYS:HE3	2.20	0.41
1:C:617:GLY:HA2	1:C:620:MET:HB3	2.02	0.41
1:C:829:ALA:HA	1:C:832:VAL:HG22	2.02	0.41
1:D:596:ASN:HA	1:D:597:PRO:HD3	1.93	0.41
1:D:702:TYR:OH	1:D:759:ILE:HD12	2.20	0.41
1:D:711:SER:OG	1:D:712:ARG:HG3	2.21	0.41
2:E:71:GLU:HA	2:E:140:LYS:HE2	2.02	0.41
2:E:155:LYS:NZ	2:E:157:SER:OG	2.53	0.41
1:A:716:VAL:HA	1:A:727:ARG:NH2	2.35	0.41
1:B:157:SER:CB	1:B:187:GLU:HB2	2.50	0.41
1:B:358:ARG:NH1	1:B:362:LEU:HD21	2.35	0.41
1:B:546:ASN:ND2	4:B:1002:NAG:O7	2.53	0.41
1:C:337:PHE:HZ	1:C:355:PHE:HB3	1.84	0.41
1:C:420:LYS:HG2	1:C:424:ILE:O	2.21	0.41
1:C:498:TRP:HB3	1:C:502:VAL:HB	2.03	0.41
1:C:820:ILE:H	1:C:820:ILE:HG12	1.62	0.41
1:D:213:PRO:O	1:D:217:GLU:HG2	2.20	0.41
1:D:438:ILE:HD12	1:D:438:ILE:HA	1.92	0.41
1:D:445:LEU:HD12	1:D:460:GLU:HB3	2.03	0.41
1:D:797:LYS:NZ	1:D:798:TRP:HE1	2.18	0.41
1:A:467:LEU:O	1:A:470:LEU:HG	2.20	0.41
1:A:543:ARG:HD3	1:A:729:LEU:HA	2.03	0.41
1:B:57:PHE:HB2	1:B:323:MET:HE1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:465:ASP:O	1:B:468:ARG:NH2	2.54	0.41
1:C:345:LEU:HD21	1:C:353:TRP:CD1	2.55	0.41
1:C:451:LYS:HA	1:C:452:PRO:HD3	1.93	0.41
1:C:579:PHE:HD2	1:C:611:SER:CB	2.34	0.41
1:C:750:CYS:HB3	4:C:1001:NAG:N2	2.36	0.41
1:D:536:LEU:HD22	1:D:762:LYS:HG3	2.03	0.41
2:E:111:PRO:HA	2:E:138:TRP:CD1	2.54	0.41
1:A:558:PRO:HB3	1:A:654:ASN:OD1	2.21	0.41
1:A:574:VAL:HG11	1:A:640:TRP:CZ3	2.55	0.41
1:B:208:THR:O	1:B:211:ALA:N	2.52	0.41
1:B:343:SER:OG	1:B:354:ARG:NH1	2.53	0.41
1:C:129:HIS:HD2	1:C:130:ILE:N	2.19	0.41
1:C:183:ILE:CD1	1:D:183:ILE:HD11	2.49	0.41
1:C:323:MET:O	1:C:327:VAL:HG23	2.21	0.41
1:D:254:TYR:CD1	1:D:254:TYR:N	2.87	0.41
1:D:560:SER:HB3	1:D:563:ILE:HD13	2.03	0.41
1:D:575:SER:HB3	1:D:612:PHE:HD1	1.85	0.41
1:A:474:LEU:HD23	1:A:474:LEU:HA	1.86	0.41
1:B:57:PHE:HB2	1:B:323:MET:CE	2.51	0.41
1:B:724:GLY:O	1:B:728:VAL:HG12	2.21	0.41
1:B:815:LEU:HD23	1:B:815:LEU:HA	1.91	0.41
1:C:68:ARG:HE	1:C:72:PRO:HA	1.85	0.41
1:D:85:LEU:HB2	1:D:86:TYR:CD2	2.56	0.41
1:D:170:LYS:HE2	1:D:170:LYS:HA	2.03	0.41
1:D:224:PHE:HE1	1:D:251:TYR:HB3	1.84	0.41
1:D:780:ILE:HD11	2:E:134:GLY:HA3	2.03	0.41
1:A:142:LYS:HD3	1:A:142:LYS:HA	1.83	0.41
1:A:324:TYR:CZ	1:A:328:HIS:NE2	2.89	0.41
1:B:750:CYS:SG	1:B:751:ASN:N	2.94	0.41
1:C:172:VAL:HG22	1:C:173:THR:H	1.86	0.41
1:C:253:HIS:HD1	1:C:275:ASN:HB2	1.85	0.41
1:D:42:PHE:CG	1:D:54:GLU:HB2	2.56	0.41
1:A:376:THR:OG1	1:A:377:PHE:N	2.53	0.41
1:A:451:LYS:HA	1:A:452:PRO:HD3	1.96	0.41
1:A:613:TRP:CZ3	1:D:634:ARG:HB3	2.56	0.41
1:A:737:MET:SD	1:A:742:ILE:HG13	2.61	0.41
1:A:858:CYS:O	1:A:862:VAL:HG23	2.21	0.41
1:B:295:LYS:HA	1:B:298:MET:CE	2.51	0.41
1:B:537:GLY:HA3	1:B:758:LEU:HD22	2.03	0.41
1:B:719:LYS:N	1:B:723:GLU:OE2	2.43	0.41
1:B:793:MET:SD	1:B:794:MET:N	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:THR:HB	1:C:75:THR:HB	2.03	0.41
1:C:70:LEU:HD21	1:C:331:SER:CB	2.48	0.41
1:C:145:PHE:HD1	1:C:145:PHE:HA	1.75	0.41
1:C:453:LEU:O	1:C:458:ARG:HB3	2.21	0.41
1:C:563:ILE:HD11	1:D:817:VAL:N	2.35	0.41
1:C:627:MET:HE1	1:C:628:PRO:O	2.20	0.41
1:C:682:TYR:HA	1:C:734:ALA:HB3	2.03	0.41
1:C:751:ASN:O	1:C:752:LEU:HD23	2.20	0.41
1:C:775:ARG:O	1:C:778:ILE:HG22	2.21	0.41
1:C:791:LEU:HD12	1:C:792:HIS:N	2.35	0.41
1:D:35:VAL:HA	1:D:75:THR:O	2.21	0.41
1:D:212:LYS:HG2	1:D:245:MET:CE	2.50	0.41
1:D:533:PHE:CZ	1:D:764:TYR:HB3	2.56	0.41
1:D:607:THR:H	1:D:610:ASN:CB	2.27	0.41
1:D:627:MET:SD	1:D:627:MET:N	2.94	0.41
1:D:718:VAL:CG2	1:D:723:GLU:HG3	2.51	0.41
2:E:142:SER:OG	2:E:143:SER:N	2.53	0.41
1:A:161:LEU:CD1	1:A:187:GLU:HG3	2.51	0.41
1:A:378:ASN:CA	3:G:1:NAG:C8	2.99	0.41
1:A:783:LEU:O	1:A:786:GLN:HB3	2.20	0.41
1:B:289:VAL:O	1:B:293:ILE:HG13	2.21	0.41
1:B:325:ASP:OD2	1:B:371:LEU:N	2.51	0.41
1:B:590:TYR:CE2	1:B:592:PRO:HG3	2.56	0.41
1:C:172:VAL:HG22	1:C:173:THR:N	2.36	0.41
1:C:349:ARG:HH11	1:C:351:LYS:CB	2.33	0.41
1:C:683:GLY:O	1:C:736:LEU:N	2.50	0.41
2:E:101:ARG:HA	2:E:120:ARG:NH2	2.33	0.41
1:A:788:GLU:O	1:A:790:LYS:N	2.54	0.40
1:B:71:LEU:H	1:B:335:GLN:NE2	2.18	0.40
1:B:531:LYS:HA	1:C:531:LYS:HZ1	1.86	0.40
1:B:831:LEU:O	1:B:835:VAL:HG23	2.21	0.40
1:C:169:TRP:HZ2	1:C:253:HIS:HD2	1.69	0.40
1:D:85:LEU:HD13	1:D:86:TYR:CD2	2.55	0.40
1:D:153:PHE:CD1	1:D:156:LEU:HD12	2.56	0.40
2:E:84:ILE:HG23	2:E:158:PHE:CE1	2.52	0.40
1:A:460:GLU:OE2	1:A:798:TRP:HZ2	2.04	0.40
1:A:491:GLN:OE1	1:A:497:GLN:N	2.54	0.40
1:B:531:LYS:HZ3	1:C:531:LYS:HA	1.86	0.40
1:C:522:VAL:O	1:C:525:LYS:HB2	2.21	0.40
1:D:228:PHE:HE2	1:D:254:TYR:CD2	2.37	0.40
1:D:434:ILE:HD12	1:D:511:ASP:OD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:555:PHE:CE2	1:D:823:ILE:HG12	2.56	0.40
1:B:98:GLN:O	1:B:102:GLY:N	2.54	0.40
1:B:224:PHE:O	1:B:225:HIS:CG	2.74	0.40
1:C:561:PRO:CA	1:C:564:TRP:HD1	2.28	0.40
1:D:229:ASP:HA	1:D:257:THR:HG22	2.02	0.40
1:D:231:SER:O	1:D:234:MET:N	2.40	0.40
1:D:274:VAL:HG12	1:D:275:ASN:N	2.36	0.40
1:D:563:ILE:HD12	1:D:563:ILE:H	1.86	0.40
1:D:699:ILE:HD13	1:D:702:TYR:CD2	2.56	0.40
1:A:289:VAL:O	1:A:293:ILE:HG13	2.22	0.40
1:A:353:TRP:CZ2	1:A:355:PHE:HB2	2.56	0.40
1:A:551:GLY:HA2	1:A:819:ASN:O	2.21	0.40
1:A:628:PRO:HB3	1:A:633:THR:CG2	2.51	0.40
1:B:57:PHE:O	1:B:61:VAL:HG23	2.21	0.40
1:B:297:SER:O	1:B:301:LEU:HD22	2.21	0.40
1:C:81:GLN:HG2	1:C:98:GLN:NE2	2.36	0.40
1:C:134:TRP:NE1	1:C:135:LYS:O	2.55	0.40
1:C:176:TYR:CE1	1:C:203:GLN:HG3	2.56	0.40
1:C:591:ASN:HD21	1:C:599:SER:N	2.18	0.40
1:C:660:THR:O	1:C:664:MET:HG3	2.21	0.40
1:C:851:GLN:O	1:C:852:LEU:HG	2.21	0.40
1:A:433:LEU:HA	1:A:511:ASP:OD2	2.21	0.40
1:A:682:TYR:CZ	1:A:705:MET:SD	3.15	0.40
1:B:70:LEU:HD12	1:B:335:GLN:OE1	2.22	0.40
1:B:341:THR:O	1:B:354:ARG:NH2	2.54	0.40
1:B:406:ASP:OD1	1:B:409:SER:N	2.32	0.40
1:B:441:GLU:HB3	1:B:442:PRO:HD3	2.04	0.40
1:B:443:TYR:HA	1:B:462:TYR:HB3	2.03	0.40
1:B:581:ILE:HG22	1:B:633:THR:HG22	2.04	0.40
1:C:65:ASN:CG	1:C:75:THR:HG23	2.41	0.40
1:C:169:TRP:HZ2	1:C:253:HIS:CD2	2.40	0.40
1:C:259:LEU:O	1:C:261:LEU:N	2.55	0.40
1:C:328:HIS:O	1:C:332:VAL:HG23	2.20	0.40
1:C:681:GLU:HG2	1:C:716:VAL:HG11	2.04	0.40
1:C:712:ARG:HA	1:C:712:ARG:HD3	1.80	0.40
1:D:622:GLN:OE1	1:D:622:GLN:N	2.55	0.40
1:D:675:ALA:C	1:D:677:GLN:H	2.24	0.40
2:E:55:GLY:O	2:E:155:LYS:HD2	2.22	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	829/908 (91%)	757 (91%)	72 (9%)	0	100	100
1	B	829/908 (91%)	736 (89%)	93 (11%)	0	100	100
1	C	833/908 (92%)	754 (90%)	79 (10%)	0	100	100
1	D	816/908 (90%)	706 (86%)	110 (14%)	0	100	100
2	E	149/525 (28%)	137 (92%)	12 (8%)	0	100	100
All	All	3456/4157 (83%)	3090 (89%)	366 (11%)	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	722/794 (91%)	718 (99%)	4 (1%)	84	88
1	B	721/794 (91%)	719 (100%)	2 (0%)	91	92
1	C	724/794 (91%)	719 (99%)	5 (1%)	81	86
1	D	709/794 (89%)	707 (100%)	2 (0%)	91	92
2	E	134/465 (29%)	134 (100%)	0	100	100
All	All	3010/3641 (83%)	2997 (100%)	13 (0%)	88	91

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	415	GLU
1	A	519	ILE
1	A	754	GLN
1	A	820	ILE
1	B	380	THR
1	B	420	LYS
1	C	426	ASP
1	C	433	LEU
1	C	710	SER
1	C	711	SER
1	C	819	ASN
1	D	262	PHE
1	D	426	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	ASN
1	A	129	HIS
1	A	131	GLN
1	A	137	GLN
1	A	497	GLN
1	A	622	GLN
1	A	677	GLN
1	A	818	GLN
1	B	34	HIS
1	B	111	HIS
1	B	350	HIS
1	B	654	ASN
1	B	819	ASN
1	C	119	GLN
1	C	123	ASN
1	C	131	GLN
1	C	136	HIS
1	D	98	GLN
1	D	123	ASN
1	D	253	HIS
1	D	499	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

12 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	F	1	3,1	14,14,15	0.38	0	17,19,21	1.16	2 (11%)
3	NAG	F	2	3	14,14,15	0.32	0	17,19,21	1.73	4 (23%)
3	BMA	F	3	3	11,11,12	0.22	0	15,15,17	0.61	0
3	NAG	G	1	3,1	14,14,15	0.31	0	17,19,21	0.88	1 (5%)
3	NAG	G	2	3	14,14,15	0.33	0	17,19,21	0.58	0
3	BMA	G	3	3	11,11,12	0.22	0	15,15,17	0.60	0
3	NAG	H	1	3,1	14,14,15	0.53	0	17,19,21	1.45	2 (11%)
3	NAG	H	2	3	14,14,15	0.30	0	17,19,21	0.86	1 (5%)
3	BMA	H	3	3	11,11,12	0.32	0	15,15,17	1.06	1 (6%)
3	NAG	I	1	3,1	14,14,15	0.35	0	17,19,21	0.99	1 (5%)
3	NAG	I	2	3	14,14,15	0.46	0	17,19,21	1.16	2 (11%)
3	BMA	I	3	3	11,11,12	0.20	0	15,15,17	0.67	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	F	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	4/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
3	NAG	G	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
3	NAG	H	1	3,1	1/1/5/7	5/6/23/26	0/1/1/1
3	NAG	H	2	3	-	4/6/23/26	0/1/1/1
3	BMA	H	3	3	-	1/2/19/22	0/1/1/1
3	NAG	I	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	3/6/23/26	0/1/1/1
3	BMA	I	3	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1	NAG	C1-O5-C5	-4.50	106.09	112.19
3	F	2	NAG	C2-N2-C7	3.89	128.44	122.90
3	I	2	NAG	C1-O5-C5	3.46	116.87	112.19
3	F	2	NAG	C1-C2-N2	3.30	116.12	110.49
3	F	2	NAG	O5-C1-C2	-3.14	106.33	111.29
3	H	3	BMA	C1-C2-C3	2.70	112.98	109.67
3	F	1	NAG	C3-C4-C5	-2.67	105.48	110.24
3	H	1	NAG	C2-N2-C7	2.48	126.43	122.90
3	F	2	NAG	C4-C3-C2	-2.38	107.54	111.02
3	H	2	NAG	C1-O5-C5	2.28	115.28	112.19
3	F	1	NAG	O5-C5-C6	2.21	110.67	107.20
3	G	1	NAG	C1-O5-C5	2.20	115.17	112.19
3	I	1	NAG	O4-C4-C5	2.17	114.69	109.30
3	I	2	NAG	C1-C2-N2	2.01	113.93	110.49

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	H	1	NAG	C1

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	1	NAG	C3-C2-N2-C7
3	H	1	NAG	C8-C7-N2-C2
3	H	1	NAG	O7-C7-N2-C2
3	H	2	NAG	C8-C7-N2-C2
3	H	2	NAG	O7-C7-N2-C2
3	F	1	NAG	C8-C7-N2-C2

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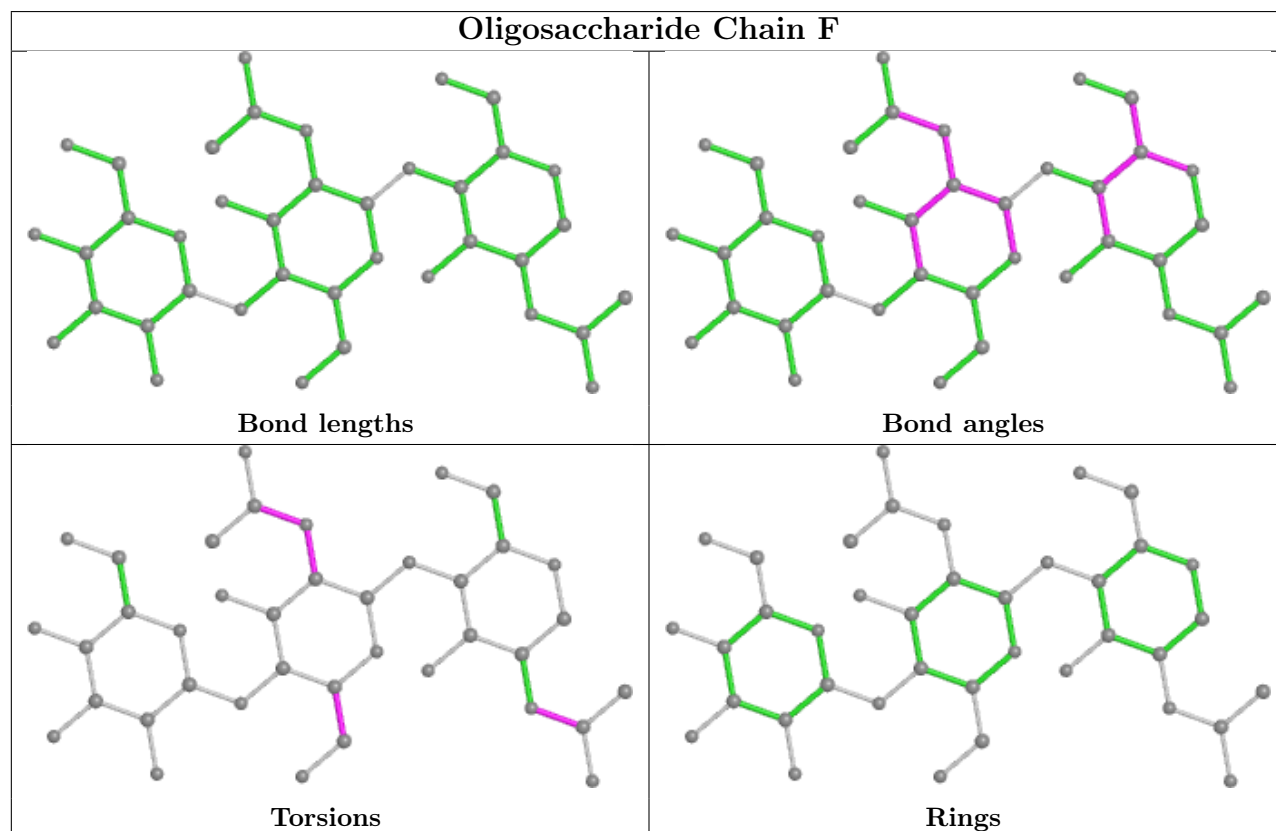
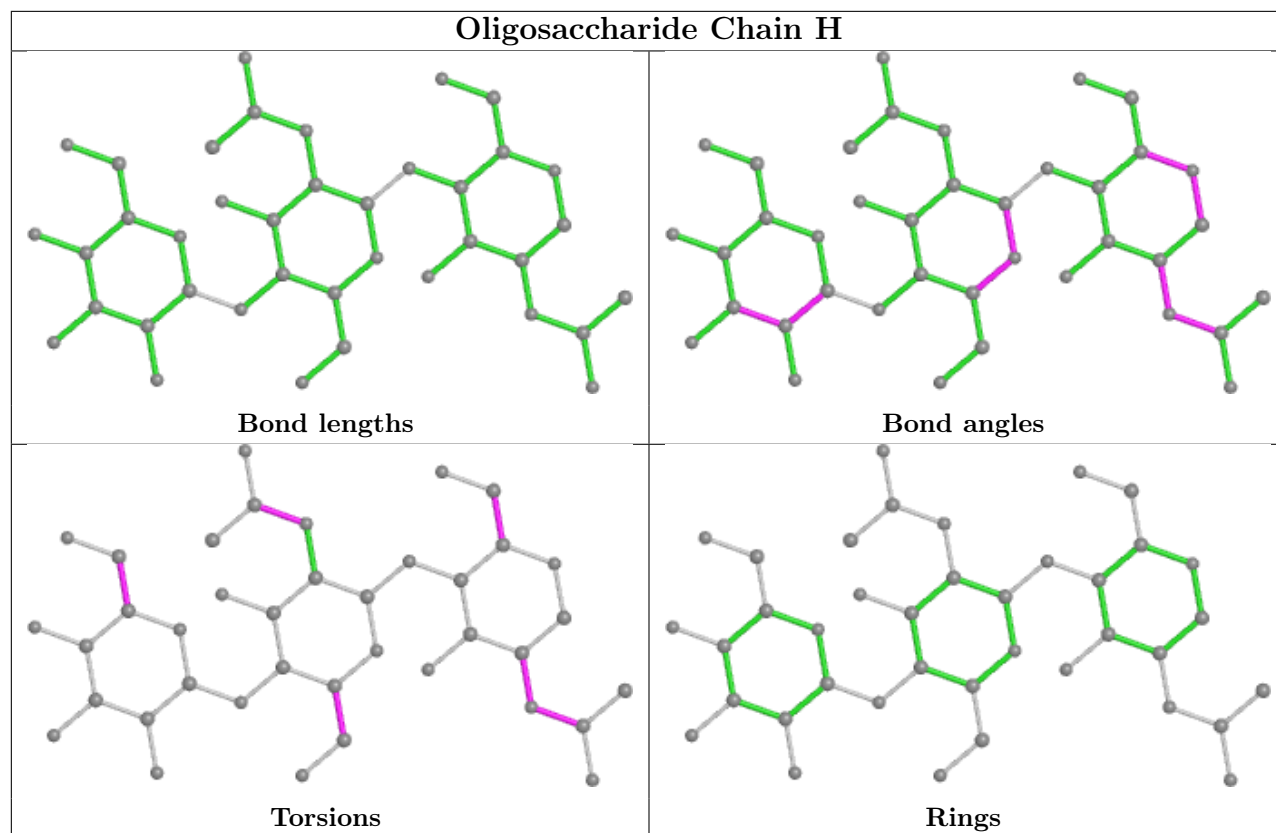
Mol	Chain	Res	Type	Atoms
3	F	1	NAG	O7-C7-N2-C2
3	G	1	NAG	C8-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2
3	G	2	NAG	C8-C7-N2-C2
3	G	2	NAG	O7-C7-N2-C2
3	H	1	NAG	C4-C5-C6-O6
3	I	2	NAG	C8-C7-N2-C2
3	I	2	NAG	O7-C7-N2-C2
3	H	1	NAG	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	F	2	NAG	C1-C2-N2-C7
3	H	3	BMA	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2

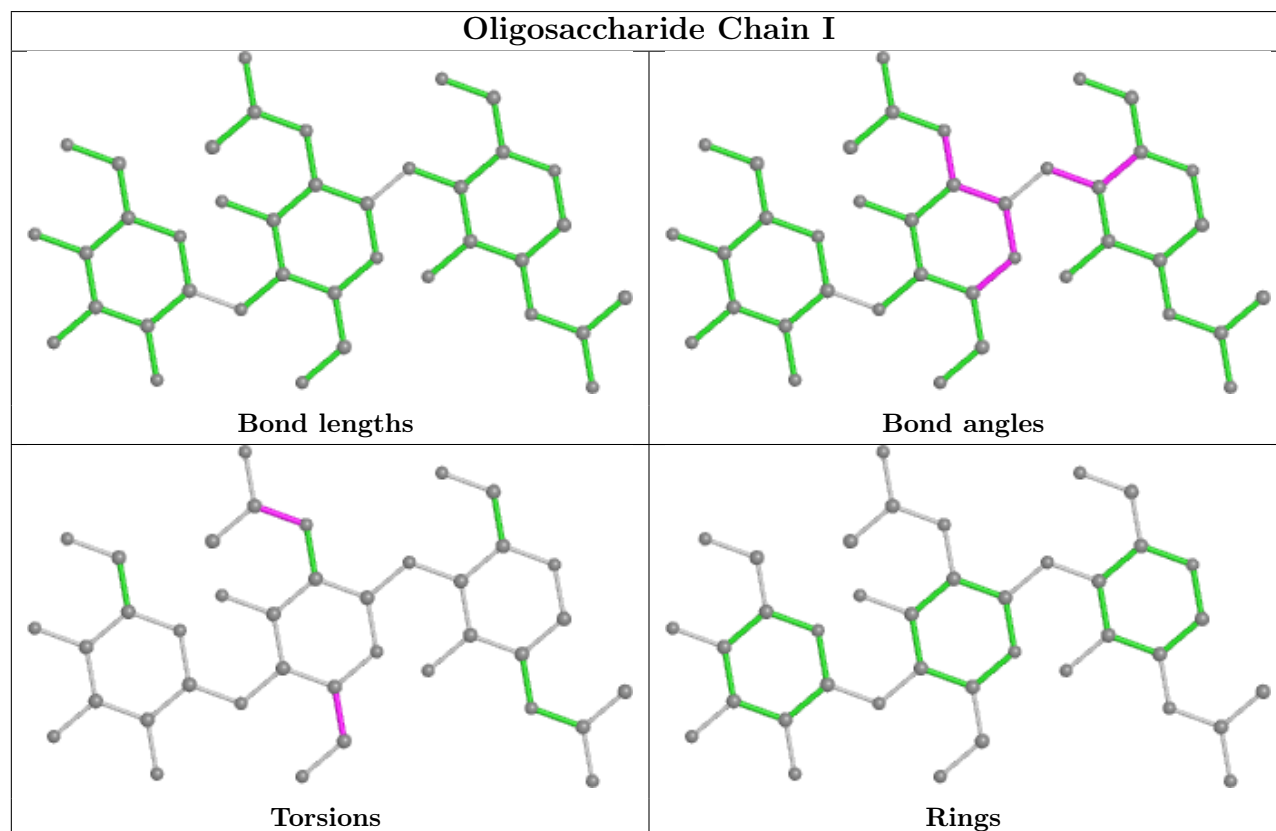
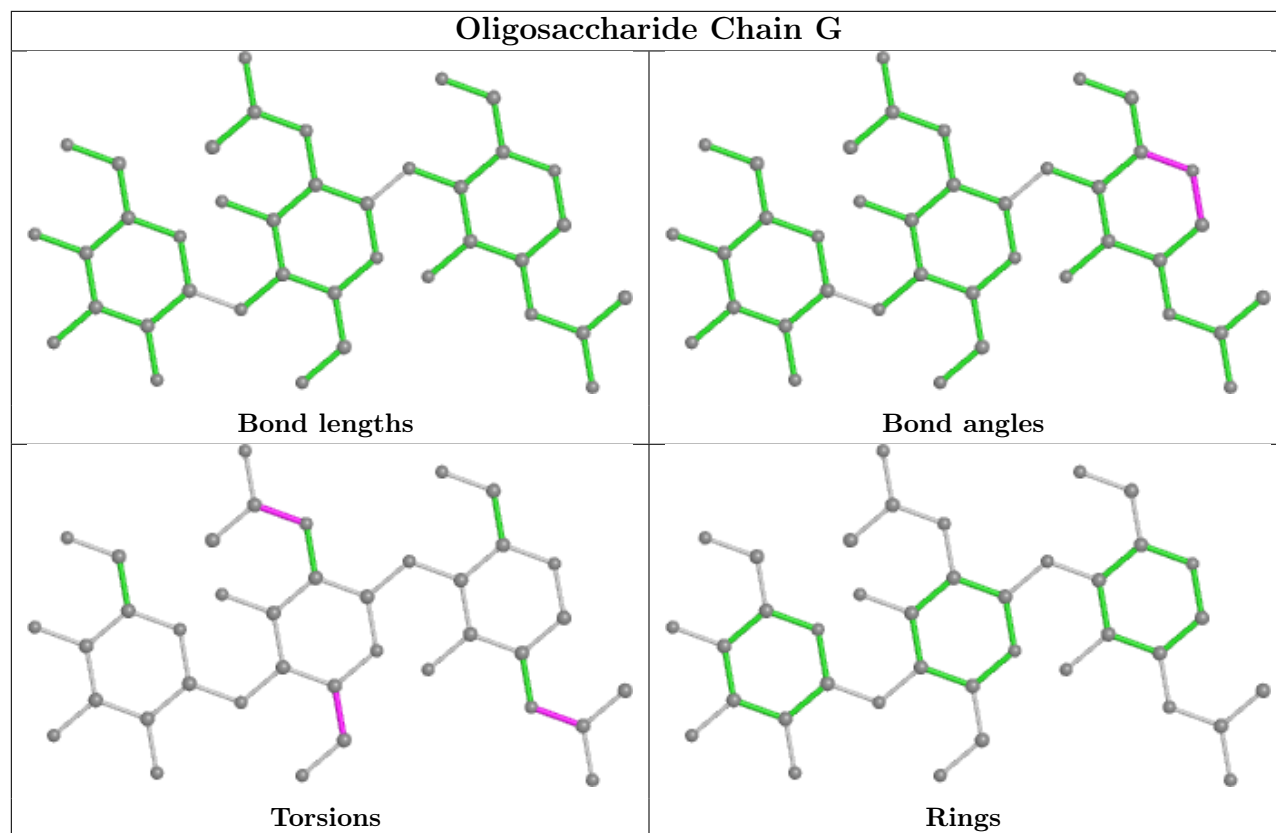
There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	1	NAG	1	0
3	G	1	NAG	11	0
3	I	2	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	1003	1	14,14,15	0.26	0	17,19,21	0.92	1 (5%)
4	NAG	A	1002	1	14,14,15	0.46	0	17,19,21	0.38	0
4	NAG	B	1001	1	14,14,15	0.23	0	17,19,21	0.50	0
4	NAG	C	1001	1	14,14,15	0.18	0	17,19,21	0.38	0
4	NAG	C	1003	1	14,14,15	0.23	0	17,19,21	0.84	0
4	NAG	D	1003	-	14,14,15	0.34	0	17,19,21	1.12	2 (11%)
4	NAG	A	1001	1	14,14,15	0.26	0	17,19,21	0.47	0
4	NAG	C	1005	1	14,14,15	0.24	0	17,19,21	0.79	0
4	NAG	A	1003	-	14,14,15	0.27	0	17,19,21	0.57	0
4	NAG	B	1002	1	14,14,15	0.51	0	17,19,21	0.41	0
4	NAG	C	1002	1	14,14,15	0.51	0	17,19,21	0.69	1 (5%)
4	NAG	D	1004	1	14,14,15	0.26	0	17,19,21	0.49	0
4	NAG	D	1001	1	14,14,15	0.23	0	17,19,21	0.65	0
4	NAG	C	1004	1	14,14,15	0.24	0	17,19,21	1.01	2 (11%)
4	NAG	D	1002	1	14,14,15	0.74	1 (7%)	17,19,21	0.77	0
4	NAG	B	1004	1	14,14,15	0.24	0	17,19,21	0.96	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1003	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1002	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1001	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1001	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1003	1	-	3/6/23/26	0/1/1/1
4	NAG	D	1003	-	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1001	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1005	1	-	5/6/23/26	0/1/1/1
4	NAG	A	1003	-	-	1/6/23/26	0/1/1/1
4	NAG	B	1002	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1002	1	-	3/6/23/26	0/1/1/1
4	NAG	D	1004	1	-	3/6/23/26	0/1/1/1
4	NAG	D	1001	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1004	1	-	4/6/23/26	0/1/1/1
4	NAG	D	1002	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1004	1	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1002	NAG	O5-C1	-2.60	1.39	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1003	NAG	C1-O5-C5	2.86	116.06	112.19
4	B	1003	NAG	C2-N2-C7	2.57	126.57	122.90
4	B	1004	NAG	C2-N2-C7	2.57	126.57	122.90
4	C	1004	NAG	C2-N2-C7	2.37	126.27	122.90
4	D	1003	NAG	O5-C1-C2	2.29	114.90	111.29
4	C	1002	NAG	C1-O5-C5	2.17	115.13	112.19
4	C	1004	NAG	C1-O5-C5	2.08	115.01	112.19

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1003	NAG	C8-C7-N2-C2
4	B	1003	NAG	O7-C7-N2-C2
4	B	1004	NAG	C3-C2-N2-C7
4	B	1004	NAG	C8-C7-N2-C2
4	B	1004	NAG	O7-C7-N2-C2
4	C	1003	NAG	C8-C7-N2-C2
4	C	1003	NAG	O7-C7-N2-C2
4	C	1005	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	C	1005	NAG	O7-C7-N2-C2
4	B	1001	NAG	C4-C5-C6-O6
4	A	1001	NAG	C4-C5-C6-O6
4	C	1004	NAG	C8-C7-N2-C2
4	C	1004	NAG	O7-C7-N2-C2
4	C	1002	NAG	O5-C5-C6-O6
4	B	1001	NAG	O5-C5-C6-O6
4	D	1001	NAG	O5-C5-C6-O6
4	A	1001	NAG	O5-C5-C6-O6
4	D	1002	NAG	O5-C5-C6-O6
4	C	1001	NAG	C8-C7-N2-C2
4	C	1001	NAG	O7-C7-N2-C2
4	D	1004	NAG	C8-C7-N2-C2
4	D	1001	NAG	C4-C5-C6-O6
4	B	1003	NAG	C1-C2-N2-C7
4	C	1003	NAG	C1-C2-N2-C7
4	C	1004	NAG	C1-C2-N2-C7
4	D	1004	NAG	O7-C7-N2-C2
4	D	1003	NAG	C8-C7-N2-C2
4	C	1002	NAG	C4-C5-C6-O6
4	B	1003	NAG	O5-C5-C6-O6
4	D	1003	NAG	O7-C7-N2-C2
4	D	1004	NAG	O5-C5-C6-O6
4	A	1003	NAG	O5-C5-C6-O6
4	B	1004	NAG	O5-C5-C6-O6
4	C	1004	NAG	O5-C5-C6-O6
4	C	1005	NAG	O5-C5-C6-O6
4	D	1002	NAG	C4-C5-C6-O6
4	A	1002	NAG	C4-C5-C6-O6
4	C	1002	NAG	C3-C2-N2-C7
4	D	1001	NAG	C3-C2-N2-C7
4	D	1002	NAG	C3-C2-N2-C7
4	D	1001	NAG	C1-C2-N2-C7
4	D	1002	NAG	C1-C2-N2-C7
4	C	1005	NAG	C3-C2-N2-C7
4	A	1002	NAG	C1-C2-N2-C7
4	C	1005	NAG	C1-C2-N2-C7

There are no ring outliers.

6 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1002	NAG	2	0
4	C	1001	NAG	1	0
4	D	1003	NAG	5	0
4	A	1003	NAG	4	0
4	B	1002	NAG	1	0
4	B	1004	NAG	7	0

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.

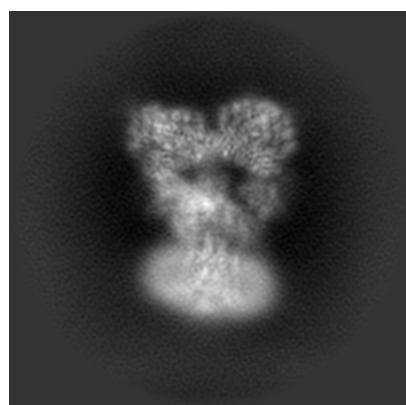
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31459. These allow visual inspection of the internal detail of the map and identification of artifacts.

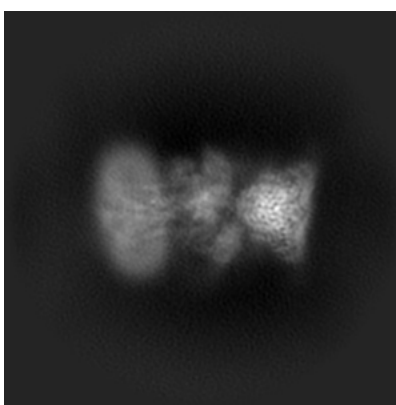
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

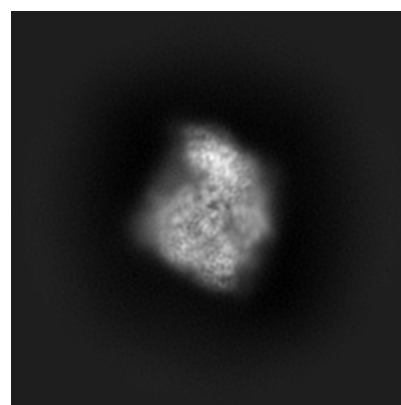
6.1.1 Primary map



X



Y

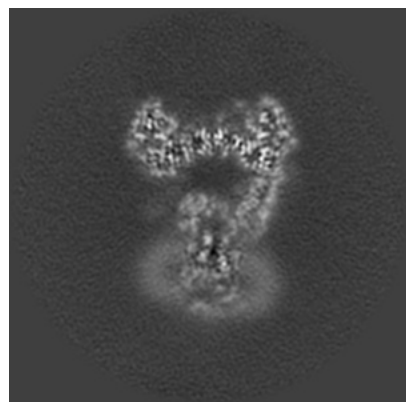


Z

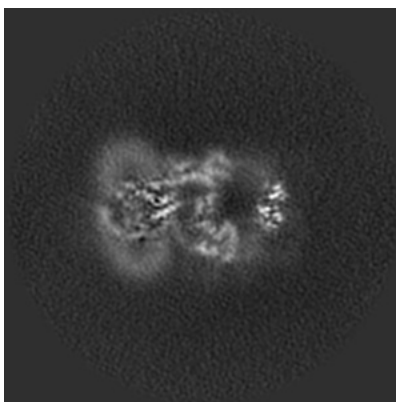
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

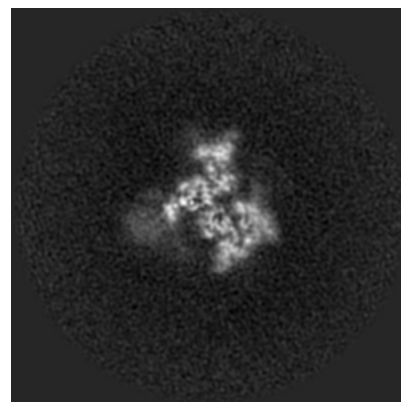
6.2.1 Primary map



X Index: 128



Y Index: 128

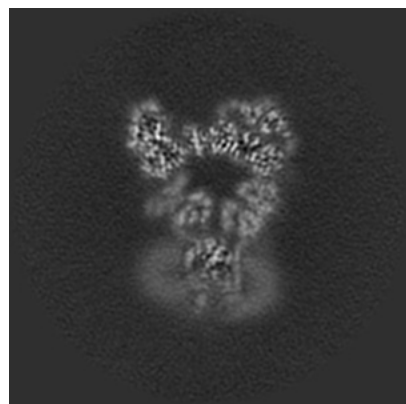


Z Index: 128

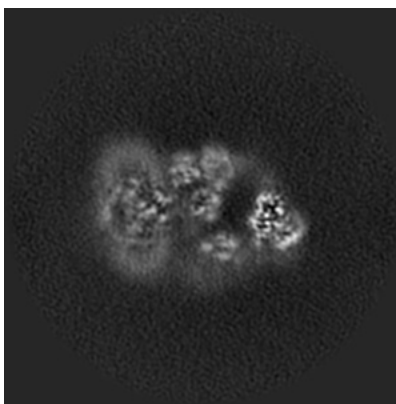
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

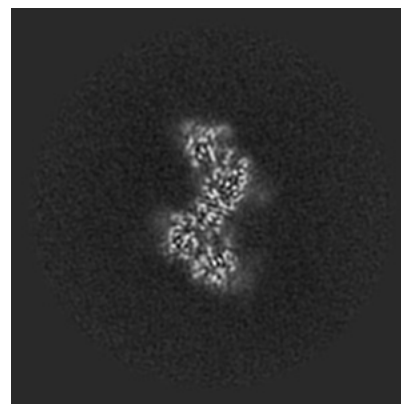
6.3.1 Primary map



X Index: 133



Y Index: 121

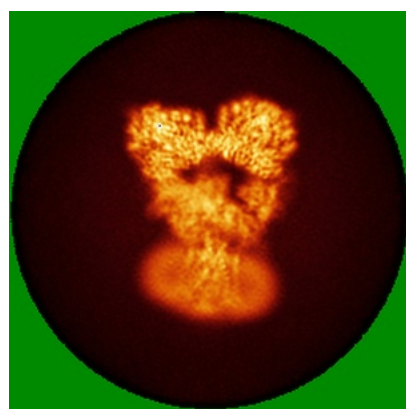


Z Index: 175

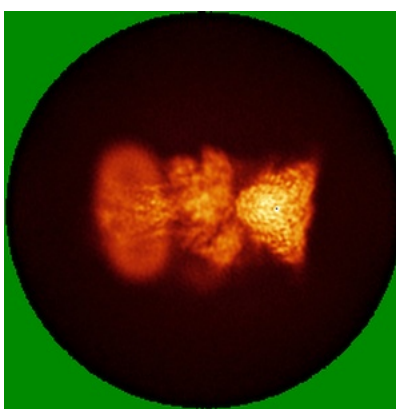
The images above show the largest variance slices of the map in three orthogonal directions.

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

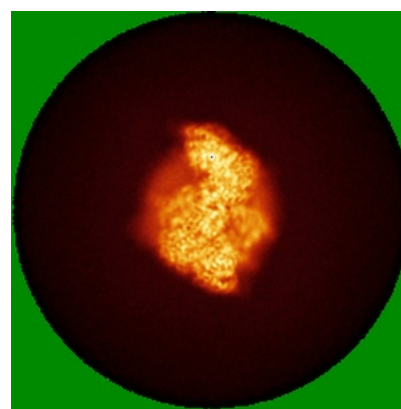
6.4.1 Primary map



X



Y

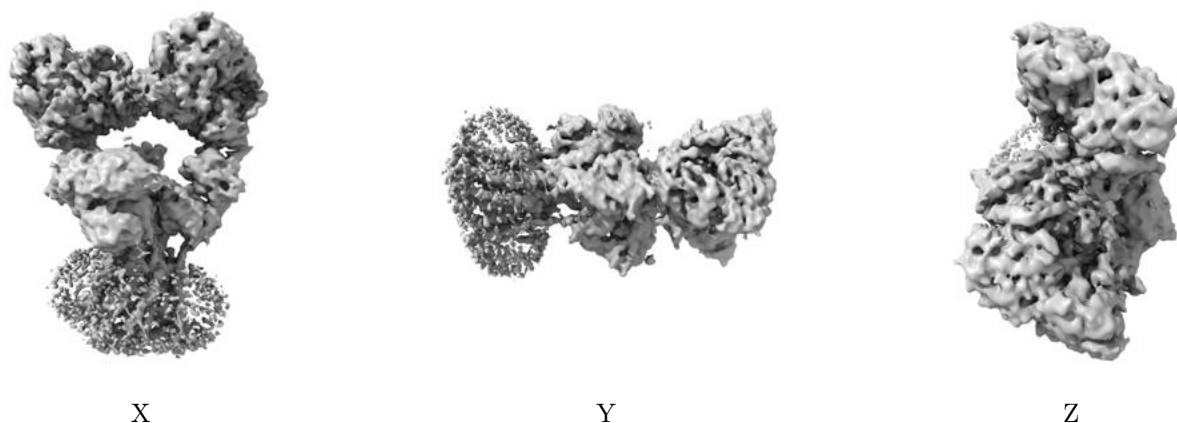


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.455. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

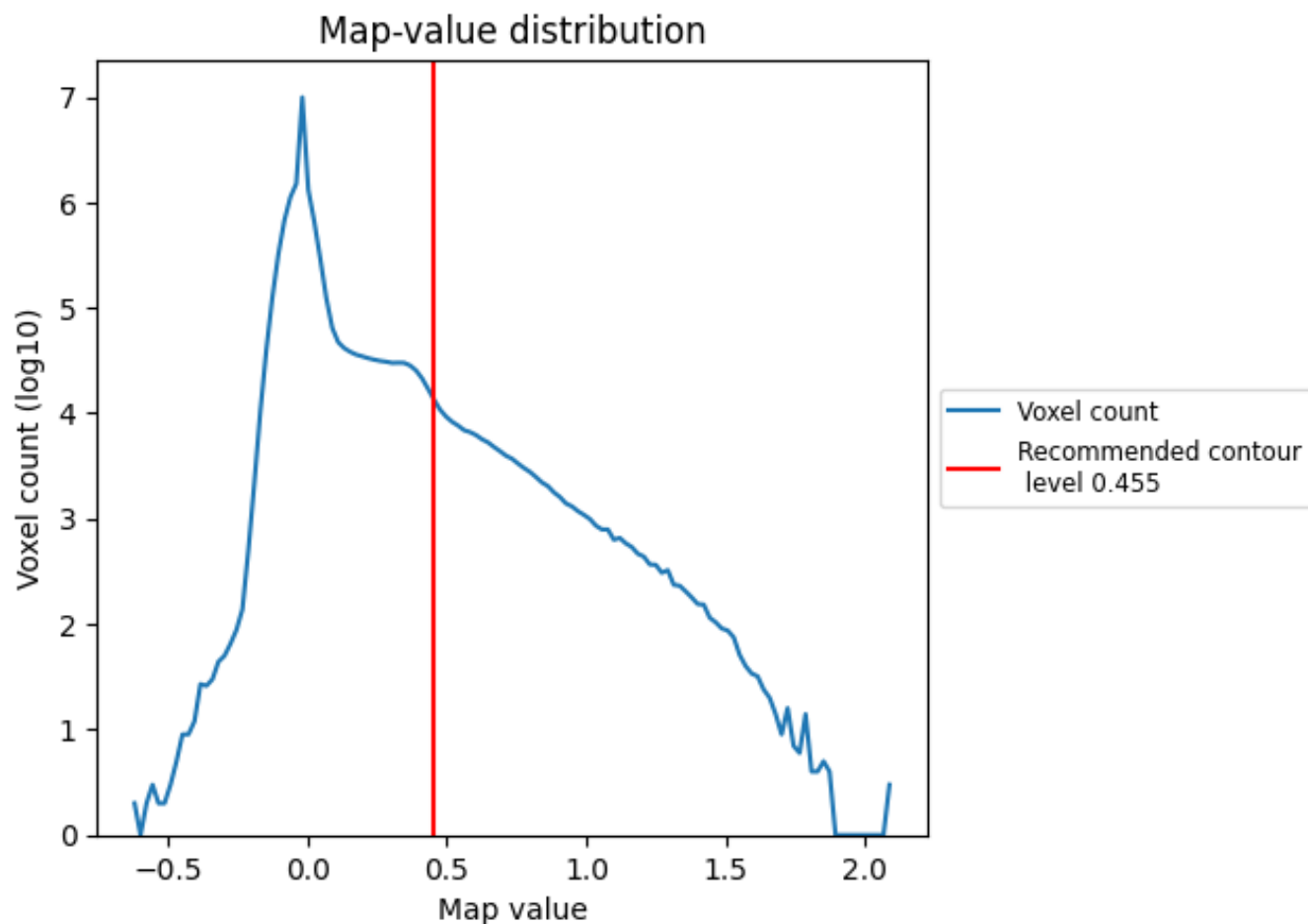
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

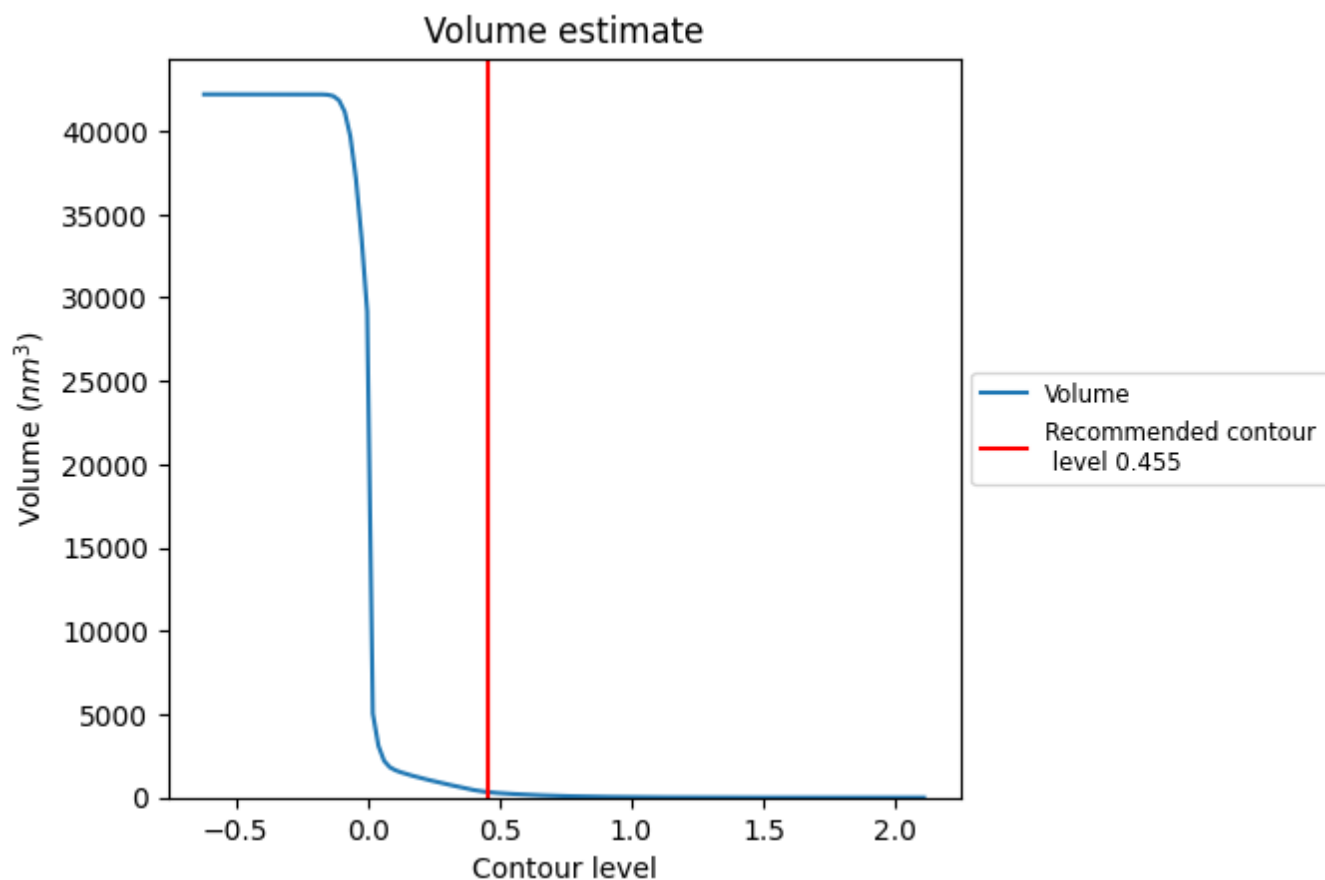
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

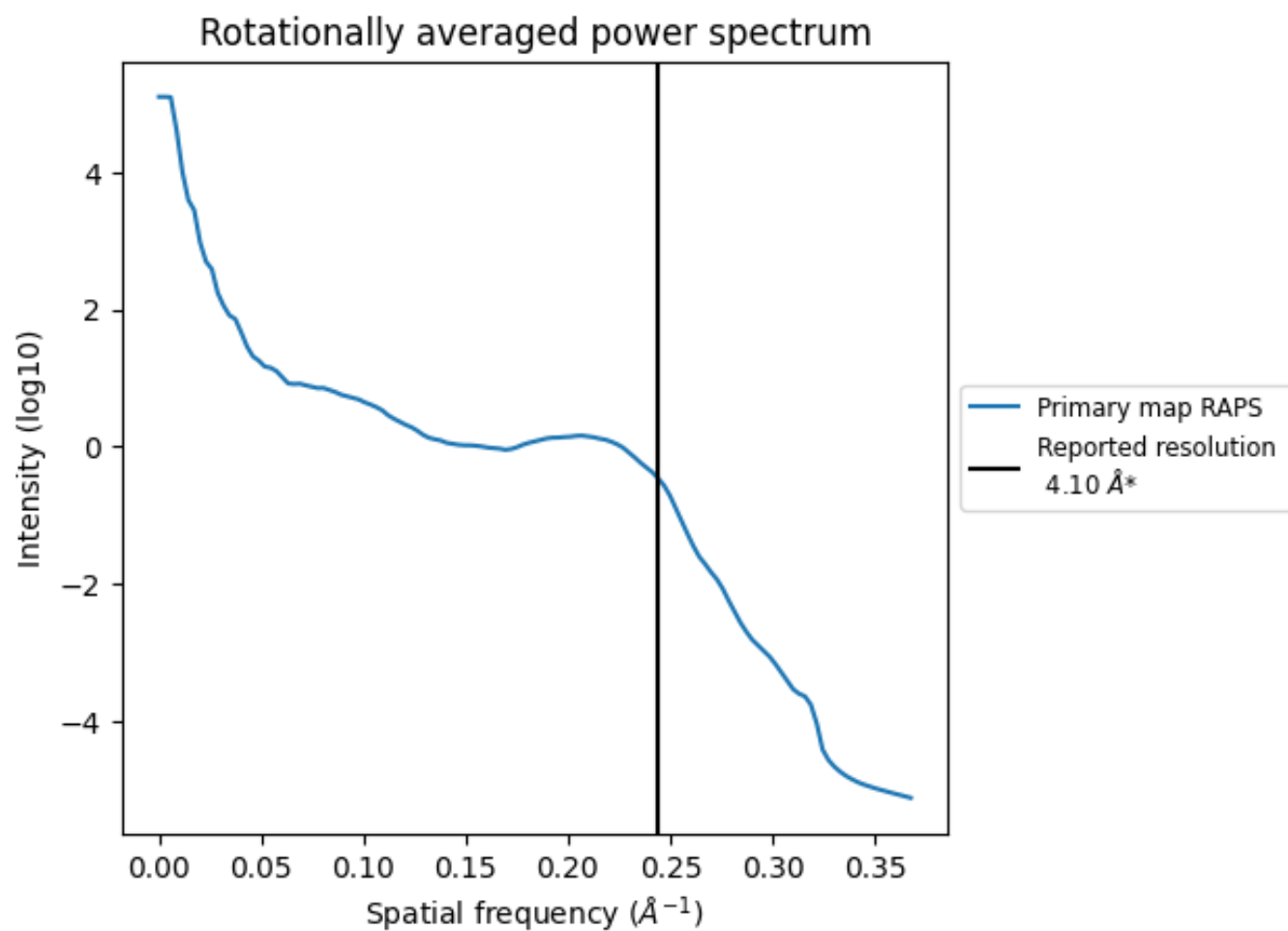
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 330 nm³; this corresponds to an approximate mass of 298 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 0.244 Å⁻¹

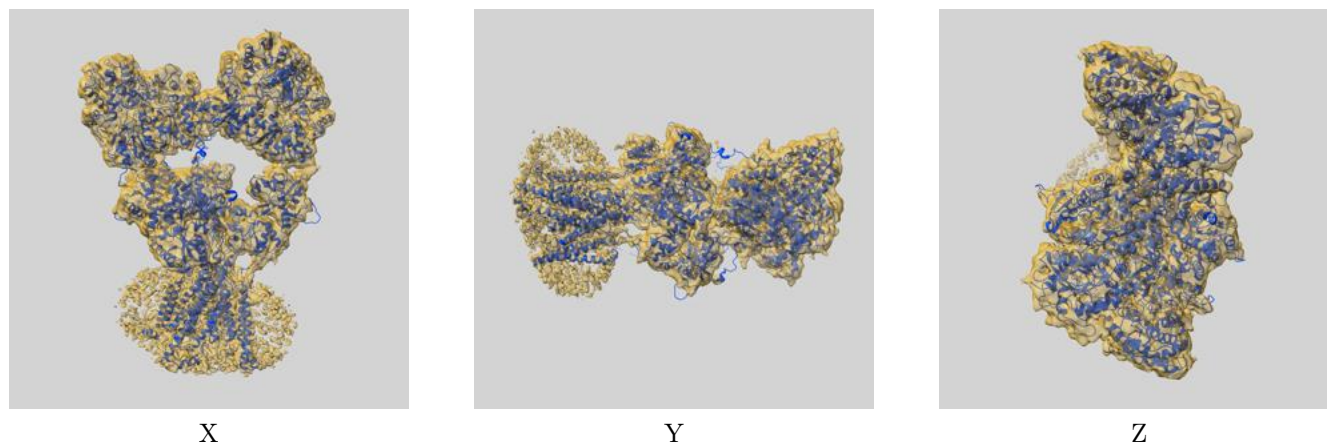
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

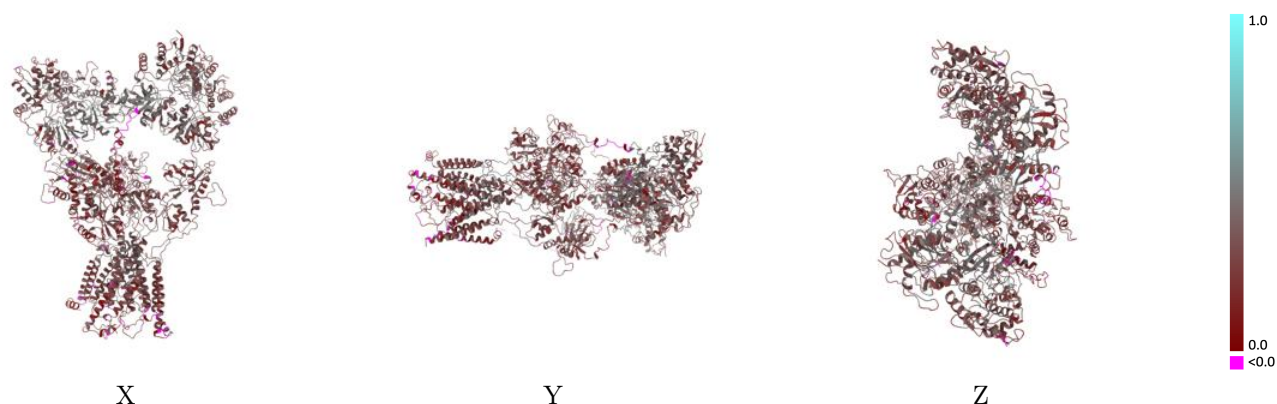
This section contains information regarding the fit between EMDB map EMD-31459 and PDB model 7F56. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



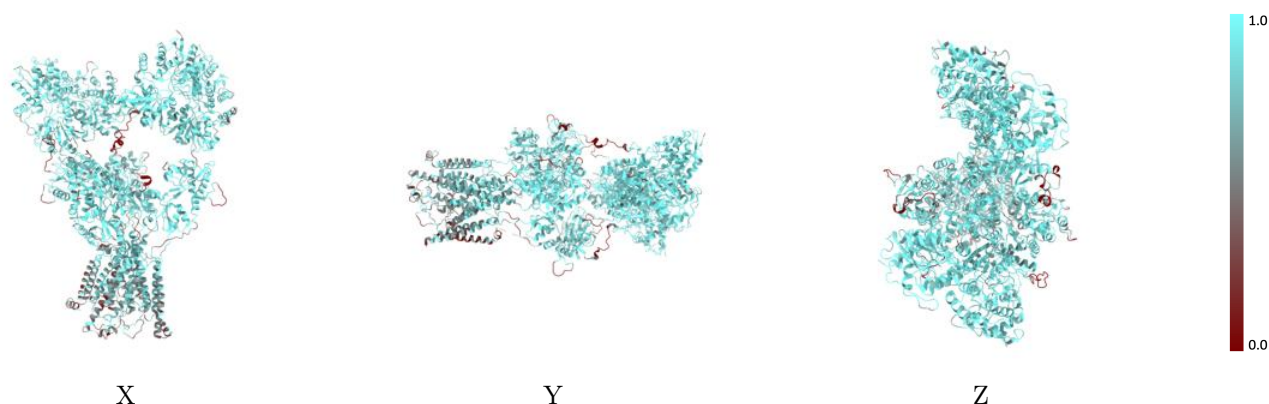
The images above show the 3D surface view of the map at the recommended contour level 0.455 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



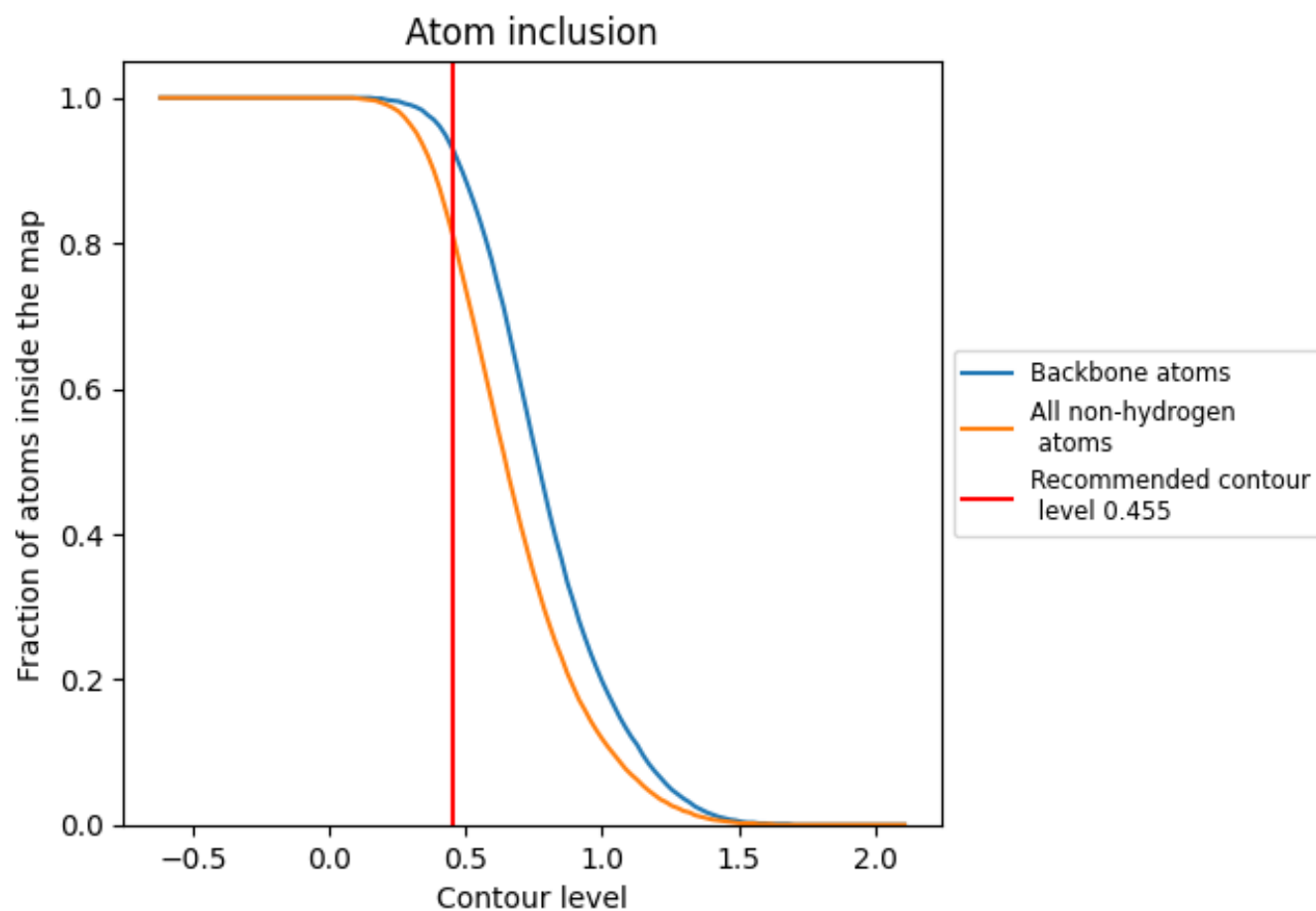
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.455).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 81% 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 (0.455) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8070	<div></div> 0.3090
A	<div></div> 0.8250	<div></div> 0.3060
B	<div></div> 0.8130	<div></div> 0.3060
C	<div></div> 0.8010	<div></div> 0.3000
D	<div></div> 0.8150	<div></div> 0.3300
E	<div></div> 0.6540	<div></div> 0.2680
F	<div></div> 0.8210	<div></div> 0.4550
G	<div></div> 0.9230	<div></div> 0.4210
H	<div></div> 0.8720	<div></div> 0.4230
I	<div></div> 0.9490	<div></div> 0.4250

1.0

0.0

<0.0