



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 06:53 AM UTC

PDB ID : 6WHR / pdb_00006whr
EMDB ID : EMD-21673
Title : GluN1b-GluN2B NMDA receptor in non-active 2 conformation at 4 angstrom resolution
Authors : Chou, T.; Tajima, N.; Furukawa, H.
Deposited on : 2020-04-08
Resolution : 3.99 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

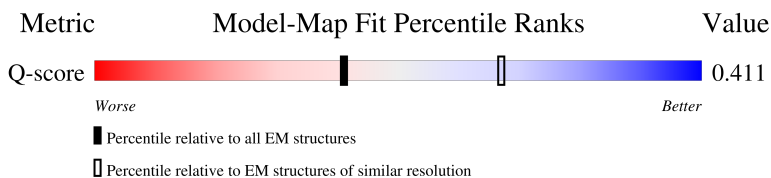
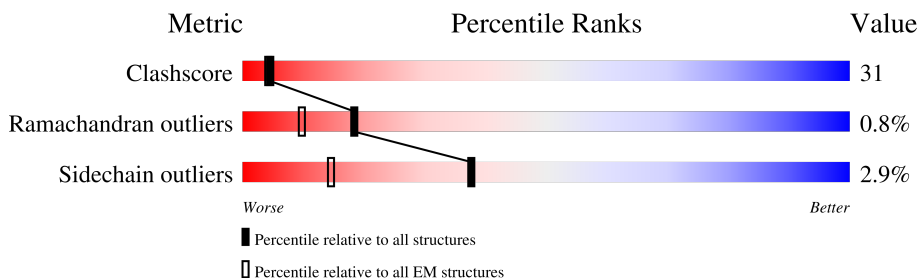
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.99 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7463 (3.49 - 4.49)

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	959	
1	C	959	
2	B	883	
2	D	883	

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Mol	Chain	Length	Quality of chain
3	E	2	 50%50%
3	F	2	 50%50%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23370 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, NMDA 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	799	Total	C	N	O	S	0	0
			5870	3757	980	1101	32		
1	C	799	Total	C	N	O	S	0	0
			5870	3757	980	1101	32		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	SER	CYS	conflict	UNP P35439
A	61	GLN	ASN	conflict	UNP P35439
A	260	ASP	ASN	conflict	UNP P35439
A	371	GLN	ASN	conflict	UNP P35439
A	492	GLN	ASN	conflict	UNP P35439
A	512	GLN	ASN	conflict	UNP P35439
A	615	GLN	GLU	conflict	UNP P35439
A	616	SER	GLU	conflict	UNP P35439
A	618	SER	GLU	conflict	UNP P35439
A	619	THR	GLU	conflict	UNP P35439
A	792	GLN	ASN	conflict	UNP P35439
A	831	CYS	PHE	conflict	UNP P35439
C	22	SER	CYS	conflict	UNP P35439
C	61	GLN	ASN	conflict	UNP P35439
C	260	ASP	ASN	conflict	UNP P35439
C	371	GLN	ASN	conflict	UNP P35439
C	492	GLN	ASN	conflict	UNP P35439
C	512	GLN	ASN	conflict	UNP P35439
C	615	GLN	GLU	conflict	UNP P35439
C	616	SER	GLU	conflict	UNP P35439
C	618	SER	GLU	conflict	UNP P35439
C	619	THR	GLU	conflict	UNP P35439
C	792	GLN	ASN	conflict	UNP P35439
C	831	CYS	PHE	conflict	UNP P35439

- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	784	Total	C	N	O	S	0	0
			5717	3679	927	1078	33		
2	D	784	Total	C	N	O	S	0	0
			5717	3679	927	1078	33		

There are 124 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-30	MET	-	expression tag	UNP Q00960
B	-29	GLY	-	expression tag	UNP Q00960
B	-28	THR	-	expression tag	UNP Q00960
B	-27	MET	-	expression tag	UNP Q00960
B	-26	ARG	-	expression tag	UNP Q00960
B	-25	LEU	-	expression tag	UNP Q00960
B	-24	PHE	-	expression tag	UNP Q00960
B	-23	LEU	-	expression tag	UNP Q00960
B	-22	LEU	-	expression tag	UNP Q00960
B	-21	ALA	-	expression tag	UNP Q00960
B	-20	VAL	-	expression tag	UNP Q00960
B	-19	LEU	-	expression tag	UNP Q00960
B	-18	PHE	-	expression tag	UNP Q00960
B	-17	LEU	-	expression tag	UNP Q00960
B	-16	PHE	-	expression tag	UNP Q00960
B	-15	SER	-	expression tag	UNP Q00960
B	-14	PHE	-	expression tag	UNP Q00960
B	-13	ALA	-	expression tag	UNP Q00960
B	-12	ARG	-	expression tag	UNP Q00960
B	-11	ALA	-	expression tag	UNP Q00960
B	-10	THR	-	expression tag	UNP Q00960
B	-9	GLY	-	expression tag	UNP Q00960
B	-8	TRP	-	expression tag	UNP Q00960
B	-7	SER	-	expression tag	UNP Q00960
B	-6	HIS	-	expression tag	UNP Q00960
B	-5	PRO	-	expression tag	UNP Q00960
B	-4	GLN	-	expression tag	UNP Q00960
B	-3	PHE	-	expression tag	UNP Q00960
B	-2	GLU	-	expression tag	UNP Q00960
B	-1	LYS	-	expression tag	UNP Q00960
B	0	GLY	-	expression tag	UNP Q00960
B	1	GLY	-	expression tag	UNP Q00960
B	2	GLY	-	expression tag	UNP Q00960
B	3	SER	-	expression tag	UNP Q00960
B	4	GLY	-	expression tag	UNP Q00960

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Chain	Residue	Modelled	Actual	Comment	Reference
B	5	GLY	-	expression tag	UNP Q00960
B	6	GLY	-	expression tag	UNP Q00960
B	7	SER	-	expression tag	UNP Q00960
B	8	GLY	-	expression tag	UNP Q00960
B	9	GLY	-	expression tag	UNP Q00960
B	10	SER	-	expression tag	UNP Q00960
B	11	ALA	-	expression tag	UNP Q00960
B	12	TRP	-	expression tag	UNP Q00960
B	13	SER	-	expression tag	UNP Q00960
B	14	HIS	-	expression tag	UNP Q00960
B	15	PRO	-	expression tag	UNP Q00960
B	16	GLN	-	expression tag	UNP Q00960
B	17	PHE	-	expression tag	UNP Q00960
B	18	GLU	-	expression tag	UNP Q00960
B	19	LYS	-	expression tag	UNP Q00960
B	20	GLY	-	expression tag	UNP Q00960
B	21	ALA	-	expression tag	UNP Q00960
B	22	LEU	-	expression tag	UNP Q00960
B	23	VAL	-	expression tag	UNP Q00960
B	24	PRO	-	expression tag	UNP Q00960
B	25	ARG	-	expression tag	UNP Q00960
B	26	GLY	-	expression tag	UNP Q00960
B	348	ASP	ASN	conflict	UNP Q00960
B	557	CYS	ASP	conflict	UNP Q00960
B	588	SER	CYS	conflict	UNP Q00960
B	838	SER	CYS	conflict	UNP Q00960
B	849	SER	CYS	conflict	UNP Q00960
D	-30	MET	-	expression tag	UNP Q00960
D	-29	GLY	-	expression tag	UNP Q00960
D	-28	THR	-	expression tag	UNP Q00960
D	-27	MET	-	expression tag	UNP Q00960
D	-26	ARG	-	expression tag	UNP Q00960
D	-25	LEU	-	expression tag	UNP Q00960
D	-24	PHE	-	expression tag	UNP Q00960
D	-23	LEU	-	expression tag	UNP Q00960
D	-22	LEU	-	expression tag	UNP Q00960
D	-21	ALA	-	expression tag	UNP Q00960
D	-20	VAL	-	expression tag	UNP Q00960
D	-19	LEU	-	expression tag	UNP Q00960
D	-18	PHE	-	expression tag	UNP Q00960
D	-17	LEU	-	expression tag	UNP Q00960
D	-16	PHE	-	expression tag	UNP Q00960

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-15	SER	-	expression tag	UNP Q00960
D	-14	PHE	-	expression tag	UNP Q00960
D	-13	ALA	-	expression tag	UNP Q00960
D	-12	ARG	-	expression tag	UNP Q00960
D	-11	ALA	-	expression tag	UNP Q00960
D	-10	THR	-	expression tag	UNP Q00960
D	-9	GLY	-	expression tag	UNP Q00960
D	-8	TRP	-	expression tag	UNP Q00960
D	-7	SER	-	expression tag	UNP Q00960
D	-6	HIS	-	expression tag	UNP Q00960
D	-5	PRO	-	expression tag	UNP Q00960
D	-4	GLN	-	expression tag	UNP Q00960
D	-3	PHE	-	expression tag	UNP Q00960
D	-2	GLU	-	expression tag	UNP Q00960
D	-1	LYS	-	expression tag	UNP Q00960
D	0	GLY	-	expression tag	UNP Q00960
D	1	GLY	-	expression tag	UNP Q00960
D	2	GLY	-	expression tag	UNP Q00960
D	3	SER	-	expression tag	UNP Q00960
D	4	GLY	-	expression tag	UNP Q00960
D	5	GLY	-	expression tag	UNP Q00960
D	6	GLY	-	expression tag	UNP Q00960
D	7	SER	-	expression tag	UNP Q00960
D	8	GLY	-	expression tag	UNP Q00960
D	9	GLY	-	expression tag	UNP Q00960
D	10	SER	-	expression tag	UNP Q00960
D	11	ALA	-	expression tag	UNP Q00960
D	12	TRP	-	expression tag	UNP Q00960
D	13	SER	-	expression tag	UNP Q00960
D	14	HIS	-	expression tag	UNP Q00960
D	15	PRO	-	expression tag	UNP Q00960
D	16	GLN	-	expression tag	UNP Q00960
D	17	PHE	-	expression tag	UNP Q00960
D	18	GLU	-	expression tag	UNP Q00960
D	19	LYS	-	expression tag	UNP Q00960
D	20	GLY	-	expression tag	UNP Q00960
D	21	ALA	-	expression tag	UNP Q00960
D	22	LEU	-	expression tag	UNP Q00960
D	23	VAL	-	expression tag	UNP Q00960
D	24	PRO	-	expression tag	UNP Q00960
D	25	ARG	-	expression tag	UNP Q00960
D	26	GLY	-	expression tag	UNP Q00960

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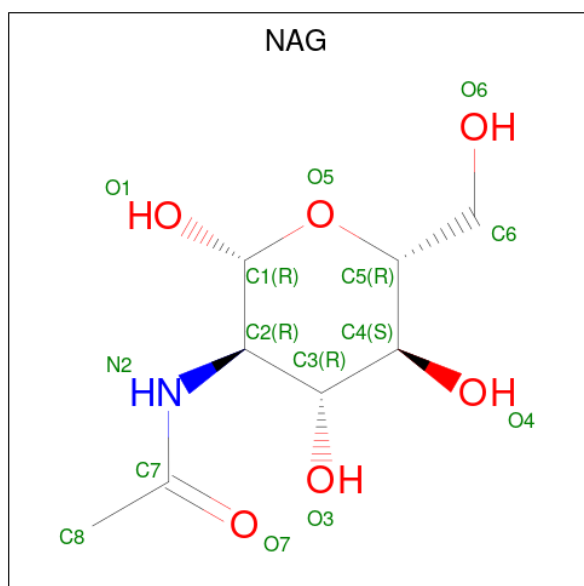
Chain	Residue	Modelled	Actual	Comment	Reference
D	348	ASP	ASN	conflict	UNP Q00960
D	557	CYS	ASP	conflict	UNP Q00960
D	588	SER	CYS	conflict	UNP Q00960
D	838	SER	CYS	conflict	UNP Q00960
D	849	SER	CYS	conflict	UNP Q00960

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



Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	F	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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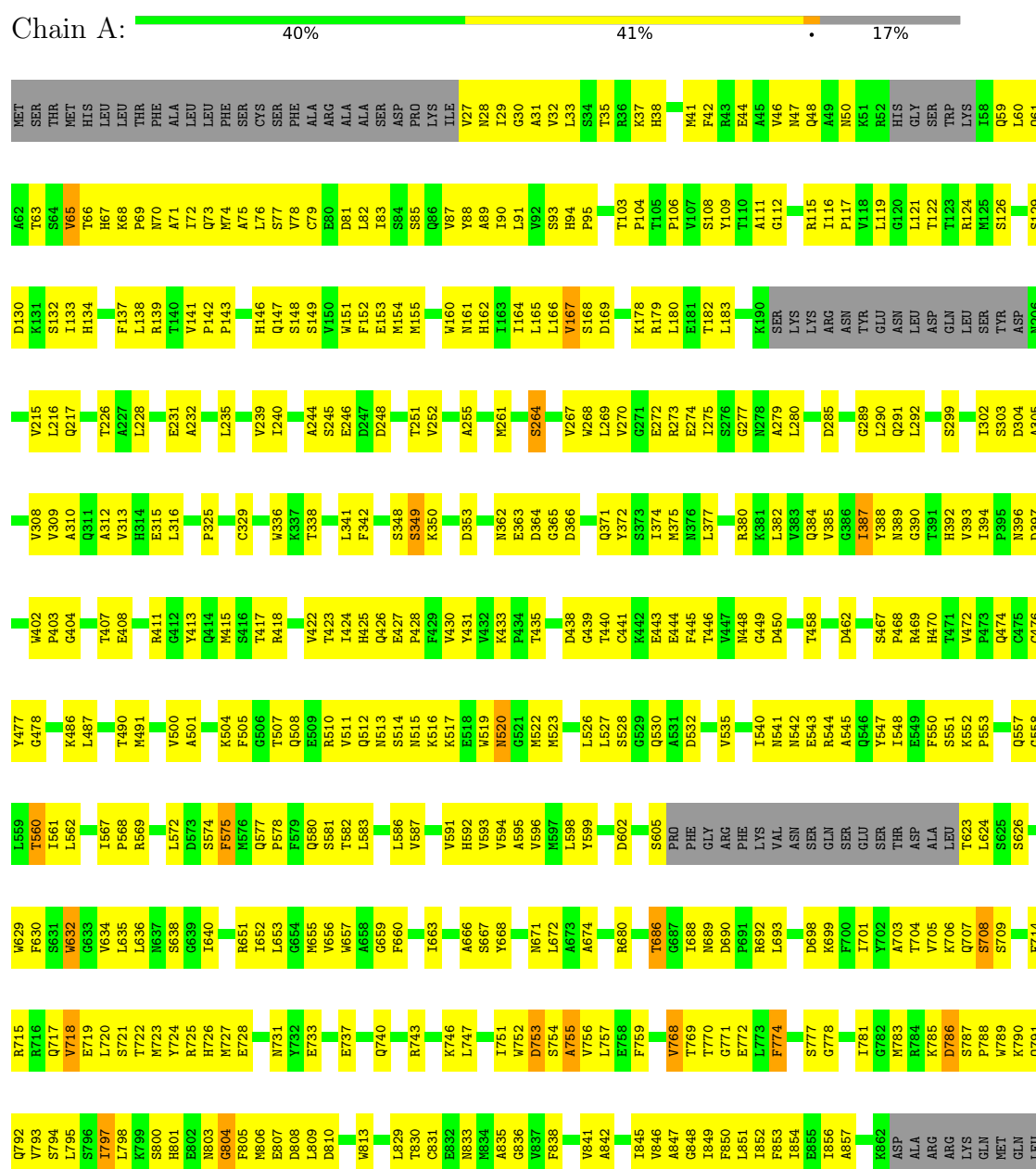
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Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C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



[illegible]

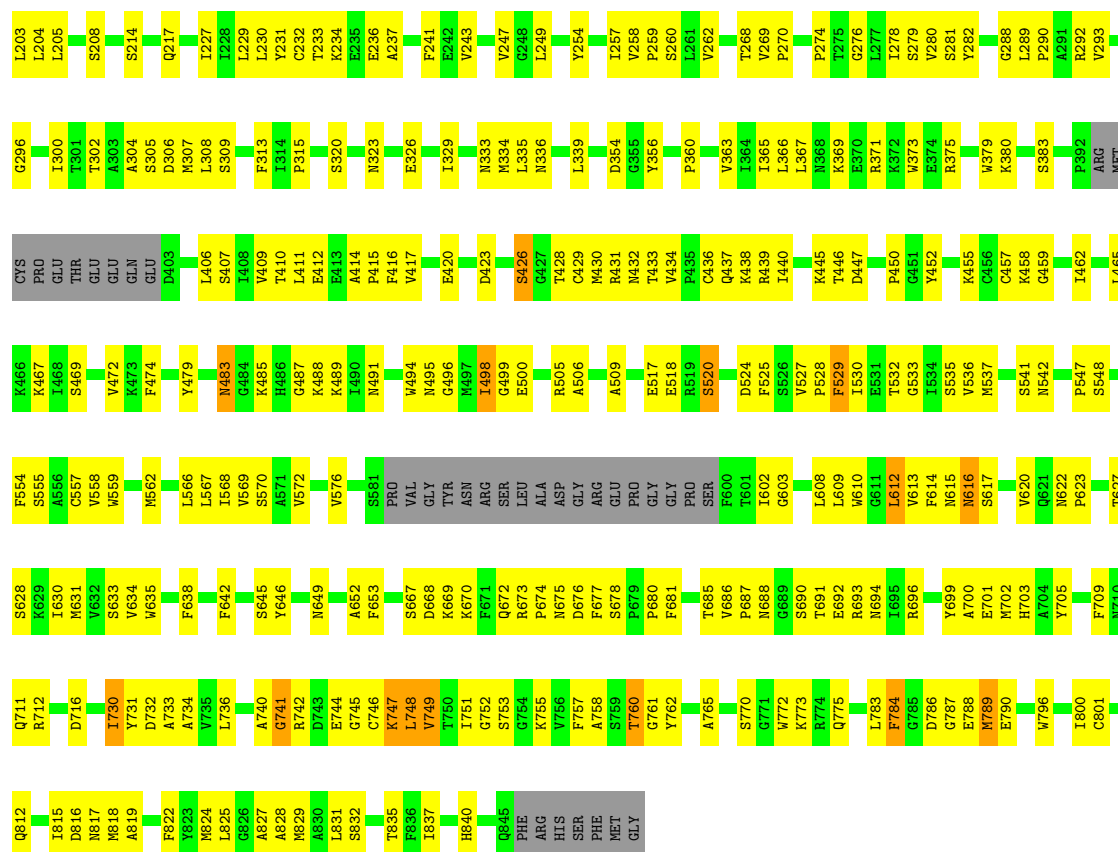
- Molecule 1: Glutamate receptor ionotropic, NMDA 1



GLN	PHE	V793	F714	L624	P553	P473	N396	A305	ASP	D130	A62
LYS	ALA	S794	R715	S625	Q57	Q474	D397	V308	N206	R131	T63
ASP	ALA	L795	R716	S626	Q57	Q475	Q475	V309	N206	S132	S64
THR	VAL	S796	Q717	S626	Q558	Q476	Q403	V310	N206	H133	P65
VAL	ASN	I797	W718	W629	L559	Q477	Q404	A310	N206	H134	HIS
LEU	VAL	L798	E719	F630	W560	Q478	Q404	Q311	N206	L135	H67
PRO	TRP	R799	L720	S631	L561	Q479	Q404	A312	N206	S136	K68
ARG	ARG	S800	S721	W632	L562	K486	T407	V312	N206	F137	P69
ARG	ALA	H801	T722	G633	L563	L487	E408	V313	N206	L138	PHE
ALA	ASN	E902	M723	V634	L564	Q488	E408	H314	N206	R139	ALA
ILE	LEU	N803	R724	L635	L565	T490	R411	L316	N206	T140	LEU
GLU	GLN	G804	R725	L636	L566	M491	G412	E231	N206	V141	LEU
ARG	ASP	F805	H726	W637	L567	Q491	V413	A232	N206	P142	PHE
GLU	ARG	M806	M727	S638	L568	Q492	Q414	A232	N206	P143	LEU
GLU	LYS	E807	E728	G639	L569	A501	M415	L235	N206	A75	SER
GLY	SER	D808	E729	I640	L570	Q493	M416	L235	N206		CYS
GLN	GLY	L809	M731	S641	L571	K504	T417	V336	N206	H146	PHE
LEU	ARG	D810	Y732	R651	L572	F505	R418	K337	N206	V78	ALA
GLN	ALA	W813	E733	L652	L573	G506	Q419	T338	N206	C79	ARG
LEU	GLU	Q814	E734	L653	L574	Q507	V422	A244	N206	E80	ALA
LEU	GLU	Q815	E735	L654	L575	T507	Q423	S245	N206	D81	ALA
CYS	PRO	F816	E736	F655	L576	Q508	T424	S245	N206	F152	ALA
SER	ASP	G817	E737	G656	L577	Q509	I424	S248	N206	E153	SER
ARG	PRO	L829	Q740	M656	L578	Q510	H425	D248	N206	M154	ALA
ARG	PRO	T830	Q741	V657	L579	R511	Q426	S248	N206	M154	PRO
HIS	LYS	C831	Q742	W657	L580	V511	Q427	S248	N206	S85	ALA
ARG	LYS	E832	K746	A658	L581	Q512	E427	S248	N206	Q86	LYS
GLU	LYS	N833	L747	F659	L582	Q513	P428	V252	N206	V87	ILE
GLU	ALA	M834	L747	G660	L583	N513	K350	V252	N206	W88	ALA
ALA	ALA	F835	I751	F661	L584	S514	F429	A255	N206	M160	N28
THR	THR	G836	W752	M662	L585	N515	V430	A255	N206	N161	I29
PHE	PHE	G837	W753	G663	L586	K516	Y431	D353	N206	H162	G30
ARG	ARG	W837	D753	I663	L587	V517	V432	S264	N206	L91	ALA
ILE	ILE	F838	S754	A666	L588	Q518	K433	N362	N206	I164	S31
THR	THR	W841	W756	S667	L589	W519	P434	E363	N206	L165	V32
SER	SER	A842	W757	V668	L590	N520	T435	D364	N206	L166	L33
THR	THR	E843	E758	V669	L591	G521	D436	G365	N206	V167	S34
LEU	LEU	I845	F759	R680	L592	W522	D438	D366	N206	S168	T35
ALA	ALA	V846	W760	Q681	L593	W523	Q439	D366	N206	D169	R36
SER	SER	A847	W761	T686	L594	E524	T440	Q371	N206	E272	K37
SER	SER	G848	T762	G687	L595	L526	Q441	Y372	N206	K178	H38
PHE	PHE	I849	T763	I688	D602	L527	K442	R273	N206	R179	
LYS	LYS	F850	G771	N689	L603	S5	E443	E274	N206	L180	M41
ARG	ARG	L851	E772	D690	S605	G528	E444	M375	N206	S108	F42
ARG	ARG	L852	L773	P691		Q530	F445	R376	N206	Y109	R43
ARG	ARG	F853	F774	R692	PAO	A831	T446	L377	N206	T110	E44
SER	SER	I854		R693	PHE	D532	V447		N206	L183	A45
SER	SER	E855	S777	R694	GLY	A831		R380	N206	L184	A45
LYS	LYS	I856	G778		ARG	K381	N448	R281	N206	G112	V46
ASP	ASP	A857		D698	PHE	V535	D450	L382	N206	K190	M47
THR	THR		T781	K699	LYS			V383	N206		Q48
SER	SER	K862	G782	K699	VAL	T540	T456	L384	N206		Q48
THR	THR	ASP	M783	F700	ASN	N541		Q384	N206		Q48
GLY	GLY	ALA		T701	SER	N542	C457	V385	N206		A49
GLY	GLY	ARG		R784	GLN	E543	T458	G386	N206		A49
GLY	GLY	ARG	K785	A702	SER	A544		L387	N206		A49
ARG	ARG		D786	T704	GLU	A545	D462	Y388	N206		A49
LYS	ARG		S787	V705	SER				N206		A49
GLN	GLN		P788	K706	THR		S467		N206		A49
ALA	ALA		W789	Q707	THR				N206		A49
LEU	LEU		K790	S708	ALA				N206		A49
GLN	GLN		Q791	S709	LEU				N206		A49
ALA	ALA								N206		A49
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- Molecule 2: Glutamate receptor ionotropic, NMDA 2B





- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	134688	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	64.5	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	18.999	Depositor
Minimum map value	-8.082	Depositor
Average map value	0.015	Depositor
Map value standard deviation	0.684	Depositor
Recommended contour level	2.3	Depositor
Map size ($\text{\AA}$)	350.72, 350.72, 350.72	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.37, 1.37, 1.37	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.74	1/5996 (0.0%)	0.73	0/8192
1	C	0.74	1/5996 (0.0%)	0.73	0/8192
2	B	0.68	2/5835 (0.0%)	0.70	3/7968 (0.0%)
2	D	0.68	2/5835 (0.0%)	0.70	3/7968 (0.0%)
All	All	0.71	6/23662 (0.0%)	0.72	6/32320 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	2
2	B	0	2
2	D	0	2
All	All	0	8

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	755	ALA	CA-C	-8.24	1.41	1.52
1	C	755	ALA	CA-C	-8.21	1.41	1.52
2	D	520	SER	CA-C	-6.65	1.43	1.52
2	B	520	SER	CA-C	-6.61	1.44	1.52
2	B	789	MET	CA-C	-5.32	1.40	1.52
2	D	789	MET	CA-C	-5.32	1.40	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	747	LYS	CA-C-N	-6.33	114.05	121.64
2	D	747	LYS	C-N-CA	-6.33	114.05	121.64
2	B	747	LYS	CA-C-N	-6.29	114.09	121.64
2	B	747	LYS	C-N-CA	-6.29	114.09	121.64
2	D	529	PHE	CB-CA-C	-5.26	103.02	111.39
2	B	529	PHE	CB-CA-C	-5.23	103.08	111.39

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	426	GLN	Peptide
1	A	774	PHE	Peptide
2	B	429	CYS	Peptide
2	B	748	LEU	Peptide
1	C	426	GLN	Peptide
1	C	774	PHE	Peptide
2	D	429	CYS	Peptide
2	D	748	LEU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5870	0	5528	412	0
1	C	5870	0	5528	407	0
2	B	5717	0	5359	319	0
2	D	5717	0	5359	302	0
3	E	28	0	25	1	0
3	F	28	0	25	1	0
4	A	28	0	26	0	0
4	B	42	0	39	1	0
4	C	28	0	26	0	0
4	D	42	0	39	1	0
All	All	23370	0	21954	1400	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 31.

All (1400) 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:C:149:SER:HB2	1:C:179:ARG:HH21	1.33	0.93
1:A:149:SER:HB2	1:A:179:ARG:HH21	1.32	0.93
1:A:511:VAL:HG13	1:A:512:GLN:HG3	1.52	0.92
1:C:511:VAL:HG13	1:C:512:GLN:HG3	1.52	0.91
1:A:574:SER:HB2	1:A:577:GLN:HE21	1.36	0.91
1:C:574:SER:HB2	1:C:577:GLN:HE21	1.36	0.90
1:A:164:ILE:HD11	1:A:240:ILE:HG12	1.56	0.87
1:C:164:ILE:HD11	1:C:240:ILE:HG12	1.56	0.87
1:A:520:ASN:ND2	1:A:707:GLN:OE1	2.09	0.86
1:A:753:ASP:N	1:A:753:ASP:OD1	2.05	0.85
1:C:520:ASN:ND2	1:C:707:GLN:OE1	2.09	0.84
1:A:138:LEU:HD22	1:A:365:GLY:HA3	1.60	0.84
1:C:138:LEU:HD22	1:C:365:GLY:HA3	1.59	0.83
1:A:446:THR:OG1	1:A:448:ASN:OD1	1.97	0.83
1:C:446:THR:OG1	1:C:448:ASN:OD1	1.97	0.81
1:C:753:ASP:OD1	1:C:753:ASP:N	2.05	0.81
1:C:698:ASP:OD2	1:C:699:LYS:NZ	2.14	0.81
1:A:94:HIS:N	1:A:122:THR:OG1	2.14	0.80
2:B:488:LYS:NZ	2:B:688:ASN:OD1	2.15	0.79
1:C:94:HIS:N	1:C:122:THR:OG1	2.14	0.79
2:D:709:PHE:O	2:D:711:GLN:NE2	2.14	0.79
1:A:698:ASP:OD2	1:A:699:LYS:NZ	2.14	0.78
2:D:488:LYS:NZ	2:D:688:ASN:OD1	2.15	0.78
2:D:668:ASP:OD1	2:D:670:LYS:N	2.16	0.77
1:C:139:ARG:HH12	1:C:143:PRO:HB3	1.49	0.77
1:C:274:GLU:OE1	1:C:274:GLU:N	2.18	0.76
1:A:139:ARG:HH12	1:A:143:PRO:HB3	1.49	0.76
2:B:709:PHE:O	2:B:711:GLN:NE2	2.14	0.76
1:C:835:ALA:HA	1:C:838:PHE:HB2	1.68	0.76
2:D:326:GLU:HA	2:D:329:ILE:HB	1.67	0.75
2:B:488:LYS:HD3	2:B:688:ASN:HA	1.67	0.75
1:A:274:GLU:N	1:A:274:GLU:OE1	2.18	0.75
2:D:535:SER:OG	2:D:536:VAL:N	2.18	0.75
2:B:732:ASP:OD1	2:B:733:ALA:N	2.20	0.75
1:A:849:ILE:O	1:A:852:ILE:HB	1.87	0.75
1:A:835:ALA:HA	1:A:838:PHE:HB2	1.68	0.75
1:C:849:ILE:O	1:C:852:ILE:HB	1.87	0.75
1:A:562:LEU:HD23	1:A:757:LEU:HD13	1.69	0.74
2:B:668:ASP:OD1	2:B:670:LYS:N	2.16	0.74
2:D:488:LYS:HD3	2:D:688:ASN:HA	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:706:LYS:O	1:A:708:SER:OG	2.05	0.74
2:B:326:GLU:HA	2:B:329:ILE:HB	1.67	0.74
2:D:732:ASP:OD1	2:D:733:ALA:N	2.20	0.74
1:C:706:LYS:O	1:C:708:SER:OG	2.05	0.74
2:D:524:ASP:OD1	2:D:525:PHE:N	2.21	0.74
1:A:371:GLN:HB2	1:A:389:ASN:HA	1.70	0.74
1:A:528:SER:OG	1:A:530:GLN:OE1	2.06	0.73
1:C:44:GLU:O	1:C:48:GLN:NE2	2.19	0.73
1:A:804:GLY:O	1:A:808:ASP:N	2.20	0.73
1:A:849:ILE:HA	1:A:852:ILE:HD12	1.71	0.73
1:C:562:LEU:HD23	1:C:757:LEU:HD13	1.69	0.73
1:A:44:GLU:O	1:A:48:GLN:NE2	2.19	0.73
2:B:269:VAL:HG11	2:B:371:ARG:HB3	1.70	0.73
1:C:690:ASP:OD2	1:C:692:ARG:NH1	2.22	0.72
2:D:269:VAL:HG11	2:D:371:ARG:HB3	1.70	0.72
1:A:690:ASP:OD2	1:A:692:ARG:NH1	2.22	0.72
1:C:71:ALA:HB1	1:C:106:PRO:HG2	1.72	0.72
1:C:371:GLN:HB2	1:C:389:ASN:HA	1.70	0.72
1:C:849:ILE:HA	1:C:852:ILE:HD12	1.71	0.71
2:D:772:TRP:O	2:D:775:GLN:N	2.23	0.71
1:A:155:MET:SD	1:A:155:MET:N	2.63	0.71
2:B:815:ILE:HG13	2:B:817:ASN:OD1	1.90	0.71
1:C:528:SER:OG	1:C:530:GLN:OE1	2.06	0.71
2:D:257:ILE:HG12	2:D:278:ILE:HB	1.73	0.71
1:C:804:GLY:O	1:C:808:ASP:N	2.20	0.71
2:D:232:CYS:SG	2:D:233:THR:N	2.64	0.71
2:B:257:ILE:HG12	2:B:278:ILE:HB	1.73	0.71
1:A:777:SER:OG	1:A:778:GLY:N	2.22	0.71
2:B:524:ASP:OD1	2:B:525:PHE:N	2.21	0.71
2:B:535:SER:OG	2:B:536:VAL:N	2.18	0.71
2:B:772:TRP:O	2:B:775:GLN:N	2.23	0.71
2:D:380:LYS:O	2:D:383:SER:OG	2.08	0.71
1:A:71:ALA:HB1	1:A:106:PRO:HG2	1.72	0.70
2:B:113:ASP:O	2:B:116:SER:OG	2.09	0.70
2:B:232:CYS:SG	2:B:233:THR:N	2.64	0.70
1:A:582:THR:OG1	2:B:814:ASP:OD2	2.08	0.70
2:B:157:MET:HE1	2:B:182:PHE:HZ	1.57	0.70
1:A:446:THR:OG1	1:A:450:ASP:N	2.23	0.70
1:C:777:SER:OG	1:C:778:GLY:N	2.23	0.70
1:A:146:HIS:HA	1:A:179:ARG:HH12	1.56	0.69
2:B:178:GLY:O	2:B:182:PHE:N	2.20	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:ALA:HA	1:C:91:LEU:O	1.92	0.69
2:D:815:ILE:HG13	2:D:817:ASN:OD1	1.91	0.69
1:C:446:THR:OG1	1:C:450:ASP:N	2.23	0.69
2:D:157:MET:HE1	2:D:182:PHE:HZ	1.57	0.69
2:D:178:GLY:O	2:D:182:PHE:N	2.20	0.69
1:A:830:THR:OG1	2:D:557:CYS:SG	2.51	0.69
2:D:701:GLU:OE1	2:D:701:GLU:N	2.21	0.68
1:A:31:ALA:HA	1:A:91:LEU:O	1.92	0.68
1:C:232:ALA:HA	1:C:235:LEU:HD23	1.76	0.68
1:C:374:ILE:HB	1:C:385:VAL:HG23	1.75	0.68
1:A:797:ILE:O	1:A:800:SER:OG	2.12	0.68
1:A:374:ILE:HB	1:A:385:VAL:HG23	1.75	0.68
1:A:599:TYR:HB2	1:A:624:LEU:HD23	1.76	0.68
1:A:133:ILE:O	1:A:134:HIS:ND1	2.28	0.67
1:C:599:TYR:HB2	1:C:624:LEU:HD23	1.76	0.67
1:C:797:ILE:O	1:C:800:SER:OG	2.11	0.67
2:D:113:ASP:O	2:D:116:SER:OG	2.09	0.67
1:A:829:LEU:HD11	2:D:554:PHE:HE1	1.58	0.67
2:B:208:SER:OG	2:B:236:GLU:OE2	2.13	0.67
1:C:146:HIS:HA	1:C:179:ARG:HH12	1.56	0.67
1:C:155:MET:N	1:C:155:MET:SD	2.63	0.67
2:D:302:THR:O	2:D:305:SER:OG	2.13	0.67
1:C:133:ILE:O	1:C:134:HIS:ND1	2.28	0.67
1:A:718:VAL:O	1:A:721:SER:OG	2.13	0.67
1:C:91:LEU:HD11	1:C:119:LEU:HB2	1.77	0.67
1:A:70:ASN:HD21	1:A:72:ILE:HD12	1.59	0.66
2:D:112:LEU:HD12	2:D:112:LEU:H	1.60	0.66
1:C:415:MET:O	1:C:417:THR:HG23	1.96	0.66
1:A:232:ALA:HA	1:A:235:LEU:HD23	1.76	0.66
2:B:612:LEU:HD11	1:C:638:SER:HB3	1.78	0.66
1:C:70:ASN:HD21	1:C:72:ILE:HD12	1.59	0.66
1:A:543:GLU:OE1	1:A:543:GLU:N	2.21	0.66
2:B:112:LEU:HD12	2:B:112:LEU:H	1.60	0.66
1:C:336:TRP:O	1:C:338:THR:N	2.25	0.66
2:B:41:LEU:HA	2:B:100:ALA:HB3	1.77	0.65
1:C:60:LEU:HD21	1:C:313:VAL:HG11	1.79	0.65
1:C:543:GLU:OE1	1:C:543:GLU:N	2.21	0.65
2:D:609:LEU:HD21	2:D:635:TRP:CZ2	2.31	0.65
1:A:336:TRP:O	1:A:338:THR:N	2.25	0.65
1:A:580:GLN:H	2:B:812:GLN:HG2	1.61	0.65
2:D:154:ALA:HA	2:D:157:MET:HE2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:701:GLU:OE1	2:B:701:GLU:N	2.21	0.65
1:C:362:ASN:OD1	1:C:366:ASP:N	2.28	0.65
2:D:138:ASP:OD1	2:D:139:GLU:N	2.30	0.65
1:A:362:ASN:OD1	1:A:366:ASP:N	2.28	0.65
2:B:567:LEU:O	2:B:570:SER:OG	2.15	0.65
1:C:79:CYS:HA	1:C:83:ILE:HB	1.79	0.65
1:A:126:SER:O	1:A:129:SER:OG	2.06	0.65
2:B:380:LYS:O	2:B:383:SER:OG	2.08	0.65
2:B:430:MET:O	2:B:432:ASN:N	2.30	0.65
1:C:444:GLU:HG2	1:C:445:PHE:H	1.62	0.65
1:A:27:VAL:N	1:A:59:GLN:O	2.30	0.65
1:A:79:CYS:HA	1:A:83:ILE:HB	1.79	0.65
1:A:91:LEU:HD11	1:A:119:LEU:HB2	1.77	0.65
1:A:636:LEU:O	1:A:638:SER:OG	2.14	0.65
1:C:27:VAL:N	1:C:59:GLN:O	2.30	0.65
1:C:846:VAL:O	1:C:849:ILE:HG12	1.97	0.65
2:D:41:LEU:HA	2:D:100:ALA:HB3	1.77	0.65
2:D:102:ASP:OD1	2:D:102:ASP:N	2.28	0.65
1:A:291:GLN:O	1:A:372:TYR:HB2	1.97	0.65
2:B:176:PHE:O	2:B:178:GLY:N	2.30	0.65
1:C:636:LEU:O	1:C:638:SER:OG	2.14	0.65
1:C:155:MET:HB2	1:C:160:TRP:H	1.62	0.64
1:A:248:ASP:O	1:A:251:THR:OG1	2.12	0.64
1:A:846:VAL:O	1:A:849:ILE:HG12	1.97	0.64
2:B:102:ASP:OD1	2:B:102:ASP:N	2.28	0.64
1:C:117:PRO:HG2	1:C:342:PHE:HB3	1.79	0.64
2:D:176:PHE:O	2:D:178:GLY:N	2.30	0.64
1:A:415:MET:O	1:A:417:THR:HG23	1.96	0.64
1:C:770:THR:HG22	1:C:771:GLY:H	1.62	0.64
2:D:410:THR:OG1	2:D:411:LEU:N	2.31	0.64
2:D:732:ASP:OD2	2:D:762:TYR:OH	2.12	0.64
2:B:609:LEU:HD21	2:B:635:TRP:CZ2	2.32	0.64
2:D:134:MET:O	2:D:145:GLN:NE2	2.28	0.64
1:A:444:GLU:HG2	1:A:445:PHE:H	1.62	0.64
2:B:138:ASP:OD1	2:B:139:GLU:N	2.30	0.64
1:C:291:GLN:O	1:C:372:TYR:HB2	1.97	0.64
1:C:747:LEU:HD23	1:C:747:LEU:H	1.63	0.64
1:A:728:GLU:HA	1:A:731:ASN:HD21	1.62	0.64
1:A:772:GLU:OE1	1:A:772:GLU:N	2.31	0.64
2:D:430:MET:O	2:D:432:ASN:N	2.30	0.64
1:A:60:LEU:HD21	1:A:313:VAL:HG11	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:732:ASP:OD2	2:B:762:TYR:OH	2.12	0.64
1:C:789:TRP:CD1	1:C:789:TRP:H	2.14	0.64
3:F:2:NAG:H3	3:F:2:NAG:H83	1.80	0.64
1:A:155:MET:HB2	1:A:160:TRP:H	1.62	0.63
1:C:728:GLU:HA	1:C:731:ASN:HD21	1.62	0.63
2:B:154:ALA:HA	2:B:157:MET:HE2	1.78	0.63
2:B:760:THR:OG1	2:B:761:GLY:N	2.26	0.63
1:C:541:ASN:OD1	1:C:542:ASN:N	2.28	0.63
2:B:831:LEU:O	2:B:835:THR:HG23	1.98	0.63
1:A:789:TRP:CD1	1:A:789:TRP:H	2.14	0.63
2:D:831:LEU:O	2:D:835:THR:HG23	1.98	0.63
1:A:770:THR:HG22	1:A:771:GLY:H	1.62	0.63
1:C:228:LEU:O	1:C:231:GLU:HB3	1.98	0.63
1:C:772:GLU:OE1	1:C:772:GLU:N	2.31	0.63
1:A:747:LEU:H	1:A:747:LEU:HD23	1.63	0.63
2:B:410:THR:OG1	2:B:411:LEU:N	2.31	0.63
2:D:760:THR:OG1	2:D:761:GLY:N	2.26	0.63
1:C:580:GLN:O	1:C:582:THR:N	2.32	0.63
2:D:532:THR:OG1	2:D:533:GLY:N	2.26	0.63
2:B:302:THR:O	2:B:305:SER:OG	2.13	0.62
1:C:126:SER:O	1:C:129:SER:OG	2.06	0.62
2:D:169:PHE:HB3	2:D:227:ILE:HB	1.82	0.62
2:D:529:PHE:HB2	2:D:530:ILE:HG12	1.81	0.62
1:A:117:PRO:HG2	1:A:342:PHE:HB3	1.79	0.62
1:A:228:LEU:O	1:A:231:GLU:HB3	1.99	0.62
1:A:111:ALA:HB1	1:A:116:ILE:HD12	1.81	0.62
1:C:111:ALA:HB1	1:C:116:ILE:HD12	1.81	0.62
2:D:567:LEU:O	2:D:570:SER:OG	2.15	0.62
1:A:580:GLN:O	1:A:582:THR:N	2.32	0.62
3:E:2:NAG:H83	3:E:2:NAG:H3	1.80	0.62
2:B:169:PHE:HB3	2:B:227:ILE:HB	1.82	0.62
2:B:230:LEU:HD12	2:B:231:TYR:H	1.65	0.62
1:C:532:ASP:N	1:C:532:ASP:OD1	2.29	0.62
2:D:208:SER:OG	2:D:236:GLU:OE2	2.13	0.62
1:A:124:ARG:NH1	1:A:142:PRO:O	2.33	0.62
1:A:854:ILE:O	1:A:857:ALA:HB3	2.00	0.62
2:D:260:SER:HB2	2:D:281:SER:HB3	1.82	0.62
1:A:532:ASP:OD1	1:A:532:ASP:N	2.29	0.61
1:A:720:LEU:HB3	1:A:723:MET:HE3	1.82	0.61
1:C:124:ARG:NH1	1:C:142:PRO:O	2.33	0.61
1:A:148:SER:HG	1:A:151:TRP:HE3	1.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:260:SER:HB2	2:B:281:SER:HB3	1.82	0.61
2:B:529:PHE:HB2	2:B:530:ILE:HG12	1.81	0.61
1:A:733:GLU:N	1:A:737:GLU:OE2	2.32	0.61
1:C:733:GLU:N	1:C:737:GLU:OE2	2.32	0.61
2:B:532:THR:OG1	2:B:533:GLY:N	2.26	0.61
2:D:154:ALA:HB2	2:D:182:PHE:HE1	1.65	0.61
1:C:540:ILE:HD12	1:C:550:PHE:CD2	2.36	0.61
1:A:510:ARG:HA	1:A:517:LYS:HA	1.83	0.61
2:B:154:ALA:HB2	2:B:182:PHE:HE1	1.65	0.61
1:C:854:ILE:O	1:C:857:ALA:HB3	2.00	0.61
1:A:830:THR:HG23	1:A:831:CYS:H	1.66	0.61
1:A:853:PHE:HA	1:A:856:ILE:HD12	1.83	0.61
1:C:830:THR:HG23	1:C:831:CYS:H	1.66	0.61
1:A:640:ILE:HD12	1:A:640:ILE:H	1.66	0.61
1:C:146:HIS:HA	1:C:179:ARG:NH1	2.16	0.61
1:C:143:PRO:HG2	1:C:146:HIS:HB2	1.83	0.60
1:C:510:ARG:HA	1:C:517:LYS:HA	1.83	0.60
1:A:146:HIS:HA	1:A:179:ARG:NH1	2.16	0.60
1:C:640:ILE:HD12	1:C:640:ILE:H	1.66	0.60
2:D:230:LEU:HD12	2:D:231:TYR:H	1.65	0.60
2:B:423:ASP:HB3	2:B:428:THR:OG1	2.02	0.60
1:C:720:LEU:HB3	1:C:723:MET:HE3	1.82	0.60
1:C:853:PHE:HA	1:C:856:ILE:HD12	1.83	0.60
2:D:409:VAL:HG12	2:D:479:TYR:HD1	1.66	0.60
1:A:108:SER:OG	1:A:109:TYR:N	2.35	0.60
2:B:44:THR:HG23	2:B:46:ASP:H	1.66	0.60
2:B:411:LEU:HG	2:B:412:GLU:H	1.66	0.60
2:B:420:GLU:OE2	2:B:458:LYS:NZ	2.35	0.60
2:B:740:ALA:O	2:B:742:ARG:N	2.35	0.60
1:C:108:SER:OG	1:C:109:TYR:N	2.35	0.60
1:A:541:ASN:OD1	1:A:542:ASN:N	2.28	0.60
2:D:423:ASP:HB3	2:D:428:THR:OG1	2.02	0.60
2:B:527:VAL:HG13	2:B:528:PRO:HD2	1.84	0.59
2:D:740:ALA:O	2:D:742:ARG:N	2.35	0.59
2:B:134:MET:O	2:B:145:GLN:NE2	2.28	0.59
1:C:146:HIS:O	1:C:179:ARG:NH2	2.35	0.59
1:C:148:SER:HG	1:C:151:TRP:HE3	1.49	0.59
1:C:698:ASP:OD1	1:C:699:LYS:N	2.35	0.59
1:C:842:ALA:HA	1:C:845:ILE:HD12	1.84	0.59
2:D:527:VAL:HG13	2:D:528:PRO:HD2	1.84	0.59
1:A:143:PRO:HG2	1:A:146:HIS:HB2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:747:LYS:O	2:B:748:LEU:HD22	2.02	0.59
1:C:130:ASP:OD1	1:C:132:SER:N	2.31	0.59
1:A:486:LYS:HD3	1:A:805:PHE:CE2	2.38	0.59
1:A:698:ASP:OD1	1:A:699:LYS:N	2.35	0.59
2:D:80:SER:O	2:D:83:THR:OG1	2.20	0.59
1:A:523:MET:SD	1:A:544:ARG:HG2	2.43	0.59
1:A:540:ILE:HD12	1:A:550:PHE:CD2	2.36	0.59
1:A:842:ALA:HA	1:A:845:ILE:HD12	1.84	0.59
2:B:469:SER:HA	2:B:474:PHE:CE1	2.38	0.59
1:C:88:TYR:HA	1:C:336:TRP:HZ3	1.68	0.59
2:D:747:LYS:O	2:D:748:LEU:HD22	2.02	0.59
1:A:511:VAL:HG22	1:A:512:GLN:H	1.67	0.59
2:D:44:THR:HG23	2:D:46:ASP:H	1.66	0.59
2:D:411:LEU:HG	2:D:412:GLU:H	1.66	0.59
2:D:675:ASN:HA	2:D:680:PRO:HG3	1.85	0.59
1:A:146:HIS:O	1:A:179:ARG:NH2	2.35	0.59
1:A:715:ARG:HB3	1:A:724:TYR:CE2	2.38	0.59
2:B:409:VAL:HG12	2:B:479:TYR:HD1	1.66	0.59
1:C:511:VAL:HG22	1:C:512:GLN:H	1.67	0.59
1:C:523:MET:SD	1:C:544:ARG:HG2	2.43	0.59
2:D:469:SER:HA	2:D:474:PHE:CE1	2.38	0.59
1:C:73:GLN:HA	1:C:76:LEU:HG	1.83	0.59
2:D:334:MET:SD	2:D:334:MET:N	2.76	0.59
2:D:699:TYR:O	2:D:702:MET:N	2.36	0.59
1:A:27:VAL:O	1:A:61:GLN:N	2.36	0.58
1:A:427:GLU:HB2	1:A:428:PRO:HD3	1.85	0.58
1:A:486:LYS:HD3	1:A:805:PHE:CZ	2.38	0.58
1:A:801:HIS:CD2	1:A:806:MET:HG2	2.38	0.58
2:B:467:LYS:NZ	2:B:788:GLU:OE1	2.35	0.58
1:C:248:ASP:O	1:C:251:THR:OG1	2.12	0.58
1:A:73:GLN:HA	1:A:76:LEU:HG	1.83	0.58
1:C:27:VAL:O	1:C:61:GLN:N	2.36	0.58
1:C:486:LYS:HD3	1:C:805:PHE:CE2	2.38	0.58
1:C:486:LYS:HD3	1:C:805:PHE:CZ	2.38	0.58
1:A:353:ASP:OD1	1:A:353:ASP:N	2.34	0.58
2:B:775:GLN:N	2:B:775:GLN:OE1	2.36	0.58
1:C:569:ARG:H	1:C:680:ARG:HH12	1.51	0.58
1:C:715:ARG:HB3	1:C:724:TYR:CE2	2.38	0.58
1:C:754:SER:O	1:C:756:VAL:N	2.36	0.58
2:B:365:ILE:HG22	2:B:375:ARG:HA	1.85	0.58
1:C:88:TYR:HA	1:C:336:TRP:CZ3	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:699:TYR:O	2:B:702:MET:N	2.36	0.58
1:C:801:HIS:CD2	1:C:806:MET:HG2	2.39	0.58
1:A:88:TYR:HA	1:A:336:TRP:CZ3	2.38	0.58
2:D:420:GLU:OE2	2:D:458:LYS:NZ	2.35	0.58
2:B:78:PRO:O	2:B:82:ILE:HG12	2.04	0.58
2:D:365:ILE:HG22	2:D:375:ARG:HA	1.85	0.58
2:D:365:ILE:HD12	2:D:373:TRP:HB3	1.84	0.58
2:B:365:ILE:HD12	2:B:373:TRP:HB3	1.84	0.57
1:C:68:LYS:N	1:C:74:MET:SD	2.77	0.57
1:A:313:VAL:HG23	1:A:316:LEU:HD23	1.86	0.57
1:A:754:SER:O	1:A:756:VAL:N	2.36	0.57
1:C:313:VAL:HA	1:C:316:LEU:HB3	1.86	0.57
2:D:437:GLN:OE1	2:D:437:GLN:N	2.37	0.57
1:A:68:LYS:N	1:A:74:MET:SD	2.77	0.57
2:B:334:MET:SD	2:B:334:MET:N	2.76	0.57
2:B:491:ASN:ND2	4:B:905:NAG:O7	2.32	0.57
2:D:156:VAL:HG22	2:D:379:TRP:CE2	2.39	0.57
2:D:775:GLN:N	2:D:775:GLN:OE1	2.36	0.57
1:A:88:TYR:HA	1:A:336:TRP:HZ3	1.68	0.57
1:A:674:ALA:HA	2:B:655:ILE:HD11	1.85	0.57
2:B:675:ASN:HA	2:B:680:PRO:HG3	1.85	0.57
1:C:313:VAL:HG23	1:C:316:LEU:HD23	1.86	0.57
2:D:180:GLN:O	2:D:184:ASN:ND2	2.38	0.57
2:B:156:VAL:HG22	2:B:379:TRP:CE2	2.39	0.57
2:B:437:GLN:N	2:B:437:GLN:OE1	2.37	0.57
1:C:543:GLU:H	1:C:543:GLU:CD	2.11	0.57
1:C:718:VAL:O	1:C:721:SER:OG	2.13	0.57
2:B:180:GLN:O	2:B:184:ASN:ND2	2.38	0.57
2:B:547:PRO:HA	2:B:817:ASN:HB3	1.87	0.57
1:C:353:ASP:OD1	1:C:353:ASP:N	2.34	0.57
1:C:427:GLU:HB2	1:C:428:PRO:HD3	1.85	0.57
1:A:630:PHE:O	1:A:634:VAL:HG23	2.04	0.57
1:A:313:VAL:HA	1:A:316:LEU:HB3	1.86	0.57
1:A:299:SER:HA	1:A:302:ILE:HD12	1.86	0.57
1:A:448:ASN:OD1	1:A:449:GLY:N	2.38	0.57
1:A:569:ARG:H	1:A:680:ARG:HH12	1.51	0.57
1:A:580:GLN:HB2	2:B:812:GLN:HB3	1.87	0.57
1:C:387:ILE:HD13	1:C:396:ASN:CB	2.35	0.57
1:C:591:VAL:HG21	1:C:632:TRP:CD1	2.40	0.57
2:D:258:VAL:HG13	2:D:259:PRO:HD2	1.86	0.57
2:D:642:PHE:O	2:D:645:SER:OG	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:VAL:HG21	1:A:632:TRP:CD1	2.40	0.56
1:C:448:ASN:OD1	1:C:449:GLY:N	2.38	0.56
1:C:630:PHE:O	1:C:634:VAL:HG23	2.05	0.56
2:B:80:SER:O	2:B:83:THR:OG1	2.20	0.56
2:B:733:ALA:O	2:B:736:LEU:N	2.37	0.56
2:B:818:MET:SD	2:B:818:MET:N	2.78	0.56
1:C:71:ALA:CB	1:C:106:PRO:HG2	2.35	0.56
2:D:268:THR:O	2:D:268:THR:OG1	2.23	0.56
2:D:818:MET:SD	2:D:818:MET:N	2.78	0.56
1:A:95:PRO:HG3	1:A:103:THR:HG21	1.87	0.56
1:A:387:ILE:HD13	1:A:396:ASN:CB	2.35	0.56
1:A:577:GLN:O	2:B:812:GLN:HG3	2.05	0.56
2:B:744:GLU:CD	2:B:744:GLU:H	2.13	0.56
1:C:90:ILE:O	1:C:91:LEU:HD22	2.06	0.56
1:C:165:LEU:C	1:C:166:LEU:HD12	2.31	0.56
2:D:78:PRO:O	2:D:82:ILE:HG12	2.04	0.56
2:D:483:ASN:OD1	2:D:483:ASN:N	2.28	0.56
1:A:275:ILE:HD11	1:A:289:GLY:HA3	1.88	0.56
2:B:483:ASN:OD1	2:B:483:ASN:N	2.28	0.56
2:D:547:PRO:HA	2:D:817:ASN:HB3	1.87	0.56
2:D:685:THR:HG22	2:D:686:VAL:H	1.71	0.56
1:A:71:ALA:CB	1:A:106:PRO:HG2	2.35	0.56
1:A:90:ILE:O	1:A:91:LEU:HD22	2.06	0.56
1:A:248:ASP:OD1	1:A:248:ASP:N	2.39	0.56
1:A:769:THR:OG1	1:A:770:THR:N	2.39	0.56
1:A:842:ALA:O	1:A:845:ILE:HB	2.06	0.56
1:C:575:PHE:C	1:C:577:GLN:H	2.13	0.56
1:C:769:THR:OG1	1:C:770:THR:N	2.39	0.56
2:B:685:THR:HG22	2:B:686:VAL:H	1.71	0.56
1:C:299:SER:HA	1:C:302:ILE:HD12	1.86	0.56
1:A:602:ASP:OD2	1:A:623:THR:OG1	2.24	0.56
2:D:691:THR:OG1	2:D:692:GLU:N	2.39	0.56
2:D:733:ALA:O	2:D:736:LEU:N	2.37	0.56
2:B:258:VAL:HG13	2:B:259:PRO:HD2	1.86	0.56
1:C:490:THR:HG23	1:C:491:MET:HG2	1.88	0.56
1:A:165:LEU:C	1:A:166:LEU:HD12	2.31	0.56
1:A:833:ASN:O	1:A:836:GLY:N	2.37	0.56
2:D:467:LYS:NZ	2:D:788:GLU:OE1	2.35	0.56
1:A:543:GLU:H	1:A:543:GLU:CD	2.11	0.55
2:B:642:PHE:O	2:B:645:SER:OG	2.23	0.55
1:A:387:ILE:HD12	1:A:394:ILE:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:ASP:OD1	1:A:469:ARG:NH1	2.39	0.55
1:A:719:GLU:OE1	1:A:719:GLU:N	2.34	0.55
2:B:558:VAL:HG23	2:B:559:TRP:CD1	2.42	0.55
2:B:691:THR:OG1	2:B:692:GLU:N	2.39	0.55
1:C:790:LYS:O	1:C:793:VAL:HG12	2.06	0.55
1:C:95:PRO:HG3	1:C:103:THR:HG21	1.87	0.55
1:C:462:ASP:OD1	1:C:469:ARG:NH1	2.39	0.55
1:C:505:PHE:O	1:C:522:MET:N	2.39	0.55
1:C:540:ILE:HG12	1:C:778:GLY:O	2.07	0.55
2:D:180:GLN:N	2:D:180:GLN:OE1	2.38	0.55
1:A:290:LEU:HD13	1:A:372:TYR:CE2	2.42	0.55
1:A:540:ILE:HG12	1:A:778:GLY:O	2.07	0.55
1:C:375:MET:HE3	1:C:382:LEU:HG	1.87	0.55
1:C:833:ASN:O	1:C:836:GLY:N	2.37	0.55
2:B:741:GLY:HA2	2:B:801:CYS:SG	2.47	0.55
1:C:275:ILE:HD11	1:C:289:GLY:HA3	1.88	0.55
1:C:842:ALA:O	1:C:845:ILE:HB	2.06	0.55
2:B:40:ILE:HG23	2:B:99:PHE:HA	1.89	0.55
2:B:45:SER:O	2:B:47:GLU:N	2.40	0.55
2:B:541:SER:OG	2:B:542:ASN:N	2.39	0.55
1:A:375:MET:HE3	1:A:382:LEU:HG	1.87	0.55
1:A:510:ARG:HH21	1:A:513:ASN:HA	1.72	0.55
2:B:180:GLN:OE1	2:B:180:GLN:N	2.38	0.55
1:C:42:PHE:O	1:C:46:VAL:HG23	2.06	0.55
1:C:580:GLN:H	2:D:812:GLN:HG2	1.72	0.55
2:D:558:VAL:HG23	2:D:559:TRP:CD1	2.42	0.55
2:D:677:PHE:O	2:D:678:SER:OG	2.22	0.55
1:A:382:LEU:C	1:A:384:GLN:HE21	2.15	0.55
1:A:490:THR:HG23	1:A:491:MET:HG2	1.88	0.55
1:A:790:LYS:O	1:A:793:VAL:HG12	2.06	0.55
1:C:728:GLU:HA	1:C:731:ASN:ND2	2.21	0.55
2:D:541:SER:OG	2:D:542:ASN:N	2.39	0.55
2:B:608:LEU:HB2	2:B:620:VAL:HG21	1.89	0.55
1:C:560:THR:OG1	1:C:561:ILE:N	2.37	0.55
1:A:244:ALA:HB1	1:A:248:ASP:OD2	2.07	0.55
1:A:575:PHE:C	1:A:577:GLN:H	2.13	0.55
1:C:540:ILE:HG23	1:C:550:PHE:CD2	2.42	0.55
1:C:557:GLN:OE1	1:C:558:GLY:N	2.40	0.55
2:D:672:GLN:HA	2:D:702:MET:SD	2.47	0.55
1:A:540:ILE:HG23	1:A:550:PHE:CD2	2.42	0.54
2:B:672:GLN:HA	2:B:702:MET:SD	2.47	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:363:GLU:OE1	1:C:363:GLU:N	2.33	0.54
1:A:42:PHE:O	1:A:46:VAL:HG23	2.06	0.54
2:D:608:LEU:HB2	2:D:620:VAL:HG21	1.89	0.54
1:C:387:ILE:HD12	1:C:394:ILE:O	2.06	0.54
2:D:193:SER:O	2:D:193:SER:OG	2.25	0.54
2:D:433:THR:OG1	2:D:457:CYS:O	2.12	0.54
2:D:509:ALA:HB3	2:D:765:ALA:HB3	1.90	0.54
2:D:744:GLU:CD	2:D:744:GLU:H	2.13	0.54
2:B:268:THR:O	2:B:268:THR:OG1	2.23	0.54
2:D:45:SER:O	2:D:47:GLU:N	2.40	0.54
2:B:276:GLY:HA2	2:B:366:LEU:HD11	1.90	0.54
1:C:783:MET:HG3	1:C:790:LYS:CG	2.38	0.54
2:D:615:ASN:O	2:D:617:SER:N	2.40	0.54
2:D:741:GLY:HA2	2:D:801:CYS:SG	2.47	0.54
1:C:540:ILE:HD12	1:C:550:PHE:CE2	2.43	0.54
2:D:40:ILE:HG23	2:D:99:PHE:HA	1.89	0.54
1:A:375:MET:CE	1:A:382:LEU:HG	2.38	0.54
1:A:540:ILE:HD12	1:A:550:PHE:CE2	2.43	0.54
2:B:433:THR:OG1	2:B:434:VAL:N	2.41	0.54
1:C:290:LEU:HD13	1:C:372:TYR:CE2	2.42	0.54
1:A:728:GLU:HA	1:A:731:ASN:ND2	2.21	0.54
2:B:688:ASN:N	2:B:692:GLU:OE1	2.41	0.54
1:C:382:LEU:C	1:C:384:GLN:HE21	2.15	0.54
1:A:292:LEU:HD12	1:A:372:TYR:HB3	1.90	0.54
1:A:514:SER:OG	1:A:515:ASN:N	2.41	0.54
2:B:701:GLU:HG2	2:B:702:MET:HG2	1.90	0.54
2:B:829:MET:O	2:B:832:SER:OG	2.25	0.54
1:C:244:ALA:HB1	1:C:248:ASP:OD2	2.07	0.54
1:C:599:TYR:CD1	1:C:624:LEU:HD22	2.43	0.54
2:D:690:SER:OG	2:D:691:THR:N	2.41	0.54
1:A:783:MET:HG3	1:A:790:LYS:CG	2.38	0.53
1:C:515:ASN:O	1:C:516:LYS:HE2	2.08	0.53
1:C:583:LEU:O	1:C:587:VAL:HG23	2.08	0.53
1:C:626:SER:O	1:C:629:TRP:N	2.41	0.53
1:C:725:ARG:HG3	1:C:726:HIS:N	2.23	0.53
2:D:491:ASN:ND2	4:D:905:NAG:O7	2.32	0.53
1:A:515:ASN:O	1:A:516:LYS:HE2	2.09	0.53
1:A:557:GLN:OE1	1:A:558:GLY:N	2.40	0.53
1:A:725:ARG:HG3	1:A:726:HIS:N	2.23	0.53
2:D:276:GLY:HA2	2:D:366:LEU:HD11	1.90	0.53
2:D:701:GLU:HG2	2:D:702:MET:HG2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:GLN:N	2:B:812:GLN:HG2	2.23	0.53
1:A:304:ASP:O	1:A:308:VAL:HG23	2.08	0.53
1:A:505:PHE:O	1:A:522:MET:N	2.39	0.53
1:A:510:ARG:HB3	1:A:517:LYS:HG2	1.90	0.53
2:D:688:ASN:N	2:D:692:GLU:OE1	2.41	0.53
1:A:438:ASP:OD1	1:A:439:GLY:N	2.41	0.53
1:A:599:TYR:CD1	1:A:624:LEU:HD22	2.43	0.53
2:B:183:VAL:HG22	2:B:187:ARG:NH1	2.24	0.53
2:B:232:CYS:O	2:B:262:VAL:HG12	2.09	0.53
1:C:504:LYS:HG3	1:C:707:GLN:NE2	2.23	0.53
1:A:626:SER:O	1:A:629:TRP:N	2.41	0.53
1:A:849:ILE:HG13	1:A:850:PHE:N	2.24	0.53
1:C:304:ASP:O	1:C:308:VAL:HG23	2.08	0.53
1:C:596:VAL:HA	1:C:599:TYR:CE2	2.43	0.53
2:D:120:LEU:HB3	2:D:333:ASN:OD1	2.08	0.53
1:A:130:ASP:OD1	1:A:132:SER:N	2.31	0.53
1:A:139:ARG:HH12	1:A:143:PRO:CB	2.20	0.53
2:B:786:ASP:HA	1:C:717:GLN:HE22	1.74	0.53
1:C:228:LEU:O	1:C:231:GLU:CB	2.57	0.53
1:C:651:ARG:NH1	2:D:603:GLY:O	2.42	0.53
2:D:829:MET:O	2:D:832:SER:OG	2.25	0.53
1:A:504:LYS:HG3	1:A:707:GLN:NE2	2.23	0.53
1:A:583:LEU:O	1:A:587:VAL:HG23	2.08	0.53
2:B:509:ALA:HB3	2:B:765:ALA:HB3	1.90	0.53
1:C:438:ASP:OD1	1:C:439:GLY:N	2.41	0.53
1:A:397:ASP:OD1	1:A:397:ASP:N	2.39	0.53
2:B:49:ALA:HB1	2:B:290:PRO:HB3	1.91	0.53
1:C:74:MET:O	1:C:78:VAL:HG23	2.09	0.53
1:C:349:SER:O	1:C:349:SER:OG	2.27	0.53
2:D:77:ASP:O	2:D:80:SER:OG	2.16	0.53
2:D:232:CYS:O	2:D:262:VAL:HG12	2.09	0.53
1:A:74:MET:O	1:A:78:VAL:HG23	2.09	0.52
1:A:226:THR:HG22	1:A:255:ALA:HB1	1.91	0.52
1:C:292:LEU:HD12	1:C:372:TYR:HB3	1.90	0.52
2:D:183:VAL:HG22	2:D:187:ARG:NH1	2.24	0.52
1:A:149:SER:HB2	1:A:179:ARG:NH2	2.15	0.52
2:B:615:ASN:O	2:B:617:SER:N	2.40	0.52
1:C:397:ASP:OD1	1:C:397:ASP:N	2.39	0.52
1:C:510:ARG:HH21	1:C:513:ASN:HA	1.72	0.52
1:C:572:LEU:C	1:C:574:SER:H	2.18	0.52
1:C:578:PRO:HG2	1:C:668:TYR:HE1	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:LEU:O	1:A:231:GLU:CB	2.57	0.52
1:A:402:TRP:HB3	1:A:403:PRO:HD2	1.92	0.52
1:A:596:VAL:HA	1:A:599:TYR:CE2	2.43	0.52
1:C:248:ASP:OD1	1:C:248:ASP:N	2.39	0.52
1:C:510:ARG:HB3	1:C:517:LYS:HG2	1.90	0.52
2:D:433:THR:OG1	2:D:434:VAL:N	2.41	0.52
1:A:363:GLU:OE1	1:A:363:GLU:N	2.33	0.52
1:A:719:GLU:N	1:A:719:GLU:CD	2.68	0.52
1:A:789:TRP:O	1:A:792:GLN:HB3	2.10	0.52
2:B:120:LEU:HB3	2:B:333:ASN:OD1	2.08	0.52
2:B:152:GLN:HE22	2:B:360:PRO:HD2	1.75	0.52
2:B:436:CYS:N	2:B:455:LYS:O	2.42	0.52
1:C:602:ASP:OD2	1:C:623:THR:OG1	2.23	0.52
1:C:849:ILE:HG13	1:C:850:PHE:N	2.23	0.52
2:B:77:ASP:O	2:B:81:ILE:HG13	2.09	0.52
2:B:784:PHE:CD1	2:B:789:MET:HG3	2.44	0.52
1:C:270:VAL:HG21	1:C:274:GLU:HB2	1.91	0.52
1:C:719:GLU:OE1	1:C:719:GLU:N	2.34	0.52
2:D:517:GLU:O	2:D:520:SER:N	2.43	0.52
1:A:560:THR:OG1	1:A:561:ILE:N	2.37	0.52
1:A:572:LEU:C	1:A:574:SER:H	2.18	0.52
2:B:627:THR:OG1	2:B:628:SER:N	2.43	0.52
2:B:677:PHE:O	2:B:678:SER:OG	2.22	0.52
2:B:690:SER:OG	2:B:691:THR:N	2.41	0.52
1:C:375:MET:CE	1:C:382:LEU:HG	2.38	0.52
1:C:514:SER:OG	1:C:515:ASN:N	2.41	0.52
1:C:582:THR:OG1	1:C:583:LEU:N	2.42	0.52
2:D:49:ALA:HB1	2:D:290:PRO:HB3	1.92	0.52
2:D:152:GLN:HE22	2:D:360:PRO:HD2	1.75	0.52
2:D:249:LEU:HA	2:D:254:TYR:CE2	2.45	0.52
1:A:640:ILE:HG21	2:B:619:PRO:HB3	1.92	0.52
2:B:157:MET:HE1	2:B:182:PHE:CZ	2.43	0.52
2:D:77:ASP:O	2:D:81:ILE:HG13	2.09	0.52
2:D:784:PHE:CD1	2:D:789:MET:HG3	2.44	0.52
1:A:30:GLY:HA2	1:A:63:THR:O	2.10	0.52
1:A:362:ASN:CG	1:A:364:ASP:H	2.18	0.52
1:C:139:ARG:HH12	1:C:143:PRO:CB	2.20	0.51
1:C:789:TRP:O	1:C:792:GLN:HB3	2.10	0.51
2:D:406:LEU:HD12	2:D:474:PHE:CD2	2.45	0.51
2:D:562:MET:O	2:D:566:LEU:HG	2.10	0.51
2:D:751:ILE:HG13	2:D:752:GLY:N	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:PRO:HG2	1:A:668:TYR:HE1	1.74	0.51
1:A:595:ALA:HA	1:A:598:LEU:HD12	1.92	0.51
2:B:517:GLU:O	2:B:520:SER:N	2.43	0.51
2:B:673:ARG:HG3	2:B:677:PHE:CE2	2.45	0.51
1:C:81:ASP:O	1:C:85:SER:OG	2.27	0.51
2:D:411:LEU:HD21	2:D:485:LYS:HB3	1.91	0.51
1:A:270:VAL:HG21	1:A:274:GLU:HB2	1.91	0.51
1:A:688:ILE:HB	1:A:774:PHE:CE1	2.45	0.51
1:C:164:ILE:C	1:C:165:LEU:HD22	2.35	0.51
1:A:582:THR:OG1	1:A:583:LEU:N	2.42	0.51
1:A:790:LYS:HD2	1:A:791:GLN:N	2.25	0.51
2:B:249:LEU:HD23	2:B:254:TYR:CE2	2.46	0.51
1:C:595:ALA:HA	1:C:598:LEU:HD12	1.92	0.51
2:D:157:MET:HE1	2:D:182:PHE:CZ	2.43	0.51
1:A:508:GLN:HB2	1:A:519:TRP:NE1	2.25	0.51
2:B:751:ILE:HG13	2:B:752:GLY:N	2.24	0.51
1:C:226:THR:HG22	1:C:255:ALA:HB1	1.91	0.51
1:C:717:GLN:O	1:C:719:GLU:N	2.44	0.51
1:C:790:LYS:HD2	1:C:791:GLN:N	2.25	0.51
2:D:627:THR:OG1	2:D:628:SER:N	2.43	0.51
2:B:249:LEU:HA	2:B:254:TYR:CE2	2.45	0.51
2:B:411:LEU:HD21	2:B:485:LYS:HB3	1.91	0.51
1:C:47:ASN:HA	1:C:50:ASN:ND2	2.26	0.51
1:C:273:ARG:N	1:C:274:GLU:OE1	2.44	0.51
1:A:568:PRO:HA	1:A:680:ARG:NH1	2.26	0.51
2:B:154:ALA:HB2	2:B:182:PHE:CE1	2.45	0.51
2:B:200:GLU:CD	2:B:201:GLU:HB3	2.36	0.51
2:D:200:GLU:CD	2:D:201:GLU:HB3	2.36	0.51
2:B:673:ARG:HB3	2:B:676:ASP:HB2	1.92	0.51
2:B:691:THR:O	2:B:694:ASN:N	2.44	0.51
1:C:348:SER:O	1:C:350:LYS:N	2.44	0.51
1:C:402:TRP:HB3	1:C:403:PRO:HD2	1.92	0.51
1:C:568:PRO:HA	1:C:680:ARG:NH1	2.26	0.51
1:C:719:GLU:N	1:C:719:GLU:CD	2.68	0.51
2:D:673:ARG:HG3	2:D:677:PHE:CE2	2.45	0.51
1:C:30:GLY:HA2	1:C:63:THR:O	2.11	0.51
1:C:688:ILE:HB	1:C:774:PHE:CE1	2.45	0.51
1:A:422:VAL:O	1:A:423:THR:OG1	2.28	0.51
2:B:173:THR:HG23	2:B:231:TYR:HB3	1.94	0.51
2:B:230:LEU:HD12	2:B:231:TYR:N	2.25	0.51
2:B:562:MET:O	2:B:566:LEU:HG	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:508:GLN:HB2	1:C:519:TRP:NE1	2.25	0.51
1:C:580:GLN:HB2	2:D:812:GLN:HB3	1.93	0.51
1:C:752:TRP:CG	1:C:753:ASP:H	2.29	0.51
2:D:489:LYS:HB3	2:D:494:TRP:CZ3	2.46	0.51
2:D:772:TRP:O	2:D:773:LYS:C	2.54	0.51
1:A:164:ILE:C	1:A:165:LEU:HD22	2.35	0.50
1:A:540:ILE:HG23	1:A:550:PHE:CE2	2.47	0.50
1:A:717:GLN:O	1:A:719:GLU:N	2.44	0.50
2:B:282:TYR:CB	2:B:363:VAL:HG22	2.41	0.50
2:B:406:LEU:HD12	2:B:474:PHE:CD2	2.45	0.50
2:D:230:LEU:HD12	2:D:231:TYR:N	2.25	0.50
2:D:249:LEU:HD23	2:D:254:TYR:CE2	2.46	0.50
1:A:47:ASN:HA	1:A:50:ASN:ND2	2.26	0.50
1:A:111:ALA:HB1	1:A:116:ILE:HB	1.93	0.50
1:A:348:SER:O	1:A:350:LYS:N	2.44	0.50
1:C:362:ASN:CG	1:C:364:ASP:H	2.18	0.50
1:C:688:ILE:HG23	1:C:689:ASN:OD1	2.11	0.50
1:A:688:ILE:HG23	1:A:689:ASN:OD1	2.11	0.50
2:B:557:CYS:SG	1:C:830:THR:OG1	2.65	0.50
2:B:772:TRP:O	2:B:773:LYS:C	2.54	0.50
1:A:66:THR:OG1	1:A:67:HIS:N	2.37	0.50
2:D:547:PRO:O	2:D:817:ASN:HA	2.12	0.50
1:A:37:LYS:O	1:A:41:MET:HG2	2.12	0.50
1:A:273:ARG:N	1:A:274:GLU:OE1	2.44	0.50
1:A:349:SER:O	1:A:349:SER:OG	2.27	0.50
1:A:586:LEU:HG	2:B:822:PHE:CZ	2.47	0.50
1:A:752:TRP:CG	1:A:753:ASP:H	2.29	0.50
2:D:173:THR:HG23	2:D:231:TYR:HB3	1.94	0.50
2:D:282:TYR:CB	2:D:363:VAL:HG22	2.41	0.50
2:B:745:GLY:C	2:B:747:LYS:H	2.20	0.50
2:B:818:MET:O	2:B:822:PHE:HD1	1.95	0.50
1:C:30:GLY:O	1:C:90:ILE:HD12	2.12	0.50
1:C:277:GLY:HA2	1:C:280:LEU:HB3	1.94	0.50
2:D:673:ARG:HB3	2:D:676:ASP:HB2	1.92	0.50
1:C:111:ALA:HB1	1:C:116:ILE:HB	1.93	0.49
1:C:371:GLN:N	1:C:371:GLN:OE1	2.45	0.49
1:A:651:ARG:NH1	2:B:603:GLY:O	2.45	0.49
2:B:547:PRO:O	2:B:817:ASN:HA	2.12	0.49
1:C:37:LYS:O	1:C:41:MET:HG2	2.12	0.49
1:C:443:GLU:OE1	1:C:443:GLU:N	2.45	0.49
1:A:27:VAL:HA	1:A:87:VAL:HG11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:290:PRO:O	2:B:293:VAL:HG22	2.12	0.49
2:B:472:VAL:HG12	2:B:472:VAL:O	2.13	0.49
2:D:290:PRO:O	2:D:293:VAL:HG22	2.12	0.49
2:D:827:ALA:O	2:D:831:LEU:HG	2.12	0.49
1:A:30:GLY:O	1:A:90:ILE:HD12	2.12	0.49
1:A:73:GLN:O	1:A:76:LEU:HG	2.12	0.49
2:B:489:LYS:HB3	2:B:494:TRP:CZ3	2.47	0.49
1:C:390:GLY:O	1:C:392:HIS:N	2.45	0.49
2:D:288:GLY:O	2:D:292:ARG:N	2.41	0.49
2:D:568:ILE:O	2:D:572:VAL:HG23	2.13	0.49
2:D:745:GLY:C	2:D:747:LYS:H	2.20	0.49
1:A:338:THR:O	1:A:342:PHE:N	2.42	0.49
1:A:371:GLN:N	1:A:371:GLN:OE1	2.45	0.49
1:A:374:ILE:HD12	1:A:387:ILE:HG13	1.94	0.49
1:C:415:MET:SD	1:C:415:MET:N	2.86	0.49
1:C:714:PHE:HB3	1:C:724:TYR:HD2	1.78	0.49
2:D:154:ALA:HB2	2:D:182:PHE:CE1	2.45	0.49
2:B:70:LEU:HD12	2:B:71:VAL:H	1.77	0.49
2:B:568:ILE:O	2:B:572:VAL:HG23	2.13	0.49
1:C:540:ILE:HG23	1:C:550:PHE:CE2	2.47	0.49
2:D:472:VAL:HG12	2:D:472:VAL:O	2.13	0.49
1:A:139:ARG:N	1:A:365:GLY:O	2.35	0.49
1:A:786:ASP:OD1	1:A:786:ASP:N	2.44	0.49
2:B:230:LEU:O	2:B:258:VAL:HG13	2.13	0.49
1:C:704:THR:OG1	1:C:705:VAL:N	2.42	0.49
1:A:594:VAL:HG23	1:A:653:LEU:HD21	1.95	0.49
2:B:815:ILE:HG13	2:B:817:ASN:CG	2.38	0.49
2:B:817:ASN:OD1	2:B:818:MET:N	2.39	0.49
1:C:374:ILE:HD12	1:C:387:ILE:HG13	1.94	0.49
1:A:526:LEU:HD21	1:A:783:MET:O	2.12	0.49
1:C:27:VAL:HA	1:C:87:VAL:HG11	1.94	0.49
1:C:73:GLN:O	1:C:76:LEU:HG	2.12	0.49
1:C:139:ARG:N	1:C:365:GLY:O	2.35	0.49
1:C:336:TRP:CD1	1:C:338:THR:HG1	2.30	0.49
1:C:474:GLN:N	1:C:474:GLN:OE1	2.46	0.49
1:C:540:ILE:HG22	1:C:541:ASN:H	1.78	0.49
2:D:230:LEU:O	2:D:258:VAL:HG13	2.13	0.49
2:D:307:MET:HG3	2:D:308:LEU:N	2.28	0.49
2:D:436:CYS:N	2:D:455:LYS:O	2.42	0.49
1:A:540:ILE:HG22	1:A:541:ASN:H	1.78	0.49
1:C:635:LEU:HD12	1:C:635:LEU:HA	1.49	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:414:ALA:HB3	2:D:415:PRO:HD3	1.95	0.49
1:A:93:SER:HA	1:A:121:LEU:HB2	1.95	0.48
1:A:277:GLY:HA2	1:A:280:LEU:HB3	1.94	0.48
1:A:390:GLY:O	1:A:392:HIS:N	2.45	0.48
1:A:474:GLN:N	1:A:474:GLN:OE1	2.46	0.48
2:B:111:ILE:O	2:B:115:ILE:HG12	2.13	0.48
1:A:89:ALA:HB2	1:A:342:PHE:HE2	1.78	0.48
1:A:443:GLU:OE1	1:A:443:GLU:N	2.45	0.48
2:B:110:GLN:HA	2:B:113:ASP:OD2	2.14	0.48
1:C:285:ASP:HA	1:C:377:LEU:HD23	1.95	0.48
1:C:393:VAL:HG12	1:C:394:ILE:H	1.78	0.48
1:A:714:PHE:HB3	1:A:724:TYR:HD2	1.78	0.48
1:C:504:LYS:NZ	1:C:733:GLU:OE1	2.37	0.48
2:D:818:MET:O	2:D:822:PHE:HD1	1.95	0.48
2:B:173:THR:CG2	2:B:231:TYR:HB3	2.43	0.48
1:C:89:ALA:HB2	1:C:342:PHE:HE2	1.78	0.48
1:A:336:TRP:CD1	1:A:338:THR:HG1	2.31	0.48
2:B:489:LYS:HB3	2:B:494:TRP:CH2	2.49	0.48
2:B:712:ARG:HG3	2:B:716:ASP:OD2	2.14	0.48
1:C:526:LEU:HD21	1:C:783:MET:O	2.12	0.48
2:D:70:LEU:HD12	2:D:71:VAL:H	1.77	0.48
2:D:173:THR:CG2	2:D:231:TYR:HB3	2.44	0.48
1:A:162:HIS:NE2	1:A:413:TYR:HE2	2.11	0.48
1:A:285:ASP:HA	1:A:377:LEU:HD23	1.95	0.48
1:A:552:LYS:HB3	1:A:553:PRO:HD2	1.96	0.48
1:A:759:PHE:CD2	1:A:759:PHE:C	2.90	0.48
2:B:731:TYR:CG	2:B:732:ASP:N	2.82	0.48
1:C:719:GLU:CD	1:C:719:GLU:H	2.21	0.48
2:D:110:GLN:HA	2:D:113:ASP:OD2	2.13	0.48
1:A:139:ARG:NH2	1:A:143:PRO:HD3	2.29	0.48
1:A:535:VAL:HG22	1:A:781:ILE:CD1	2.44	0.48
1:A:580:GLN:HB2	2:B:812:GLN:C	2.39	0.48
2:B:193:SER:O	2:B:193:SER:OG	2.25	0.48
2:B:411:LEU:CG	2:B:412:GLU:H	2.26	0.48
2:B:440:ILE:HD13	2:B:450:PRO:HB3	1.95	0.48
2:B:757:PHE:CG	2:B:758:ALA:N	2.82	0.48
1:C:162:HIS:NE2	1:C:413:TYR:HE2	2.11	0.48
1:C:552:LYS:HB3	1:C:553:PRO:HD2	1.96	0.48
1:C:759:PHE:CD2	1:C:759:PHE:C	2.90	0.48
1:C:785:LYS:HD2	1:C:785:LYS:HA	1.71	0.48
2:D:173:THR:HG22	2:D:174:THR:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:MET:SD	1:A:415:MET:N	2.86	0.48
2:B:288:GLY:O	2:B:292:ARG:N	2.41	0.48
2:B:572:VAL:O	2:B:576:VAL:HG13	2.14	0.48
2:B:827:ALA:O	2:B:831:LEU:HG	2.12	0.48
2:D:85:ILE:O	2:D:88:LEU:HG	2.14	0.48
2:B:79:LYS:O	2:B:83:THR:HG23	2.14	0.48
2:B:173:THR:HG22	2:B:174:THR:N	2.28	0.48
1:C:786:ASP:OD1	1:C:786:ASP:N	2.45	0.48
1:C:810:ASP:O	1:C:813:TRP:N	2.38	0.48
2:D:79:LYS:O	2:D:83:THR:HG23	2.14	0.48
2:D:489:LYS:HB3	2:D:494:TRP:CH2	2.49	0.48
2:D:740:ALA:C	2:D:742:ARG:H	2.21	0.48
1:A:415:MET:O	1:A:417:THR:N	2.47	0.48
1:A:638:SER:HB3	2:D:612:LEU:HD11	1.96	0.48
2:B:307:MET:HG3	2:B:308:LEU:N	2.28	0.48
1:C:519:TRP:CH2	1:C:547:TYR:CD2	3.02	0.48
1:C:580:GLN:N	2:D:812:GLN:HG2	2.28	0.48
1:C:594:VAL:HG23	1:C:653:LEU:HD21	1.95	0.48
1:C:830:THR:HG23	1:C:831:CYS:N	2.29	0.48
2:D:411:LEU:CG	2:D:412:GLU:H	2.26	0.48
1:A:393:VAL:HG12	1:A:394:ILE:H	1.78	0.47
1:A:655:MET:HG2	2:B:610:TRP:CE2	2.48	0.47
1:A:830:THR:HG23	1:A:831:CYS:N	2.29	0.47
2:B:85:ILE:O	2:B:88:LEU:HG	2.14	0.47
2:B:740:ALA:C	2:B:742:ARG:H	2.21	0.47
1:C:139:ARG:NH2	1:C:143:PRO:HD3	2.29	0.47
1:C:788:PRO:O	1:C:790:LYS:N	2.47	0.47
2:D:172:VAL:HG12	2:D:203:LEU:HB2	1.95	0.47
1:A:703:ALA:HB1	1:A:731:ASN:HA	1.95	0.47
2:B:414:ALA:HB3	2:B:415:PRO:HD3	1.95	0.47
2:D:409:VAL:HG12	2:D:479:TYR:CD1	2.48	0.47
2:D:815:ILE:HG13	2:D:817:ASN:CG	2.38	0.47
1:C:149:SER:HB2	1:C:179:ARG:NH2	2.15	0.47
1:C:149:SER:OG	1:C:183:LEU:HD11	2.15	0.47
1:C:634:VAL:HA	2:D:617:SER:HB2	1.96	0.47
2:D:439:ARG:HG3	2:D:452:TYR:HB2	1.96	0.47
1:A:35:THR:HG22	1:A:38:HIS:H	1.79	0.47
1:A:803:ASN:C	1:A:805:PHE:H	2.22	0.47
2:B:204:LEU:O	2:B:205:LEU:HD23	2.14	0.47
2:B:439:ARG:HG3	2:B:452:TYR:HB2	1.96	0.47
2:B:822:PHE:O	2:B:825:LEU:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:SER:HA	1:C:121:LEU:HB2	1.95	0.47
1:C:362:ASN:OD1	1:C:365:GLY:N	2.47	0.47
1:C:411:ARG:O	1:C:413:TYR:N	2.48	0.47
1:C:803:ASN:C	1:C:805:PHE:H	2.23	0.47
2:D:204:LEU:O	2:D:205:LEU:HD23	2.14	0.47
1:A:148:SER:OG	1:A:151:TRP:HE3	1.97	0.47
1:A:519:TRP:CH2	1:A:547:TYR:CD2	3.02	0.47
1:A:788:PRO:O	1:A:790:LYS:N	2.47	0.47
2:B:35:ILE:HB	2:B:64:VAL:HG12	1.97	0.47
2:D:111:ILE:O	2:D:115:ILE:HG12	2.14	0.47
2:D:712:ARG:HG3	2:D:716:ASP:OD2	2.14	0.47
2:D:731:TYR:CG	2:D:732:ASP:N	2.82	0.47
1:A:362:ASN:OD1	1:A:365:GLY:N	2.47	0.47
1:A:740:GLN:O	1:A:740:GLN:NE2	2.48	0.47
2:B:230:LEU:HB3	2:B:258:VAL:CG2	2.45	0.47
2:B:409:VAL:HG12	2:B:479:TYR:CD1	2.48	0.47
1:A:149:SER:OG	1:A:183:LEU:HD11	2.14	0.47
1:A:806:MET:HE2	1:A:806:MET:HB2	1.71	0.47
2:B:172:VAL:HG12	2:B:203:LEU:HB2	1.95	0.47
2:B:833:LEU:HD23	2:B:833:LEU:HA	1.66	0.47
1:C:542:ASN:O	1:C:545:ALA:N	2.48	0.47
2:D:757:PHE:CG	2:D:758:ALA:N	2.82	0.47
2:D:822:PHE:O	2:D:825:LEU:HB3	2.15	0.47
1:A:82:LEU:HD12	1:A:82:LEU:H	1.80	0.47
1:C:66:THR:OG1	1:C:67:HIS:N	2.37	0.47
1:C:415:MET:O	1:C:417:THR:N	2.47	0.47
1:C:634:VAL:HG13	2:D:617:SER:OG	2.14	0.47
2:D:34:SER:HA	2:D:65:VAL:HG13	1.97	0.47
2:D:536:VAL:HG22	2:D:730:ILE:HG12	1.97	0.47
2:B:498:ILE:HD13	2:B:498:ILE:HA	1.63	0.47
2:B:687:PRO:HA	2:B:692:GLU:CD	2.40	0.47
1:C:848:GLY:HA2	1:C:851:LEU:HD12	1.96	0.47
2:D:440:ILE:HD13	2:D:450:PRO:HB3	1.96	0.47
1:A:810:ASP:O	1:A:813:TRP:N	2.38	0.47
1:A:829:LEU:HD11	2:D:554:PHE:CE1	2.46	0.47
1:C:82:LEU:HD12	1:C:82:LEU:H	1.80	0.47
1:C:148:SER:OG	1:C:151:TRP:HE3	1.97	0.47
1:C:215:VAL:C	1:C:216:LEU:HD23	2.40	0.47
1:C:703:ALA:HB1	1:C:731:ASN:HA	1.95	0.47
2:D:572:VAL:O	2:D:576:VAL:HG13	2.14	0.47
1:A:567:ILE:HG13	1:A:568:PRO:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:SER:O	1:A:577:GLN:N	2.48	0.46
1:A:583:LEU:HD22	2:B:813:LEU:O	2.15	0.46
1:C:655:MET:HG2	2:D:610:TRP:NE1	2.30	0.46
1:C:690:ASP:OD1	1:C:692:ARG:N	2.34	0.46
1:C:806:MET:HA	1:C:809:LEU:HD12	1.97	0.46
2:D:609:LEU:HG	2:D:635:TRP:NE1	2.31	0.46
1:A:516:LYS:HE2	1:A:516:LYS:HA	1.98	0.46
1:C:35:THR:HG22	1:C:38:HIS:H	1.79	0.46
1:C:740:GLN:O	1:C:740:GLN:NE2	2.48	0.46
2:D:35:ILE:HB	2:D:64:VAL:HG12	1.97	0.46
2:D:687:PRO:HA	2:D:692:GLU:CD	2.40	0.46
1:A:139:ARG:HH22	1:A:143:PRO:HD3	1.80	0.46
2:B:433:THR:OG1	2:B:457:CYS:O	2.12	0.46
2:B:500:GLU:OE2	2:B:505:ARG:NH1	2.49	0.46
2:B:536:VAL:HG22	2:B:730:ILE:HG12	1.97	0.46
2:D:415:PRO:C	2:D:416:PHE:HD1	2.23	0.46
2:D:437:GLN:HE21	2:D:439:ARG:NH1	2.13	0.46
2:D:770:SER:OG	2:D:772:TRP:HB2	2.16	0.46
1:A:848:GLY:HA2	1:A:851:LEU:HD12	1.96	0.46
2:B:34:SER:HA	2:B:65:VAL:HG13	1.97	0.46
2:B:609:LEU:HG	2:B:635:TRP:NE1	2.31	0.46
1:C:422:VAL:HG22	1:C:423:THR:N	2.30	0.46
1:C:535:VAL:HG22	1:C:781:ILE:CD1	2.44	0.46
1:A:215:VAL:C	1:A:216:LEU:HD23	2.40	0.46
1:A:245:SER:N	1:A:248:ASP:OD2	2.42	0.46
1:A:422:VAL:HG22	1:A:423:THR:N	2.30	0.46
1:A:719:GLU:CD	1:A:719:GLU:H	2.21	0.46
1:A:806:MET:HA	1:A:809:LEU:HD12	1.97	0.46
1:A:842:ALA:HA	1:A:845:ILE:CD1	2.45	0.46
2:B:178:GLY:HA2	2:B:181:ASP:HB3	1.97	0.46
2:B:415:PRO:C	2:B:416:PHE:HD1	2.23	0.46
2:B:825:LEU:O	2:B:828:ALA:N	2.35	0.46
2:D:500:GLU:OE2	2:D:505:ARG:NH1	2.49	0.46
2:D:752:GLY:O	2:D:753:SER:OG	2.31	0.46
2:D:783:LEU:HD12	2:D:783:LEU:HA	1.73	0.46
1:A:73:GLN:HA	1:A:76:LEU:CG	2.46	0.46
2:B:437:GLN:HE21	2:B:439:ARG:NH1	2.13	0.46
1:C:387:ILE:HG21	1:C:396:ASN:N	2.30	0.46
1:C:567:ILE:HG13	1:C:568:PRO:HD2	1.98	0.46
1:C:574:SER:O	1:C:577:GLN:N	2.48	0.46
1:C:754:SER:C	1:C:756:VAL:N	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:230:LEU:HB3	2:D:258:VAL:CG2	2.45	0.46
2:D:612:LEU:HD13	2:D:616:ASN:HB3	1.98	0.46
1:C:847:ALA:O	1:C:851:LEU:HG	2.15	0.46
1:A:387:ILE:HG21	1:A:396:ASN:N	2.30	0.46
1:A:411:ARG:O	1:A:413:TYR:N	2.48	0.46
1:A:444:GLU:HG2	1:A:445:PHE:N	2.29	0.46
1:A:671:ASN:HD21	2:B:813:LEU:HD11	1.81	0.46
1:C:73:GLN:HA	1:C:76:LEU:CG	2.46	0.46
1:C:667:SER:OG	1:C:668:TYR:N	2.49	0.46
2:D:127:HIS:O	2:D:131:SER:OG	2.28	0.46
1:A:542:ASN:O	1:A:545:ALA:N	2.48	0.46
1:A:656:VAL:HG11	2:B:828:ALA:HB2	1.98	0.46
2:B:736:LEU:HD23	2:B:736:LEU:HA	1.65	0.46
2:B:837:ILE:O	2:B:840:HIS:N	2.45	0.46
1:C:577:GLN:O	2:D:812:GLN:HG3	2.15	0.46
2:D:157:MET:SD	2:D:229:LEU:HD13	2.56	0.46
2:D:612:LEU:HD13	2:D:612:LEU:HA	1.43	0.46
1:A:161:ASN:HB2	1:A:162:HIS:CD2	2.51	0.46
1:A:754:SER:C	1:A:756:VAL:N	2.73	0.46
2:B:459:GLY:HA2	2:B:796:TRP:CZ3	2.51	0.46
2:B:786:ASP:N	2:B:786:ASP:OD1	2.49	0.46
1:C:28:ASN:HA	1:C:61:GLN:O	2.16	0.46
1:C:338:THR:O	1:C:342:PHE:N	2.42	0.46
1:C:842:ALA:HA	1:C:845:ILE:CD1	2.45	0.46
2:D:77:ASP:HB3	2:D:80:SER:HB3	1.98	0.46
1:A:28:ASN:HA	1:A:61:GLN:O	2.16	0.45
1:A:183:LEU:HA	1:A:183:LEU:HD23	1.73	0.45
1:A:785:LYS:HD2	1:A:785:LYS:HA	1.71	0.45
2:B:289:LEU:N	2:B:290:PRO:HD2	2.31	0.45
2:B:770:SER:OG	2:B:772:TRP:HB2	2.15	0.45
1:C:505:PHE:O	1:C:522:MET:HG3	2.16	0.45
1:A:690:ASP:OD1	1:A:690:ASP:C	2.58	0.45
1:A:723:MET:O	1:A:724:TYR:C	2.59	0.45
2:B:147:GLY:O	2:B:356:TYR:HB2	2.17	0.45
2:B:199:LEU:HD12	2:B:199:LEU:HA	1.66	0.45
2:D:94:ILE:HG22	2:D:96:GLY:H	1.81	0.45
2:D:289:LEU:N	2:D:290:PRO:HD2	2.31	0.45
2:D:296:GLY:O	2:D:300:ILE:HG22	2.16	0.45
1:A:595:ALA:O	1:A:598:LEU:HB2	2.16	0.45
1:A:725:ARG:NH2	2:B:430:MET:HG3	2.31	0.45
2:B:320:SER:HB2	2:B:323:ASN:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:496:GLY:O	2:B:499:GLY:N	2.49	0.45
1:C:801:HIS:NE2	1:C:806:MET:HG2	2.32	0.45
2:D:176:PHE:O	2:D:179:TYR:HD1	2.00	0.45
2:D:496:GLY:O	2:D:499:GLY:N	2.50	0.45
1:A:29:ILE:HG23	1:A:89:ALA:O	2.17	0.45
1:A:505:PHE:O	1:A:522:MET:HG3	2.17	0.45
1:A:550:PHE:HD1	1:A:550:PHE:HA	1.59	0.45
2:B:230:LEU:HB3	2:B:258:VAL:HG22	1.98	0.45
2:B:296:GLY:O	2:B:300:ILE:HG22	2.16	0.45
1:C:245:SER:N	1:C:248:ASP:OD2	2.42	0.45
1:C:557:GLN:HB2	1:C:754:SER:OG	2.16	0.45
2:D:35:ILE:HG23	2:D:37:ILE:HG12	1.99	0.45
2:D:169:PHE:HA	2:D:227:ILE:O	2.16	0.45
2:D:178:GLY:HA2	2:D:181:ASP:HB3	1.97	0.45
2:D:320:SER:HB2	2:D:323:ASN:HB2	1.98	0.45
1:A:115:ARG:O	1:A:117:PRO:HD3	2.16	0.45
1:A:424:ILE:O	1:A:430:VAL:HG21	2.16	0.45
1:A:805:PHE:O	1:A:808:ASP:HB3	2.16	0.45
2:B:115:ILE:O	2:B:119:THR:N	2.43	0.45
1:C:161:ASN:HB2	1:C:162:HIS:CD2	2.51	0.45
1:C:516:LYS:HE2	1:C:516:LYS:HA	1.98	0.45
1:C:591:VAL:HG13	1:C:592:HIS:N	2.32	0.45
1:C:595:ALA:O	1:C:598:LEU:HB2	2.16	0.45
2:D:459:GLY:HA2	2:D:796:TRP:CZ3	2.51	0.45
1:A:93:SER:HB3	1:A:121:LEU:HD12	1.99	0.45
1:A:440:THR:OG1	1:A:441:CYS:N	2.50	0.45
1:A:667:SER:OG	1:A:668:TYR:N	2.49	0.45
1:A:847:ALA:O	1:A:851:LEU:HG	2.15	0.45
1:C:115:ARG:O	1:C:117:PRO:HD3	2.16	0.45
1:C:137:PHE:O	1:C:138:LEU:HD23	2.17	0.45
1:C:169:ASP:OD1	1:C:217:GLN:HB3	2.17	0.45
1:C:666:ALA:O	1:C:667:SER:C	2.60	0.45
2:D:147:GLY:O	2:D:356:TYR:HB2	2.17	0.45
1:A:591:VAL:HG13	1:A:592:HIS:N	2.32	0.45
1:A:783:MET:HB3	1:A:783:MET:HE3	1.79	0.45
2:B:146:PHE:HD1	2:B:146:PHE:HA	1.63	0.45
2:B:249:LEU:HA	2:B:254:TYR:HE2	1.80	0.45
2:B:668:ASP:OD1	2:B:669:LYS:N	2.50	0.45
2:B:748:LEU:HD13	2:B:748:LEU:HA	1.70	0.45
1:C:29:ILE:HG23	1:C:89:ALA:O	2.17	0.45
2:D:67:ARG:NH2	2:D:92:ARG:O	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:170:SER:OG	2:D:200:GLU:HB3	2.16	0.45
2:D:554:PHE:CG	2:D:558:VAL:HG21	2.52	0.45
2:D:668:ASP:OD1	2:D:669:LYS:N	2.50	0.45
1:A:73:GLN:HA	1:A:76:LEU:CD2	2.47	0.45
1:A:81:ASP:O	1:A:85:SER:OG	2.27	0.45
1:A:91:LEU:HD12	1:A:121:LEU:HD21	1.99	0.45
1:A:137:PHE:O	1:A:138:LEU:HD23	2.17	0.45
1:A:310:ALA:HA	1:A:313:VAL:HG12	1.99	0.45
1:A:341:LEU:HD12	1:A:341:LEU:H	1.82	0.45
1:A:698:ASP:OD1	1:A:698:ASP:N	2.49	0.45
1:A:754:SER:C	1:A:756:VAL:H	2.25	0.45
1:A:851:LEU:HA	1:A:854:ILE:HG12	1.99	0.45
2:B:157:MET:SD	2:B:229:LEU:HD13	2.56	0.45
2:B:268:THR:O	2:B:270:PRO:HD3	2.17	0.45
2:B:669:LYS:HA	2:B:672:GLN:HB2	1.99	0.45
2:B:784:PHE:CE1	2:B:789:MET:HG3	2.52	0.45
1:C:433:LYS:O	1:C:474:GLN:HB3	2.17	0.45
2:D:230:LEU:HB3	2:D:258:VAL:HG22	1.98	0.45
2:D:270:PRO:O	2:D:371:ARG:NH2	2.50	0.45
2:D:487:GLY:HA2	2:D:495:ASN:OD1	2.17	0.45
1:A:478:GLY:HA2	1:A:813:TRP:CH2	2.52	0.45
2:B:269:VAL:HG22	2:B:371:ARG:HH21	1.82	0.45
1:C:310:ALA:HA	1:C:313:VAL:HG12	1.99	0.45
1:C:422:VAL:O	1:C:423:THR:OG1	2.28	0.45
1:C:478:GLY:HA2	1:C:813:TRP:CH2	2.52	0.45
1:C:507:THR:C	1:C:519:TRP:HD1	2.25	0.45
1:C:794:SER:O	1:C:795:LEU:C	2.59	0.45
1:C:806:MET:HE2	1:C:806:MET:HB2	1.71	0.45
1:C:810:ASP:OD1	1:C:810:ASP:N	2.50	0.45
2:D:249:LEU:HA	2:D:254:TYR:HE2	1.80	0.45
2:D:369:LYS:C	2:D:371:ARG:H	2.25	0.45
2:D:438:LYS:O	2:D:440:ILE:N	2.50	0.45
2:D:825:LEU:O	2:D:828:ALA:N	2.35	0.45
1:A:178:LYS:O	1:A:182:THR:HG22	2.17	0.45
1:A:477:TYR:CD2	1:A:477:TYR:C	2.95	0.45
1:A:557:GLN:HB2	1:A:754:SER:OG	2.16	0.45
1:A:701:ILE:HD11	1:A:746:LYS:O	2.17	0.45
1:A:770:THR:HG22	1:A:771:GLY:N	2.31	0.45
2:B:94:ILE:HG22	2:B:96:GLY:H	1.81	0.45
2:B:270:PRO:O	2:B:371:ARG:NH2	2.50	0.45
2:B:274:PRO:O	2:B:367:LEU:HD23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:369:LYS:C	2:B:371:ARG:H	2.25	0.45
2:B:612:LEU:HD13	2:B:616:ASN:HB3	1.98	0.45
1:C:151:TRP:C	1:C:153:GLU:H	2.25	0.45
1:C:723:MET:O	1:C:724:TYR:C	2.59	0.45
1:C:768:VAL:HG22	1:C:769:THR:O	2.17	0.45
1:C:805:PHE:O	1:C:808:ASP:HB3	2.16	0.45
2:D:787:GLY:O	2:D:790:GLU:HB2	2.17	0.45
2:D:817:ASN:OD1	2:D:818:MET:N	2.39	0.45
1:A:666:ALA:O	1:A:667:SER:C	2.60	0.44
2:B:176:PHE:O	2:B:179:TYR:HD1	2.00	0.44
2:B:609:LEU:HD21	2:B:635:TRP:CE2	2.51	0.44
2:B:752:GLY:O	2:B:753:SER:OG	2.31	0.44
2:B:787:GLY:O	2:B:790:GLU:HB2	2.17	0.44
1:C:167:VAL:HG23	1:C:168:SER:O	2.17	0.44
1:C:178:LYS:O	1:C:182:THR:HG22	2.17	0.44
1:C:444:GLU:HG2	1:C:445:PHE:N	2.29	0.44
1:C:636:LEU:HD23	1:C:636:LEU:HA	1.68	0.44
1:C:754:SER:C	1:C:756:VAL:H	2.25	0.44
1:C:803:ASN:OD1	1:C:803:ASN:N	2.49	0.44
2:D:755:LYS:HD2	2:D:755:LYS:HA	1.56	0.44
1:A:151:TRP:C	1:A:153:GLU:H	2.25	0.44
1:A:487:LEU:HA	1:A:487:LEU:HD23	1.52	0.44
1:A:551:SER:OG	1:A:781:ILE:HB	2.18	0.44
2:B:77:ASP:HB3	2:B:80:SER:HB3	1.98	0.44
1:C:90:ILE:C	1:C:91:LEU:HD22	2.42	0.44
1:C:183:LEU:HA	1:C:183:LEU:HD23	1.73	0.44
1:C:264:SER:OG	1:C:404:GLY:HA3	2.17	0.44
1:C:424:ILE:O	1:C:430:VAL:HG21	2.16	0.44
1:C:804:GLY:HA2	1:C:807:GLU:HB3	1.99	0.44
2:D:498:ILE:HA	2:D:498:ILE:HD13	1.63	0.44
2:D:609:LEU:HD21	2:D:635:TRP:CE2	2.51	0.44
1:A:155:MET:H	1:A:155:MET:CE	2.30	0.44
1:A:167:VAL:HG23	1:A:168:SER:O	2.17	0.44
1:A:299:SER:O	1:A:302:ILE:HB	2.17	0.44
1:A:705:VAL:O	1:A:708:SER:OG	2.27	0.44
2:B:67:ARG:NH2	2:B:92:ARG:O	2.49	0.44
2:B:158:LEU:HD23	2:B:158:LEU:HA	1.73	0.44
2:B:170:SER:OG	2:B:200:GLU:HB3	2.16	0.44
2:B:608:LEU:HD23	2:B:609:LEU:N	2.32	0.44
1:C:124:ARG:HH11	1:C:141:VAL:CG1	2.31	0.44
2:D:268:THR:O	2:D:270:PRO:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:608:LEU:HD23	2:D:609:LEU:N	2.32	0.44
1:A:377:LEU:HD11	1:A:380:ARG:HA	2.00	0.44
1:A:388:TYR:HA	1:A:394:ILE:HG22	2.00	0.44
1:A:704:THR:OG1	1:A:705:VAL:N	2.42	0.44
1:A:768:VAL:HG22	1:A:769:THR:O	2.17	0.44
2:B:169:PHE:HA	2:B:227:ILE:O	2.16	0.44
2:B:438:LYS:O	2:B:440:ILE:N	2.50	0.44
2:B:487:GLY:HA2	2:B:495:ASN:OD1	2.17	0.44
1:C:73:GLN:HA	1:C:76:LEU:CD2	2.47	0.44
1:C:155:MET:H	1:C:155:MET:CE	2.30	0.44
1:C:274:GLU:O	1:C:279:ALA:HB3	2.18	0.44
1:C:388:TYR:HA	1:C:394:ILE:HG22	2.00	0.44
1:C:440:THR:OG1	1:C:441:CYS:N	2.50	0.44
1:C:467:SER:O	1:C:469:ARG:HG2	2.18	0.44
1:C:783:MET:HE2	1:C:790:LYS:HB2	1.99	0.44
1:A:32:VAL:O	1:A:33:LEU:HD23	2.17	0.44
1:A:264:SER:OG	1:A:404:GLY:HA3	2.17	0.44
1:A:467:SER:O	1:A:469:ARG:HG2	2.18	0.44
1:A:507:THR:C	1:A:519:TRP:HD1	2.25	0.44
1:A:783:MET:HE2	1:A:790:LYS:HB2	1.99	0.44
1:A:801:HIS:NE2	1:A:806:MET:HG2	2.32	0.44
1:C:139:ARG:HH22	1:C:143:PRO:HD3	1.80	0.44
1:C:445:PHE:HB3	1:C:449:GLY:HA2	2.00	0.44
1:C:701:ILE:HD11	1:C:746:LYS:O	2.17	0.44
2:D:784:PHE:CE1	2:D:789:MET:HG3	2.52	0.44
1:A:169:ASP:OD1	1:A:217:GLN:HB3	2.17	0.44
2:B:554:PHE:CG	2:B:558:VAL:HG21	2.52	0.44
2:B:770:SER:C	2:B:772:TRP:N	2.74	0.44
2:B:788:GLU:C	2:B:790:GLU:N	2.76	0.44
1:C:165:LEU:HD13	1:C:165:LEU:HA	1.71	0.44
1:C:299:SER:O	1:C:302:ILE:HB	2.17	0.44
1:C:470:HIS:O	1:C:472:VAL:HG23	2.17	0.44
1:C:838:PHE:O	1:C:841:VAL:HB	2.17	0.44
2:D:438:LYS:HE2	2:D:455:LYS:NZ	2.32	0.44
1:A:124:ARG:HH11	1:A:141:VAL:CG1	2.31	0.44
1:A:445:PHE:HB3	1:A:449:GLY:HA2	2.00	0.44
1:A:794:SER:O	1:A:795:LEU:C	2.59	0.44
2:B:35:ILE:HG23	2:B:37:ILE:HG12	1.99	0.44
2:B:276:GLY:N	2:B:367:LEU:O	2.41	0.44
2:B:438:LYS:HE2	2:B:455:LYS:NZ	2.32	0.44
1:C:290:LEU:HD13	1:C:372:TYR:HE2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:341:LEU:HD12	1:C:341:LEU:H	1.82	0.44
2:D:568:ILE:HG13	2:D:569:VAL:N	2.32	0.44
2:D:669:LYS:HA	2:D:672:GLN:HB2	1.99	0.44
2:D:786:ASP:OD1	2:D:786:ASP:N	2.49	0.44
1:A:433:LYS:O	1:A:474:GLN:HB3	2.17	0.44
1:A:838:PHE:O	1:A:841:VAL:HB	2.17	0.44
2:B:690:SER:O	2:B:693:ARG:HB3	2.18	0.44
2:B:701:GLU:HG2	2:B:702:MET:H	1.83	0.44
2:B:755:LYS:HD2	2:B:755:LYS:HA	1.56	0.44
1:C:417:THR:OG1	1:C:418:ARG:O	2.35	0.44
2:D:276:GLY:N	2:D:367:LEU:O	2.41	0.44
2:D:690:SER:O	2:D:693:ARG:HB3	2.18	0.44
1:A:417:THR:OG1	1:A:418:ARG:O	2.35	0.44
1:A:718:VAL:HG21	2:B:431:ARG:CZ	2.48	0.44
1:A:830:THR:O	2:D:558:VAL:HG13	2.18	0.44
2:B:78:PRO:HA	2:B:81:ILE:HD12	2.00	0.44
2:B:280:VAL:HG23	2:B:363:VAL:O	2.18	0.44
2:B:612:LEU:HD13	2:B:612:LEU:HA	1.43	0.44
2:B:631:MET:O	2:B:634:VAL:HG12	2.18	0.44
2:B:669:LYS:O	2:B:672:GLN:N	2.43	0.44
1:C:32:VAL:O	1:C:33:LEU:HD23	2.17	0.44
1:C:551:SER:OG	1:C:781:ILE:HB	2.18	0.44
1:C:662:MET:HE3	1:C:662:MET:HB3	1.83	0.44
2:D:152:GLN:NE2	2:D:360:PRO:HD2	2.32	0.44
2:D:691:THR:O	2:D:694:ASN:N	2.44	0.44
2:D:699:TYR:O	2:D:700:ALA:C	2.61	0.44
1:A:38:HIS:HA	1:A:41:MET:CG	2.48	0.43
1:A:375:MET:HE2	1:A:375:MET:HB2	1.89	0.43
1:A:798:LEU:HA	1:A:798:LEU:HD12	1.63	0.43
2:B:152:GLN:NE2	2:B:360:PRO:HD2	2.32	0.43
2:B:699:TYR:O	2:B:700:ALA:C	2.61	0.43
1:C:91:LEU:HD12	1:C:121:LEU:HD21	1.99	0.43
1:C:152:PHE:O	1:C:152:PHE:CG	2.71	0.43
1:C:377:LEU:HD11	1:C:380:ARG:HA	2.00	0.43
1:C:690:ASP:OD1	1:C:690:ASP:C	2.59	0.43
1:C:798:LEU:HA	1:C:798:LEU:HD12	1.63	0.43
2:D:701:GLU:HG2	2:D:702:MET:H	1.83	0.43
1:A:235:LEU:HA	1:A:235:LEU:HD13	1.71	0.43
1:A:312:ALA:HA	1:A:315:GLU:OE1	2.18	0.43
1:A:527:LEU:HD23	1:A:527:LEU:HA	1.71	0.43
2:B:701:GLU:HG2	2:B:702:MET:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:SER:HB3	1:C:121:LEU:HD12	1.99	0.43
1:C:550:PHE:HD1	1:C:550:PHE:HA	1.59	0.43
1:C:714:PHE:HD1	1:C:714:PHE:HA	1.61	0.43
1:A:87:VAL:O	1:A:325:PRO:HB3	2.19	0.43
1:A:152:PHE:O	1:A:152:PHE:CG	2.71	0.43
1:A:267:VAL:C	1:A:268:TRP:CD1	2.97	0.43
1:A:803:ASN:OD1	1:A:803:ASN:N	2.49	0.43
2:B:635:TRP:O	2:B:638:PHE:HB3	2.18	0.43
2:B:783:LEU:HD12	2:B:783:LEU:HA	1.73	0.43
1:C:435:THR:HB	1:C:440:THR:O	2.18	0.43
1:C:540:ILE:HG22	1:C:541:ASN:N	2.33	0.43
2:D:123:ILE:C	2:D:124:LEU:HD22	2.43	0.43
1:A:470:HIS:O	1:A:472:VAL:HG23	2.17	0.43
1:A:657:TRP:O	1:A:660:PHE:HB3	2.19	0.43
1:A:830:THR:HB	2:D:555:SER:HB3	2.00	0.43
2:B:674:PRO:HB2	2:B:705:TYR:CE2	2.53	0.43
2:D:99:PHE:O	2:D:126:ILE:HG22	2.18	0.43
2:D:269:VAL:HG22	2:D:371:ARG:HH21	1.82	0.43
2:D:280:VAL:HG23	2:D:363:VAL:O	2.18	0.43
2:D:649:ASN:O	2:D:652:ALA:HB3	2.19	0.43
1:A:90:ILE:C	1:A:91:LEU:HD22	2.42	0.43
1:A:274:GLU:O	1:A:279:ALA:HB3	2.18	0.43
1:A:557:GLN:CD	1:A:557:GLN:C	2.86	0.43
2:B:243:VAL:O	2:B:247:VAL:HG23	2.19	0.43
2:B:446:THR:HG22	2:B:447:ASP:N	2.34	0.43
2:B:568:ILE:HG13	2:B:569:VAL:N	2.32	0.43
1:C:851:LEU:HA	1:C:854:ILE:HG12	1.99	0.43
2:D:701:GLU:HG2	2:D:702:MET:N	2.33	0.43
1:A:856:ILE:H	1:A:856:ILE:HG13	1.61	0.43
2:B:784:PHE:HD1	2:B:784:PHE:HA	1.63	0.43
1:C:657:TRP:O	1:C:660:PHE:HB3	2.19	0.43
1:C:724:TYR:O	1:C:727:MET:HG2	2.18	0.43
2:D:115:ILE:O	2:D:119:THR:N	2.43	0.43
2:D:274:PRO:O	2:D:367:LEU:HD23	2.17	0.43
2:D:770:SER:C	2:D:772:TRP:N	2.74	0.43
1:A:435:THR:HB	1:A:440:THR:O	2.18	0.43
1:A:724:TYR:O	1:A:727:MET:HG2	2.19	0.43
1:A:846:VAL:O	1:A:847:ALA:C	2.62	0.43
2:B:786:ASP:C	1:C:717:GLN:HE22	2.25	0.43
1:C:38:HIS:HA	1:C:41:MET:CG	2.48	0.43
2:D:78:PRO:HA	2:D:81:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:129:GLY:C	2:D:131:SER:H	2.26	0.43
2:D:445:LYS:HA	2:D:445:LYS:HD3	1.83	0.43
2:D:635:TRP:O	2:D:638:PHE:HB3	2.18	0.43
2:D:674:PRO:HB2	2:D:705:TYR:CE2	2.53	0.43
1:A:500:VAL:HG22	1:A:501:ALA:H	1.83	0.43
1:A:810:ASP:OD1	1:A:810:ASP:N	2.49	0.43
2:B:234:LYS:O	2:B:237:ALA:HB3	2.18	0.43
1:C:781:ILE:HD13	1:C:781:ILE:HA	1.82	0.43
2:D:304:ALA:O	2:D:307:MET:HG2	2.18	0.43
1:A:387:ILE:HD12	1:A:394:ILE:HB	2.00	0.43
1:A:804:GLY:HA2	1:A:807:GLU:HB3	1.99	0.43
2:B:99:PHE:O	2:B:126:ILE:HG22	2.18	0.43
2:B:123:ILE:C	2:B:124:LEU:HD22	2.43	0.43
2:B:649:ASN:O	2:B:652:ALA:HB3	2.19	0.43
2:B:781:LEU:HD23	2:B:781:LEU:HA	1.68	0.43
1:C:87:VAL:O	1:C:325:PRO:HB3	2.19	0.43
1:C:312:ALA:HA	1:C:315:GLU:OE1	2.18	0.43
1:C:387:ILE:O	1:C:394:ILE:HG22	2.19	0.43
1:C:598:LEU:HG	1:C:653:LEU:HD23	2.01	0.43
2:D:199:LEU:HD12	2:D:199:LEU:HA	1.66	0.43
2:D:234:LYS:O	2:D:237:ALA:HB3	2.18	0.43
2:D:670:LYS:HD3	2:D:681:PHE:CZ	2.54	0.43
2:D:696:ARG:HE	2:D:703:HIS:HE1	1.67	0.43
2:D:770:SER:C	2:D:772:TRP:H	2.27	0.43
2:D:788:GLU:C	2:D:790:GLU:N	2.76	0.43
2:D:824:MET:O	2:D:827:ALA:HB3	2.19	0.43
1:A:634:VAL:HA	2:B:617:SER:HB2	2.01	0.43
2:B:696:ARG:HE	2:B:703:HIS:CE1	2.37	0.43
1:C:659:GLY:HA2	2:D:614:PHE:CD2	2.53	0.43
1:C:698:ASP:OD1	1:C:698:ASP:N	2.49	0.43
2:D:77:ASP:HA	2:D:78:PRO:HD2	1.90	0.43
2:D:243:VAL:O	2:D:247:VAL:HG23	2.19	0.43
2:D:354:ASP:HB3	2:D:356:TYR:CE2	2.54	0.43
2:D:446:THR:HG22	2:D:447:ASP:N	2.34	0.43
2:D:631:MET:O	2:D:634:VAL:HG12	2.18	0.43
2:D:837:ILE:O	2:D:840:HIS:N	2.45	0.43
1:A:635:LEU:HA	1:A:635:LEU:HD12	1.49	0.42
1:A:805:PHE:CZ	1:A:809:LEU:HD11	2.53	0.42
2:B:129:GLY:C	2:B:131:SER:H	2.26	0.42
2:B:258:VAL:CG1	2:B:259:PRO:HD2	2.49	0.42
2:B:407:SER:O	2:B:407:SER:OG	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:554:PHE:HE1	1:C:829:LEU:HD11	1.83	0.42
1:C:575:PHE:C	1:C:577:GLN:N	2.77	0.42
1:C:805:PHE:CZ	1:C:809:LEU:HD11	2.53	0.42
2:D:462:ILE:HA	2:D:462:ILE:HD13	1.70	0.42
1:A:507:THR:C	1:A:519:TRP:CD1	2.97	0.42
1:A:672:LEU:HA	1:A:672:LEU:HD12	1.80	0.42
2:B:770:SER:C	2:B:772:TRP:H	2.27	0.42
1:C:349:SER:O	1:C:351:TYR:N	2.48	0.42
1:C:500:VAL:HG22	1:C:501:ALA:H	1.83	0.42
1:C:520:ASN:OD1	1:C:520:ASN:N	2.51	0.42
1:C:557:GLN:CD	1:C:557:GLN:C	2.86	0.42
2:D:517:GLU:O	2:D:518:GLU:C	2.62	0.42
2:B:304:ALA:O	2:B:307:MET:HG2	2.18	0.42
2:B:670:LYS:HD3	2:B:681:PHE:CZ	2.54	0.42
1:C:267:VAL:C	1:C:268:TRP:CD1	2.97	0.42
1:C:387:ILE:HD12	1:C:394:ILE:HB	2.00	0.42
1:C:548:ILE:HG23	1:C:783:MET:O	2.18	0.42
1:C:568:PRO:HA	1:C:680:ARG:HH12	1.84	0.42
1:C:705:VAL:O	1:C:708:SER:OG	2.27	0.42
1:A:47:ASN:HB2	1:A:48:GLN:NE2	2.35	0.42
2:B:77:ASP:O	2:B:80:SER:OG	2.16	0.42
2:B:696:ARG:HE	2:B:703:HIS:HE1	1.67	0.42
1:C:507:THR:C	1:C:519:TRP:CD1	2.97	0.42
1:C:540:ILE:HD12	1:C:540:ILE:HG23	1.81	0.42
1:C:785:LYS:HE2	1:C:786:ASP:OD2	2.20	0.42
2:D:439:ARG:HD3	2:D:452:TYR:HD2	1.84	0.42
2:D:439:ARG:O	2:D:439:ARG:HG2	2.20	0.42
1:A:268:TRP:C	1:A:269:LEU:HD12	2.45	0.42
1:A:548:ILE:HG23	1:A:783:MET:O	2.19	0.42
1:A:690:ASP:OD1	1:A:692:ARG:N	2.34	0.42
1:A:785:LYS:HE2	1:A:786:ASP:OD2	2.20	0.42
2:B:532:THR:HG22	2:B:761:GLY:HA2	2.02	0.42
2:D:44:THR:HG23	2:D:45:SER:N	2.34	0.42
2:D:258:VAL:CG1	2:D:259:PRO:HD2	2.49	0.42
2:D:691:THR:H	2:D:691:THR:HG23	1.49	0.42
1:A:44:GLU:HA	1:A:47:ASN:ND2	2.35	0.42
1:A:103:THR:OG1	1:A:104:PRO:HD3	2.20	0.42
1:A:387:ILE:O	1:A:394:ILE:HG22	2.19	0.42
1:A:423:THR:OG1	1:A:535:VAL:O	2.37	0.42
1:A:693:LEU:HA	1:A:693:LEU:HD23	1.83	0.42
2:B:190:ILE:HA	2:B:190:ILE:HD13	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:645:SER:OG	2:B:646:TYR:N	2.53	0.42
2:B:745:GLY:O	2:B:747:LYS:N	2.52	0.42
1:C:75:ALA:O	1:C:78:VAL:HB	2.20	0.42
1:C:790:LYS:O	1:C:791:GLN:C	2.62	0.42
2:D:407:SER:O	2:D:407:SER:OG	2.37	0.42
2:D:622:ASN:HA	2:D:623:PRO:HD3	1.89	0.42
2:D:630:ILE:HD13	2:D:630:ILE:HA	1.81	0.42
1:A:540:ILE:HG22	1:A:541:ASN:N	2.33	0.42
2:B:179:TYR:O	2:B:183:VAL:HG12	2.19	0.42
2:D:179:TYR:O	2:D:183:VAL:HG12	2.19	0.42
1:A:139:ARG:HH22	1:A:143:PRO:HG3	1.84	0.42
2:B:48:VAL:C	2:B:50:ILE:N	2.78	0.42
1:C:103:THR:OG1	1:C:104:PRO:HD3	2.20	0.42
1:C:184:LEU:HD23	1:C:184:LEU:HA	1.70	0.42
1:C:423:THR:OG1	1:C:535:VAL:O	2.37	0.42
1:C:477:TYR:CD2	1:C:477:TYR:C	2.95	0.42
1:C:544:ARG:HH12	1:C:709:SER:HB3	1.85	0.42
1:C:596:VAL:HG12	1:C:599:TYR:CE2	2.55	0.42
2:D:745:GLY:O	2:D:747:LYS:N	2.52	0.42
1:A:124:ARG:HH12	1:A:142:PRO:HG2	1.85	0.42
1:A:277:GLY:HA2	1:A:280:LEU:CB	2.50	0.42
1:A:634:VAL:HA	2:B:617:SER:CB	2.50	0.42
2:B:38:ALA:O	2:B:97:VAL:HA	2.20	0.42
2:B:335:LEU:HD23	2:B:335:LEU:H	1.85	0.42
2:B:439:ARG:O	2:B:439:ARG:HG2	2.20	0.42
2:B:602:ILE:HD13	2:B:602:ILE:HA	1.81	0.42
2:B:630:ILE:HD13	2:B:630:ILE:HA	1.81	0.42
1:C:47:ASN:HB2	1:C:48:GLN:NE2	2.35	0.42
1:C:124:ARG:HH12	1:C:142:PRO:HG2	1.85	0.42
1:C:292:LEU:HA	1:C:372:TYR:CB	2.50	0.42
2:D:38:ALA:O	2:D:97:VAL:HA	2.20	0.42
1:A:126:SER:O	1:A:126:SER:OG	2.36	0.42
1:A:568:PRO:HA	1:A:680:ARG:HH12	1.84	0.42
1:A:692:ARG:NH2	2:B:800:ILE:HG21	2.34	0.42
2:B:641:ILE:HD13	1:C:668:TYR:HE2	1.84	0.42
1:C:135:LEU:HD23	1:C:135:LEU:HA	1.91	0.42
1:C:147:GLN:HE22	1:C:272:GLU:H	1.68	0.42
2:D:562:MET:HE3	2:D:562:MET:HB3	1.98	0.42
2:D:800:ILE:HD12	2:D:800:ILE:HA	1.76	0.42
1:A:596:VAL:HG12	1:A:599:TYR:CE2	2.54	0.41
2:B:824:MET:O	2:B:827:ALA:HB3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:500:VAL:HG22	1:C:501:ALA:N	2.35	0.41
1:C:599:TYR:CD1	1:C:599:TYR:C	2.98	0.41
1:C:694:ARG:HD3	1:C:694:ARG:HA	1.82	0.41
2:D:109:ALA:HA	2:D:112:LEU:HD13	2.01	0.41
2:D:124:LEU:HD13	2:D:124:LEU:HA	1.91	0.41
1:A:83:ILE:HG21	1:A:329:CYS:HB2	2.02	0.41
1:A:431:TYR:O	1:A:476:CYS:HA	2.19	0.41
1:A:598:LEU:HG	1:A:653:LEU:HD23	2.01	0.41
1:A:783:MET:HG3	1:A:790:LYS:HG3	2.02	0.41
2:B:44:THR:HG23	2:B:45:SER:N	2.34	0.41
2:B:655:ILE:HD13	2:B:655:ILE:HA	1.85	0.41
2:B:789:MET:HE3	2:B:789:MET:HB3	1.89	0.41
2:B:800:ILE:HA	2:B:800:ILE:HD12	1.76	0.41
1:C:44:GLU:HA	1:C:47:ASN:ND2	2.35	0.41
1:C:431:TYR:O	1:C:476:CYS:HA	2.20	0.41
1:C:663:ILE:HA	1:C:663:ILE:HD13	1.74	0.41
2:D:289:LEU:O	2:D:293:VAL:HG13	2.20	0.41
2:D:696:ARG:HE	2:D:703:HIS:CE1	2.37	0.41
2:B:214:SER:HA	2:B:217:GLN:CD	2.46	0.41
2:B:439:ARG:HD3	2:B:452:TYR:HD2	1.84	0.41
1:C:277:GLY:HA2	1:C:280:LEU:CB	2.50	0.41
1:C:415:MET:C	1:C:417:THR:HG23	2.45	0.41
2:D:339:LEU:HA	2:D:339:LEU:HD13	1.74	0.41
2:D:796:TRP:CD1	2:D:796:TRP:N	2.89	0.41
1:A:500:VAL:HG22	1:A:501:ALA:N	2.35	0.41
1:A:544:ARG:HH12	1:A:709:SER:HB3	1.85	0.41
1:A:583:LEU:O	1:A:586:LEU:HB3	2.21	0.41
1:A:743:ARG:HA	1:A:743:ARG:HD2	1.69	0.41
1:A:806:MET:O	1:A:809:LEU:N	2.52	0.41
2:B:354:ASP:HB3	2:B:356:TYR:CE2	2.54	0.41
2:B:462:ILE:HD13	2:B:462:ILE:HA	1.70	0.41
1:C:32:VAL:HG22	1:C:65:VAL:HG13	2.02	0.41
1:C:402:TRP:NE1	1:C:408:GLU:O	2.53	0.41
1:C:783:MET:HE3	1:C:783:MET:HB3	1.79	0.41
2:D:335:LEU:HD23	2:D:335:LEU:H	1.85	0.41
1:A:251:THR:OG1	1:A:252:VAL:N	2.53	0.41
1:A:261:MET:HE3	1:A:261:MET:HB3	1.80	0.41
1:A:290:LEU:HD13	1:A:372:TYR:HE2	1.83	0.41
1:A:292:LEU:HA	1:A:372:TYR:CB	2.50	0.41
1:C:151:TRP:C	1:C:153:GLU:N	2.78	0.41
1:C:787:SER:O	1:C:788:PRO:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:806:MET:O	1:C:809:LEU:N	2.52	0.41
2:D:172:VAL:O	2:D:173:THR:OG1	2.35	0.41
2:D:633:SER:OG	2:D:634:VAL:N	2.54	0.41
2:D:645:SER:OG	2:D:646:TYR:N	2.53	0.41
2:B:336:ASN:HA	2:B:339:LEU:HB2	2.02	0.41
2:B:551:LEU:HD12	2:B:551:LEU:HA	1.95	0.41
1:C:83:ILE:HG21	1:C:329:CYS:HB2	2.02	0.41
1:C:126:SER:O	1:C:126:SER:OG	2.36	0.41
1:C:154:MET:HE2	1:C:154:MET:N	2.35	0.41
1:C:268:TRP:C	1:C:269:LEU:HD12	2.45	0.41
1:C:375:MET:C	1:C:375:MET:SD	3.04	0.41
1:C:544:ARG:NH1	1:C:709:SER:HB3	2.36	0.41
2:D:336:ASN:HA	2:D:339:LEU:HB2	2.02	0.41
1:A:112:GLY:O	1:A:115:ARG:NH1	2.54	0.41
1:A:154:MET:HE2	1:A:154:MET:N	2.35	0.41
1:A:375:MET:SD	1:A:375:MET:C	3.04	0.41
1:A:390:GLY:C	1:A:392:HIS:N	2.79	0.41
2:B:82:ILE:HD12	2:B:115:ILE:HD11	2.03	0.41
2:B:512:SER:C	2:B:513:LEU:HD12	2.46	0.41
2:B:816:ASP:O	2:B:819:ALA:HB3	2.20	0.41
1:C:305:ALA:O	1:C:309:VAL:HG12	2.21	0.41
1:C:561:ILE:HG22	1:C:562:LEU:N	2.36	0.41
1:C:583:LEU:O	1:C:586:LEU:HB3	2.21	0.41
1:C:783:MET:HG3	1:C:790:LYS:HG3	2.02	0.41
2:D:48:VAL:C	2:D:50:ILE:H	2.29	0.41
2:D:417:VAL:O	2:D:417:VAL:HG22	2.21	0.41
2:D:532:THR:HG22	2:D:761:GLY:HA2	2.02	0.41
2:D:537:MET:HG3	2:D:749:VAL:O	2.21	0.41
1:A:245:SER:OG	1:A:246:GLU:N	2.52	0.41
1:A:305:ALA:O	1:A:309:VAL:HG12	2.21	0.41
1:A:540:ILE:HD12	1:A:540:ILE:HG23	1.81	0.41
2:B:109:ALA:HA	2:B:112:LEU:HD13	2.01	0.41
2:B:289:LEU:O	2:B:293:VAL:HG13	2.20	0.41
2:B:417:VAL:HG22	2:B:417:VAL:O	2.21	0.41
2:B:515:ILE:HD12	2:B:515:ILE:HG23	1.80	0.41
2:B:669:LYS:O	2:B:673:ARG:N	2.45	0.41
1:C:548:ILE:HG22	1:C:549:GLU:N	2.36	0.41
1:C:686:THR:HG22	1:C:690:ASP:OD2	2.21	0.41
2:D:748:LEU:O	2:D:749:VAL:HB	2.21	0.41
1:A:32:VAL:HG22	1:A:65:VAL:HG13	2.02	0.41
1:A:70:ASN:ND2	1:A:72:ILE:HD12	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ALA:O	1:A:78:VAL:HB	2.20	0.41
1:A:147:GLN:HE22	1:A:272:GLU:H	1.68	0.41
1:A:424:ILE:HD12	1:A:425:HIS:H	1.86	0.41
1:A:544:ARG:NH1	1:A:709:SER:HB3	2.36	0.41
1:A:599:TYR:CD1	1:A:599:TYR:C	2.98	0.41
1:A:663:ILE:HD13	1:A:663:ILE:HA	1.74	0.41
1:A:787:SER:O	1:A:788:PRO:C	2.64	0.41
1:A:803:ASN:C	1:A:805:PHE:N	2.79	0.41
1:A:803:ASN:O	1:A:805:PHE:N	2.53	0.41
2:B:307:MET:HG3	2:B:313:PHE:HA	2.03	0.41
2:B:517:GLU:O	2:B:518:GLU:C	2.62	0.41
2:B:795:LEU:HA	2:B:795:LEU:HD12	1.76	0.41
2:B:800:ILE:HG13	2:B:801:CYS:H	1.86	0.41
2:B:825:LEU:HD23	2:B:826:GLY:N	2.36	0.41
1:C:91:LEU:HD13	1:C:119:LEU:O	2.21	0.41
1:C:112:GLY:O	1:C:115:ARG:NH1	2.54	0.41
1:C:382:LEU:HB3	1:C:384:GLN:NE2	2.36	0.41
1:C:470:HIS:O	1:C:472:VAL:N	2.54	0.41
1:C:527:LEU:HD23	1:C:527:LEU:HA	1.71	0.41
1:C:803:ASN:C	1:C:805:PHE:N	2.79	0.41
2:D:130:SER:C	2:D:132:MET:H	2.29	0.41
2:D:214:SER:HA	2:D:217:GLN:CD	2.46	0.41
2:D:354:ASP:CG	2:D:356:TYR:HD2	2.29	0.41
2:D:602:ILE:HD13	2:D:602:ILE:HA	1.81	0.41
2:D:816:ASP:O	2:D:819:ALA:HB3	2.20	0.41
1:A:415:MET:C	1:A:417:THR:HG23	2.45	0.41
1:A:468:PRO:C	1:A:470:HIS:N	2.79	0.41
2:B:237:ALA:O	2:B:241:PHE:HD1	2.04	0.41
2:B:241:PHE:HD2	2:B:274:PRO:HD3	1.86	0.41
1:C:35:THR:HB	1:C:38:HIS:CB	2.52	0.41
1:C:139:ARG:HH22	1:C:143:PRO:HG3	1.84	0.41
1:C:151:TRP:NE1	1:C:269:LEU:HB3	2.36	0.41
1:C:251:THR:OG1	1:C:252:VAL:N	2.53	0.41
1:C:456:ILE:H	1:C:456:ILE:HG13	1.55	0.41
1:C:846:VAL:O	1:C:847:ALA:C	2.62	0.41
1:A:146:HIS:HA	1:A:179:ARG:HH22	1.86	0.40
1:A:151:TRP:NE1	1:A:269:LEU:HB3	2.36	0.40
1:A:659:GLY:HA2	2:B:614:PHE:CD2	2.56	0.40
1:A:686:THR:HG22	1:A:690:ASP:OD2	2.21	0.40
1:A:847:ALA:O	1:A:848:GLY:C	2.64	0.40
2:B:170:SER:O	2:B:171:ILE:HD13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:272:GLU:O	2:B:274:PRO:HD3	2.21	0.40
2:B:407:SER:OG	2:B:506:ALA:HA	2.21	0.40
2:B:437:GLN:HG3	2:B:452:TYR:CE2	2.56	0.40
2:B:518:GLU:OE2	2:B:693:ARG:NE	2.30	0.40
2:B:537:MET:HG3	2:B:749:VAL:O	2.21	0.40
1:C:139:ARG:NH1	1:C:143:PRO:HB3	2.28	0.40
1:C:847:ALA:O	1:C:848:GLY:C	2.64	0.40
2:D:170:SER:O	2:D:171:ILE:HD13	2.21	0.40
2:D:613:VAL:C	2:D:614:PHE:HD1	2.29	0.40
1:A:91:LEU:HD13	1:A:91:LEU:HA	1.74	0.40
1:A:402:TRP:NE1	1:A:408:GLU:O	2.53	0.40
1:A:636:LEU:HA	1:A:636:LEU:HD23	1.68	0.40
1:A:653:LEU:HD12	1:A:653:LEU:HA	1.80	0.40
2:B:108:ILE:H	2:B:108:ILE:HG12	1.71	0.40
2:B:461:CYS:O	2:B:464:ILE:HG22	2.22	0.40
2:B:748:LEU:O	2:B:749:VAL:HB	2.21	0.40
2:B:796:TRP:CD1	2:B:796:TRP:N	2.89	0.40
1:C:38:HIS:O	1:C:42:PHE:HD1	2.04	0.40
1:C:279:ALA:O	1:C:282:TYR:N	2.37	0.40
1:C:803:ASN:O	1:C:805:PHE:N	2.53	0.40
1:A:793:VAL:O	1:A:794:SER:C	2.64	0.40
2:B:313:PHE:O	2:B:315:PRO:HD3	2.20	0.40
2:B:656:GLN:N	2:B:656:GLN:OE1	2.54	0.40
1:C:76:LEU:HD12	1:C:77:SER:N	2.37	0.40
1:C:271:GLY:N	1:C:274:GLU:OE2	2.54	0.40
1:C:487:LEU:HD23	1:C:487:LEU:HA	1.53	0.40
2:D:82:ILE:HD12	2:D:115:ILE:HD11	2.03	0.40
2:D:306:ASP:O	2:D:309:SER:OG	2.29	0.40
2:D:407:SER:OG	2:D:506:ALA:HA	2.21	0.40
2:D:465:LEU:HD12	2:D:465:LEU:HA	1.75	0.40
2:D:748:LEU:HD13	2:D:748:LEU:HA	1.70	0.40
1:A:76:LEU:HD12	1:A:77:SER:N	2.37	0.40
1:A:561:ILE:HG22	1:A:562:LEU:N	2.36	0.40
2:B:48:VAL:C	2:B:50:ILE:H	2.29	0.40
1:C:424:ILE:HD12	1:C:425:HIS:H	1.86	0.40
1:C:435:THR:HA	1:C:441:CYS:HB3	2.04	0.40
2:D:190:ILE:HA	2:D:190:ILE:HD13	1.81	0.40
2:D:237:ALA:O	2:D:241:PHE:HD1	2.04	0.40
2:D:313:PHE:O	2:D:315:PRO:HD3	2.20	0.40
2:D:653:PHE:HD1	2:D:653:PHE:HA	1.67	0.40
1:A:593:VAL:HG12	2:B:829:MET:HE1	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:652:ILE:HD13	1:A:652:ILE:HA	1.87	0.40
2:B:287:TYR:CE2	2:B:292:ARG:HA	2.57	0.40
2:D:183:VAL:HG13	2:D:184:ASN:N	2.37	0.40
2:D:241:PHE:HD2	2:D:274:PRO:HD3	1.86	0.40
2:D:279:SER:OG	2:D:280:VAL:N	2.55	0.40
2:D:426:SER:H	2:D:428:THR:HG23	1.87	0.40
2:D:733:ALA:O	2:D:734:ALA:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	791/959 (82%)	603 (76%)	182 (23%)	6 (1%)	16	52
1	C	791/959 (82%)	604 (76%)	181 (23%)	6 (1%)	16	52
2	B	778/883 (88%)	620 (80%)	151 (19%)	7 (1%)	14	48
2	D	778/883 (88%)	620 (80%)	151 (19%)	7 (1%)	14	48
All	All	3138/3684 (85%)	2447 (78%)	665 (21%)	26 (1%)	18	52

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	749	VAL
2	D	749	VAL
1	A	581	SER
2	B	431	ARG
1	C	581	SER
2	D	431	ARG
2	B	131	SER
2	D	131	SER

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Mol	Chain	Res	Type
1	A	755	ALA
2	B	746	CYS
1	C	755	ALA
2	D	746	CYS
1	A	520	ASN
2	B	616	ASN
1	C	520	ASN
2	D	616	ASN
1	A	69	PRO
1	C	69	PRO
2	B	177	PRO
2	D	177	PRO
1	A	718	VAL
1	C	718	VAL
2	B	741	GLY
2	D	741	GLY
1	A	804	GLY
1	C	804	GLY

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	587/826 (71%)	565 (96%)	22 (4%)	30	52
1	C	587/826 (71%)	565 (96%)	22 (4%)	30	52
2	B	571/762 (75%)	559 (98%)	12 (2%)	47	65
2	D	571/762 (75%)	559 (98%)	12 (2%)	47	65
All	All	2316/3176 (73%)	2248 (97%)	68 (3%)	38	58

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	VAL
1	A	167	VAL
1	A	180	LEU

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Mol	Chain	Res	Type
1	A	239	VAL
1	A	264	SER
1	A	303	SER
1	A	349	SER
1	A	387	ILE
1	A	407	THR
1	A	458	THR
1	A	560	THR
1	A	575	PHE
1	A	605	SER
1	A	632	TRP
1	A	686	THR
1	A	708	SER
1	A	722	THR
1	A	751	ILE
1	A	753	ASP
1	A	768	VAL
1	A	786	ASP
1	A	797	ILE
2	B	44	THR
2	B	140	SER
2	B	146	PHE
2	B	426	SER
2	B	483	ASN
2	B	498	ILE
2	B	548	SER
2	B	612	LEU
2	B	667	SER
2	B	730	ILE
2	B	760	THR
2	B	784	PHE
1	C	65	VAL
1	C	167	VAL
1	C	180	LEU
1	C	239	VAL
1	C	264	SER
1	C	303	SER
1	C	349	SER
1	C	387	ILE
1	C	407	THR
1	C	458	THR
1	C	560	THR

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Mol	Chain	Res	Type
1	C	575	PHE
1	C	605	SER
1	C	632	TRP
1	C	686	THR
1	C	708	SER
1	C	722	THR
1	C	751	ILE
1	C	753	ASP
1	C	768	VAL
1	C	786	ASP
1	C	797	ILE
2	D	44	THR
2	D	140	SER
2	D	146	PHE
2	D	426	SER
2	D	483	ASN
2	D	498	ILE
2	D	548	SER
2	D	612	LEU
2	D	667	SER
2	D	730	ILE
2	D	760	THR
2	D	784	PHE

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	70	ASN
1	A	278	ASN
1	A	384	GLN
1	A	577	GLN
1	A	740	GLN
1	A	748	HIS
1	A	801	HIS
2	B	159	ASN
2	B	486	HIS
2	B	840	HIS
1	C	70	ASN
1	C	162	HIS
1	C	278	ASN
1	C	384	GLN
1	C	577	GLN

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Mol	Chain	Res	Type
1	C	717	GLN
1	C	740	GLN
2	D	159	ASN
2	D	486	HIS
2	D	703	HIS
2	D	840	HIS

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 ⓘ

4 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	E	1	2,3	14,14,15	0.89	1 (7%)	17,19,21	0.50	0
3	NAG	E	2	3	14,14,15	0.60	0	17,19,21	1.35	2 (11%)
3	NAG	F	1	2,3	14,14,15	0.90	1 (7%)	17,19,21	0.51	0
3	NAG	F	2	3	14,14,15	0.59	0	17,19,21	1.35	2 (11%)

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	E	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	6/6/23/26	0/1/1/1
3	NAG	F	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	6/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1	NAG	O5-C1	-3.25	1.38	1.43
3	E	1	NAG	O5-C1	-3.22	1.38	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2	NAG	C2-N2-C7	4.51	128.95	122.90
3	E	2	NAG	C2-N2-C7	4.51	128.94	122.90
3	E	2	NAG	C1-C2-N2	2.34	114.12	110.43
3	F	2	NAG	C1-C2-N2	2.34	114.11	110.43

There are no chirality outliers.

All (16) torsion outliers are listed below:

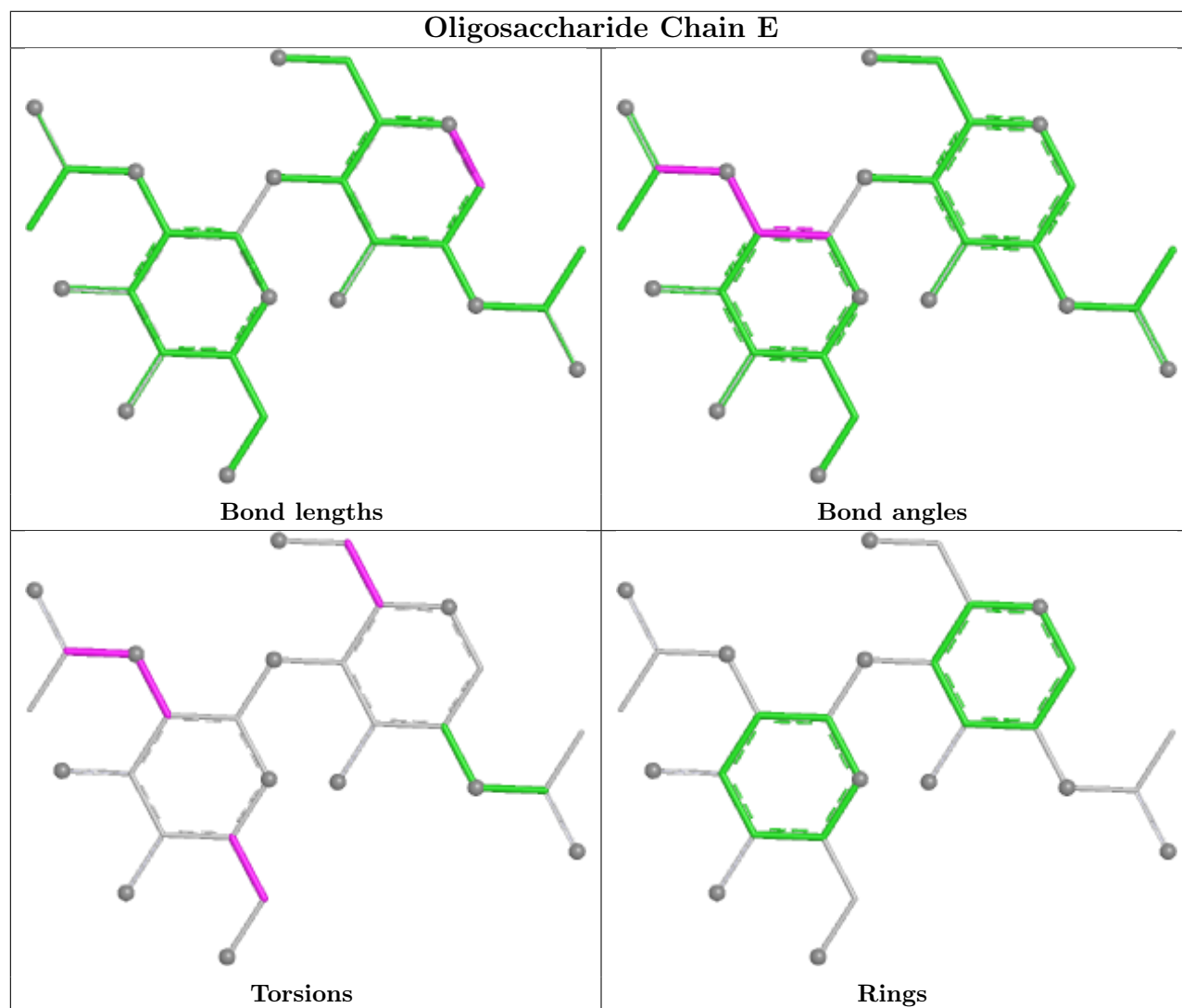
Mol	Chain	Res	Type	Atoms
3	E	2	NAG	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
3	E	2	NAG	C3-C2-N2-C7
3	F	2	NAG	C3-C2-N2-C7
3	E	2	NAG	C1-C2-N2-C7
3	F	2	NAG	C1-C2-N2-C7

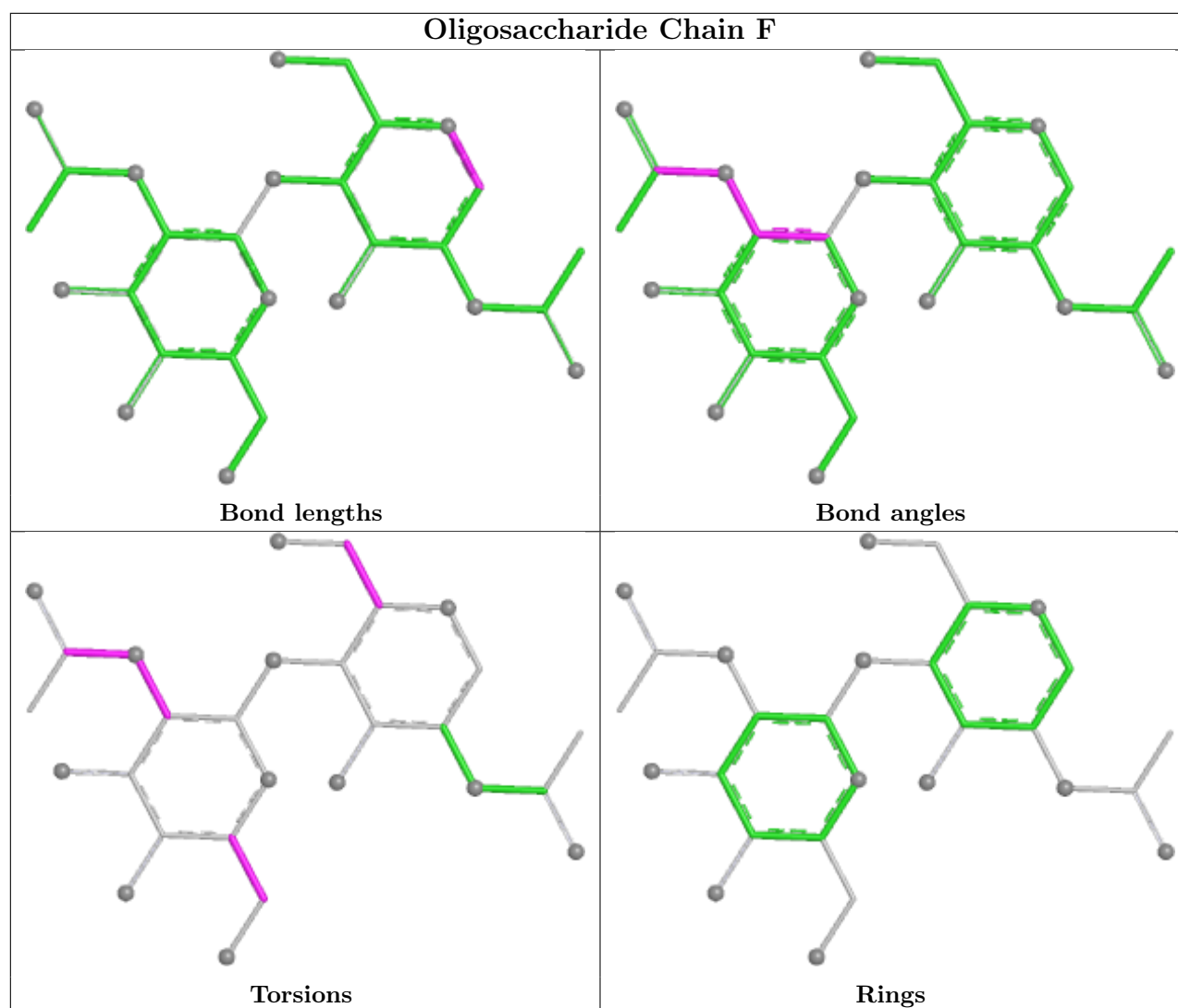
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	2	NAG	1	0
3	E	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 [i](#)

10 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	904	2	14,14,15	0.38	0	17,19,21	0.40	0
4	NAG	A	1002	1	14,14,15	0.39	0	17,19,21	0.38	0
4	NAG	C	1002	1	14,14,15	0.39	0	17,19,21	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	D	905	2	14,14,15	0.23	0	17,19,21	0.54	0
4	NAG	A	1001	1	14,14,15	0.35	0	17,19,21	0.50	0
4	NAG	D	903	2	14,14,15	0.35	0	17,19,21	0.38	0
4	NAG	D	904	2	14,14,15	0.38	0	17,19,21	0.40	0
4	NAG	B	905	2	14,14,15	0.26	0	17,19,21	0.54	0
4	NAG	B	903	2	14,14,15	0.35	0	17,19,21	0.38	0
4	NAG	C	1001	1	14,14,15	0.34	0	17,19,21	0.51	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
4	NAG	B	904	2	-	3/6/23/26	0/1/1/1
4	NAG	A	1002	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1002	1	-	4/6/23/26	0/1/1/1
4	NAG	D	905	2	-	1/6/23/26	0/1/1/1
4	NAG	A	1001	1	-	4/6/23/26	0/1/1/1
4	NAG	D	903	2	-	2/6/23/26	0/1/1/1
4	NAG	D	904	2	-	3/6/23/26	0/1/1/1
4	NAG	B	905	2	-	1/6/23/26	0/1/1/1
4	NAG	B	903	2	-	2/6/23/26	0/1/1/1
4	NAG	C	1001	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1002	NAG	O5-C5-C6-O6
4	C	1002	NAG	O5-C5-C6-O6
4	B	904	NAG	C4-C5-C6-O6
4	D	904	NAG	C4-C5-C6-O6
4	B	903	NAG	O5-C5-C6-O6
4	D	903	NAG	O5-C5-C6-O6
4	B	903	NAG	C4-C5-C6-O6
4	D	903	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	A	1001	NAG	O5-C5-C6-O6
4	C	1001	NAG	O5-C5-C6-O6
4	B	904	NAG	O5-C5-C6-O6
4	D	904	NAG	O5-C5-C6-O6
4	A	1002	NAG	C4-C5-C6-O6
4	C	1002	NAG	C4-C5-C6-O6
4	A	1001	NAG	C4-C5-C6-O6
4	C	1001	NAG	C4-C5-C6-O6
4	A	1002	NAG	C1-C2-N2-C7
4	C	1002	NAG	C1-C2-N2-C7
4	A	1001	NAG	C3-C2-N2-C7
4	B	904	NAG	C3-C2-N2-C7
4	C	1001	NAG	C3-C2-N2-C7
4	D	904	NAG	C3-C2-N2-C7
4	A	1001	NAG	C1-C2-N2-C7
4	B	905	NAG	C1-C2-N2-C7
4	C	1001	NAG	C1-C2-N2-C7
4	D	905	NAG	C1-C2-N2-C7
4	A	1002	NAG	C3-C2-N2-C7
4	C	1002	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	905	NAG	1	0
4	B	905	NAG	1	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.

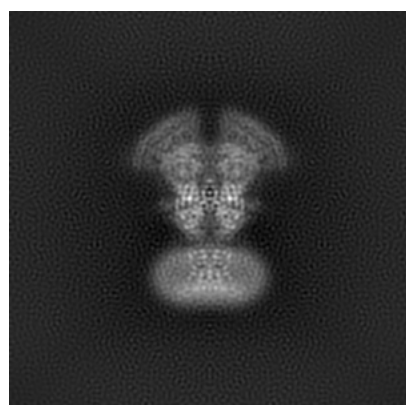
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21673. These allow visual inspection of the internal detail of the map and identification of artifacts.

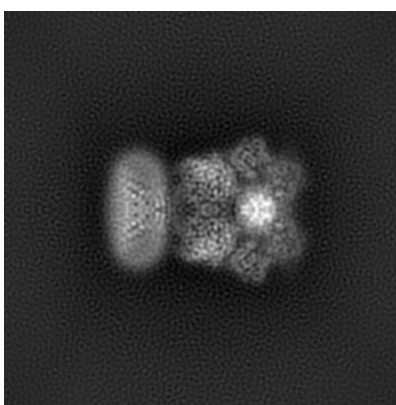
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

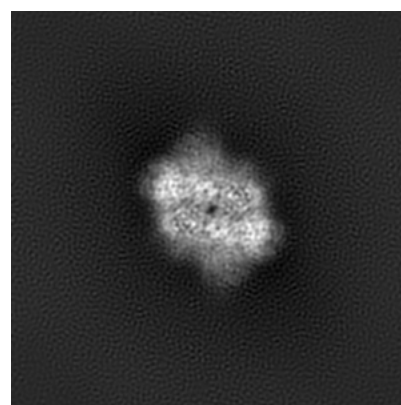
6.1.1 Primary map



X



Y

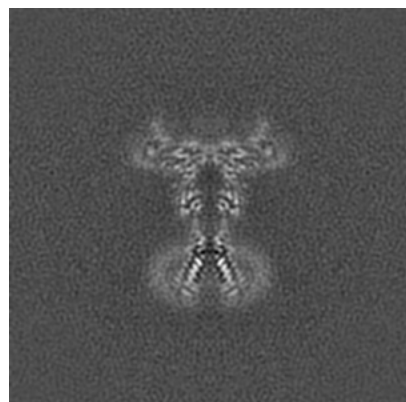


Z

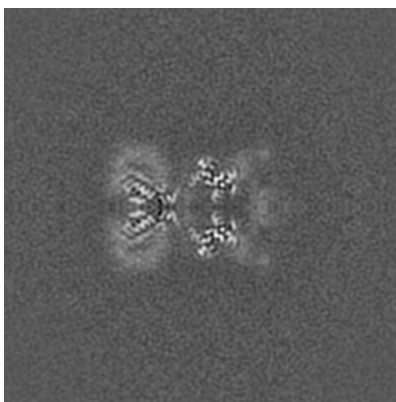
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

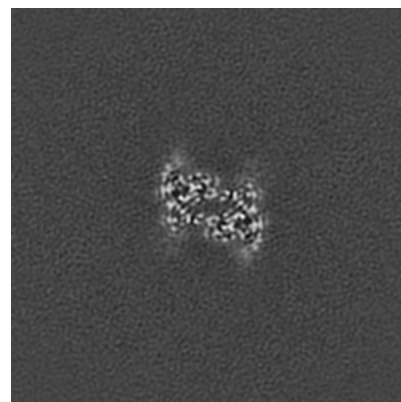
6.2.1 Primary map



X Index: 128



Y Index: 128

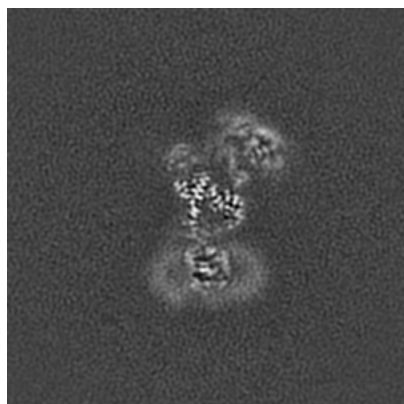


Z Index: 128

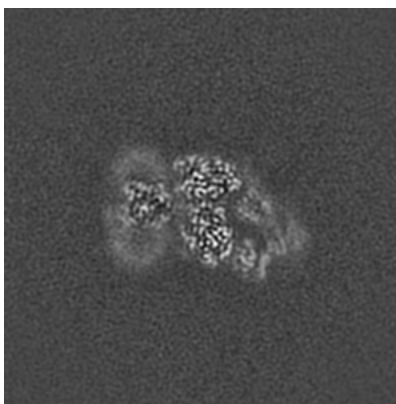
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

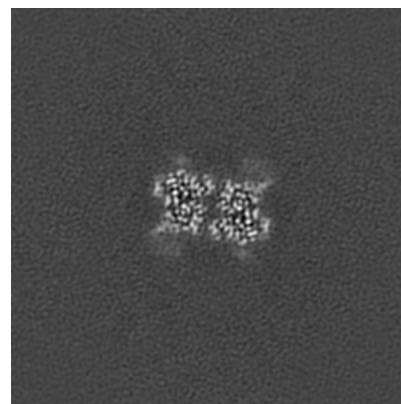
6.3.1 Primary map



X Index: 117



Y Index: 137

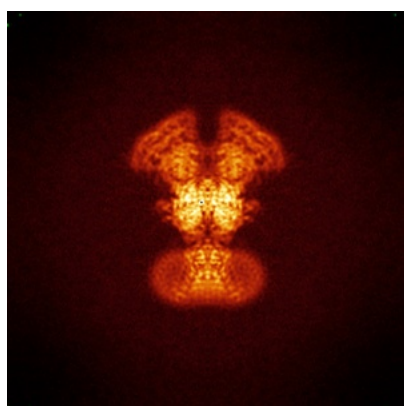


Z Index: 135

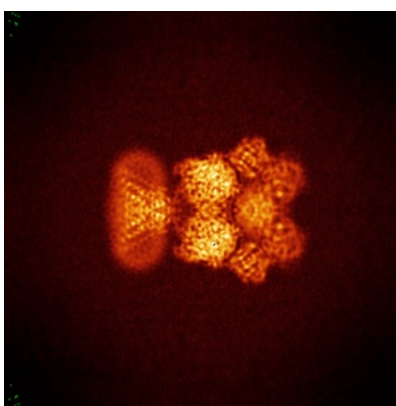
The images above show the largest variance slices of the map in three orthogonal directions.

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

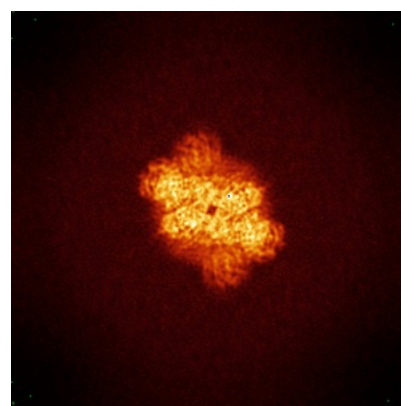
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

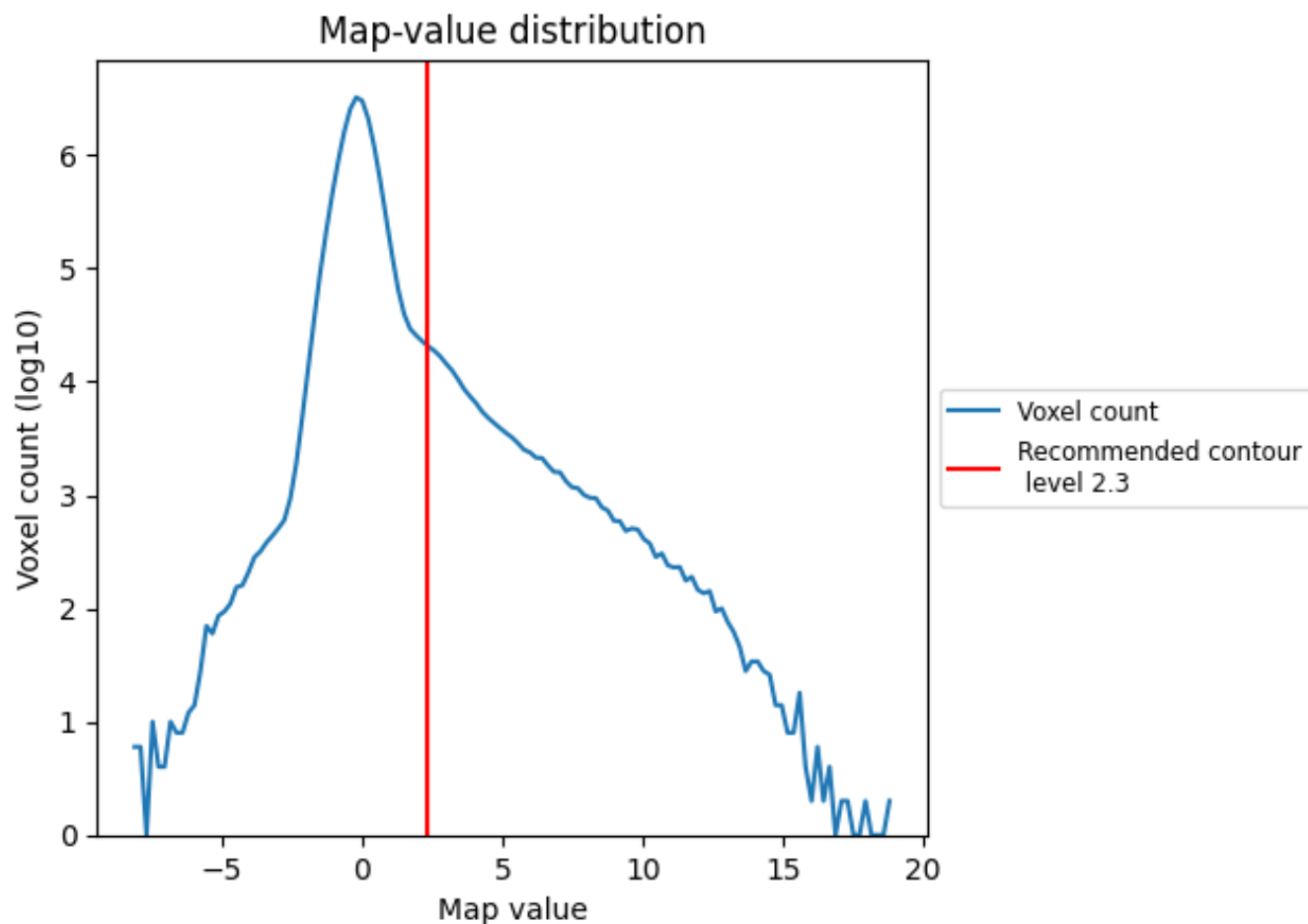
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

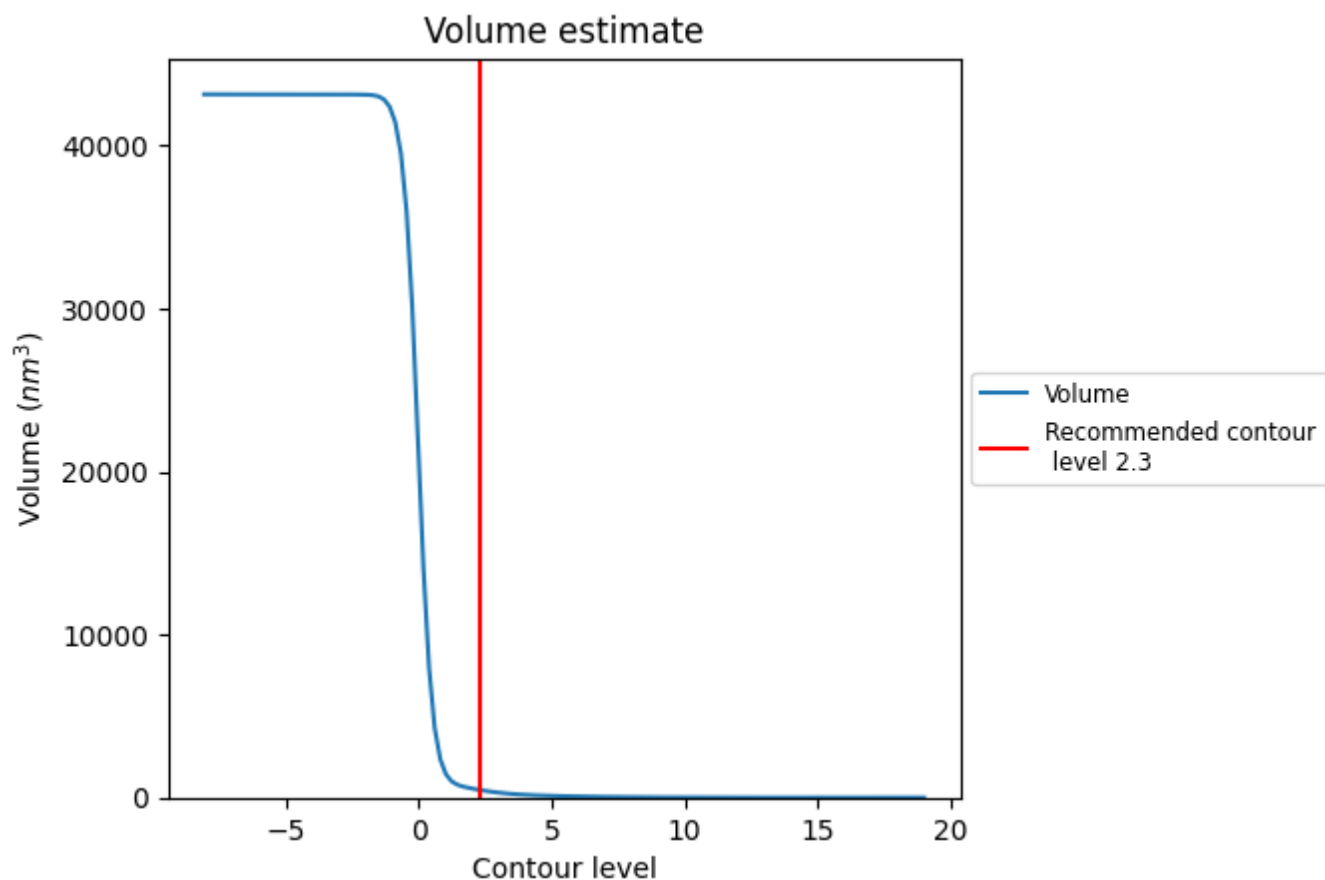
This section contains the results of statistical analysis of the map.

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.

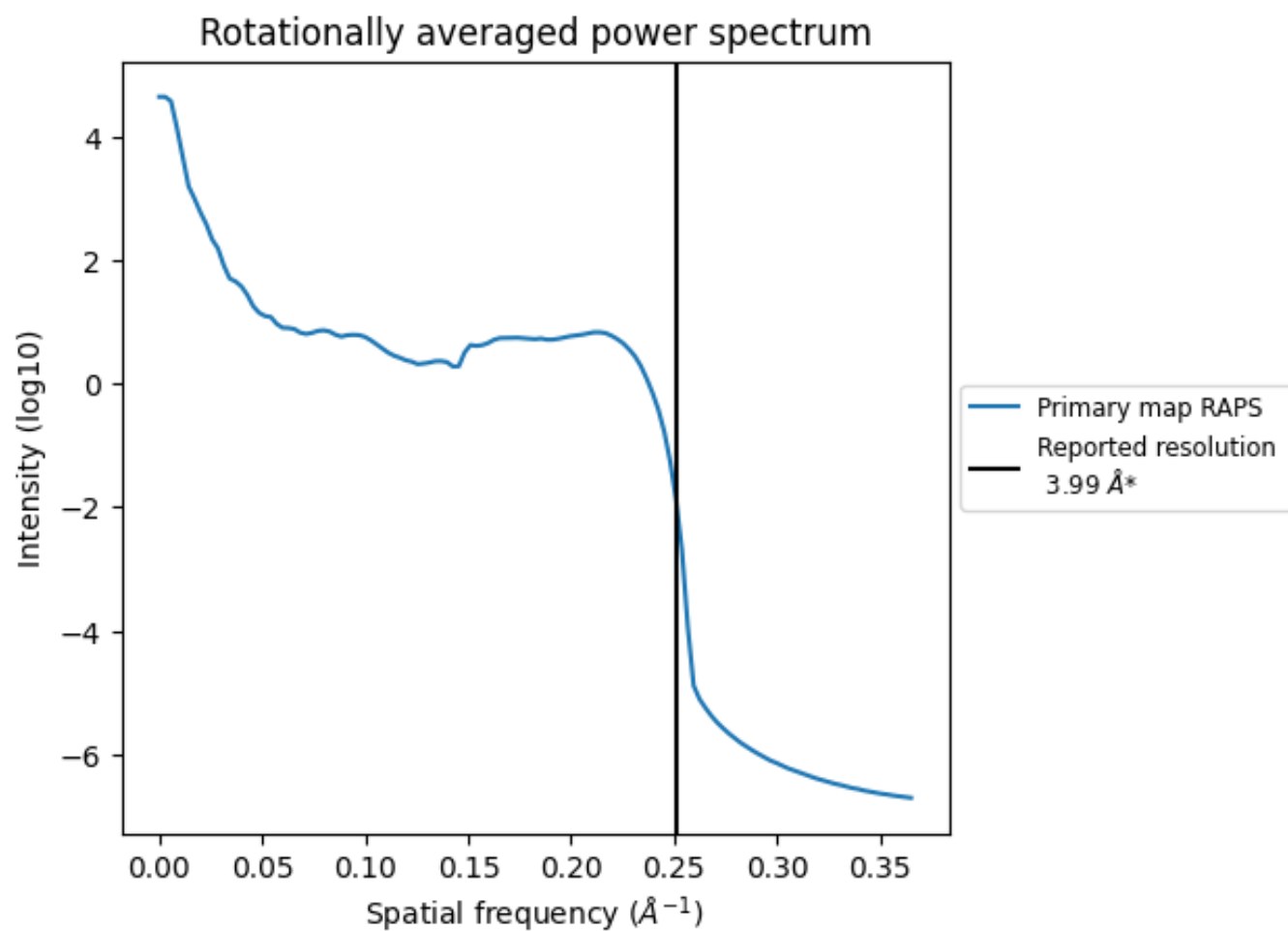
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 463 nm³; this corresponds to an approximate mass of 418 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 0.251 Å⁻¹

8 Fourier-Shell correlation

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

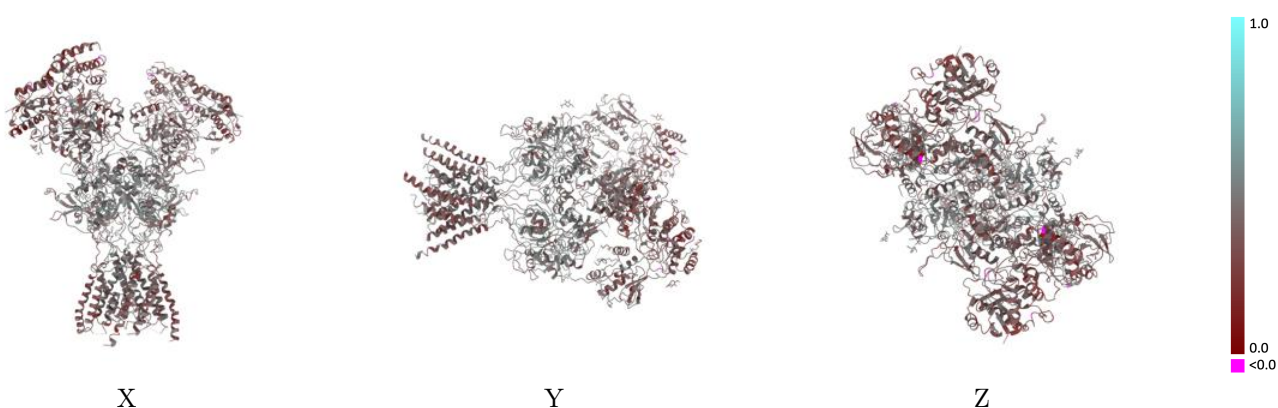
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21673 and PDB model 6WHR. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)

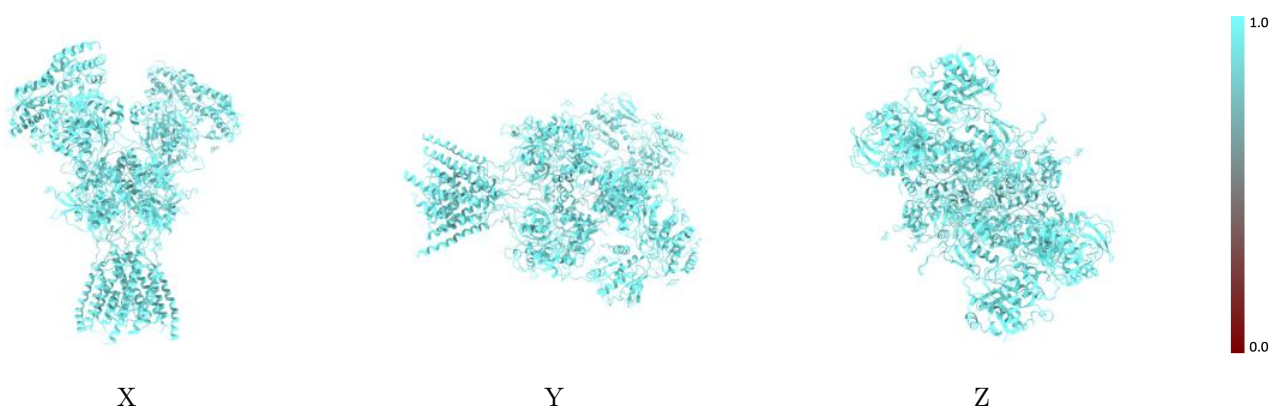
This section was not generated.

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



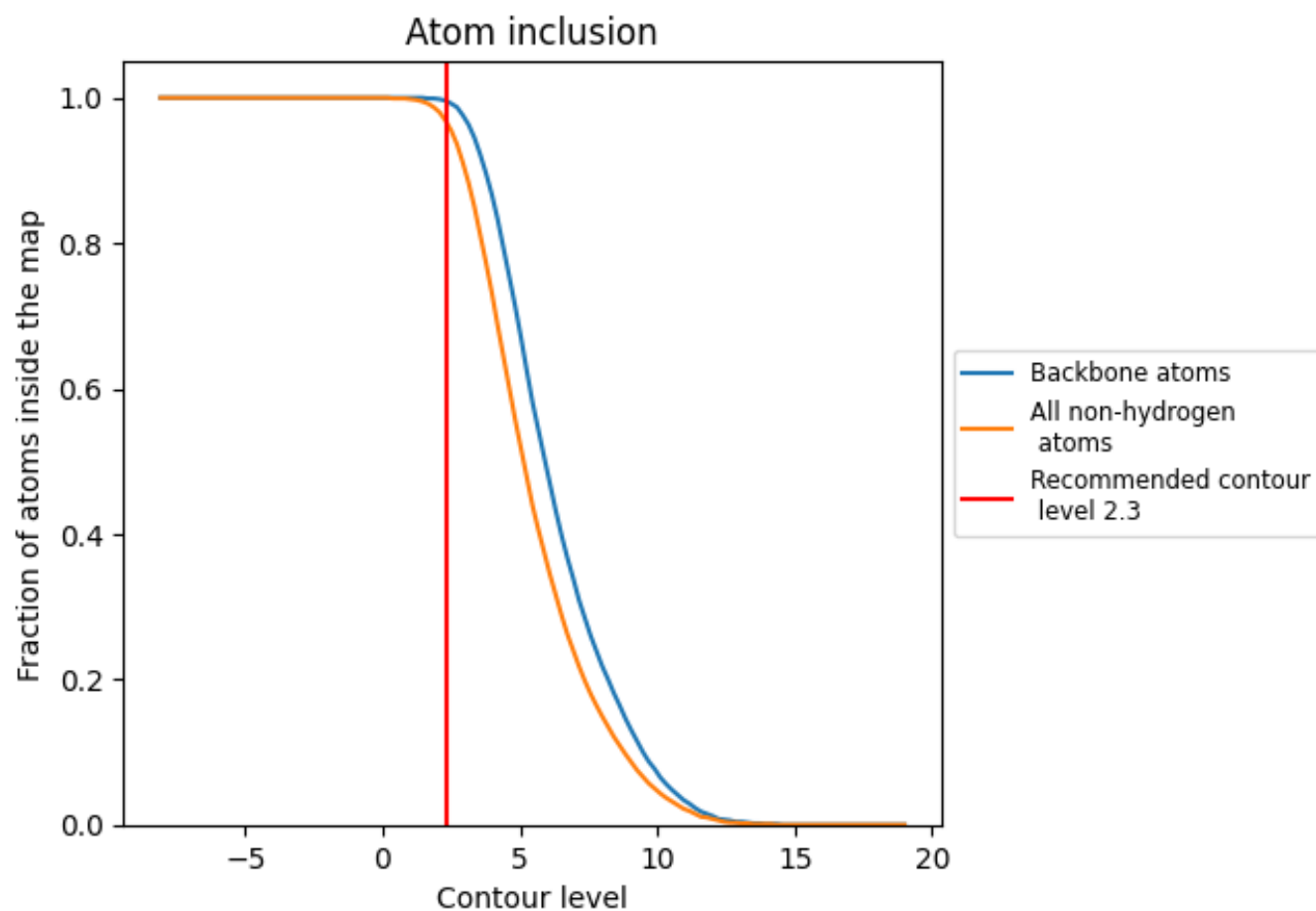
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 97% 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 (2.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9680	0.4110
A	0.9710	0.4130
B	0.9650	0.4100
C	0.9730	0.4130
D	0.9650	0.4100
E	1.0000	0.4630
F	0.9640	0.4700

1.0

0.0

<0.0