



## Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:38 AM UTC

PDB ID : 8VMC / pdb\_00008vmc  
EMDB ID : EMD-43355  
Title : Composite structure of human FASN with NADPH in State 6  
Authors : Schultz, K.; Marmorstein, R.  
Deposited on : 2024-01-13  
Resolution : 3.30 Å (reported)  
Based on initial model : 3HHD

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

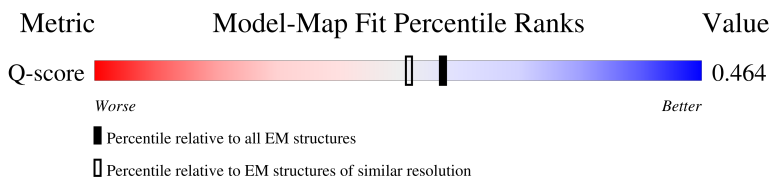
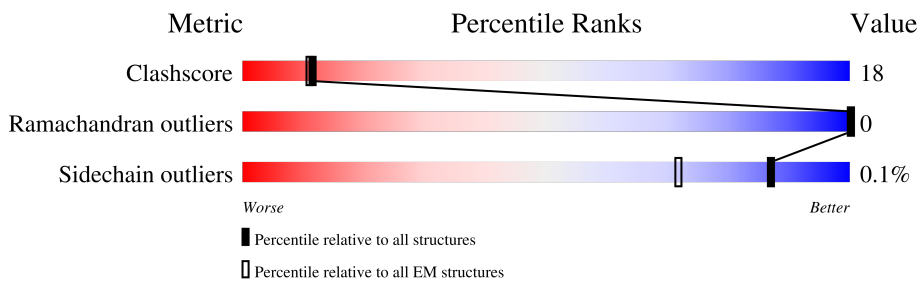
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 3.30 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	15087 ( 2.80 - 3.80 )

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  $\geq 3$ , 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	2553	57% 24% 19%
1	B	2553	59% 22% 19%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 50709 atoms, of which 18827 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 Fatty acid synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	2068	Total	C	H	N	O	S	0	0
			25176	10041	9343	2785	2934	73		
1	B	2071	Total	C	H	N	O	S	0	0
			25237	10054	9380	2789	2941	73		

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-31	MET	-	expression tag	UNP P49327
A	-30	SER	-	expression tag	UNP P49327
A	-29	TYR	-	expression tag	UNP P49327
A	-28	TYR	-	expression tag	UNP P49327
A	-27	ASP	-	expression tag	UNP P49327
A	-26	TYR	-	expression tag	UNP P49327
A	-25	LYS	-	expression tag	UNP P49327
A	-24	ASP	-	expression tag	UNP P49327
A	-23	ASP	-	expression tag	UNP P49327
A	-22	ASP	-	expression tag	UNP P49327
A	-21	ASP	-	expression tag	UNP P49327
A	-20	LYS	-	expression tag	UNP P49327
A	-19	ASP	-	expression tag	UNP P49327
A	-18	TYR	-	expression tag	UNP P49327
A	-17	ASP	-	expression tag	UNP P49327
A	-16	ILE	-	expression tag	UNP P49327
A	-15	PRO	-	expression tag	UNP P49327
A	-14	THR	-	expression tag	UNP P49327
A	-13	THR	-	expression tag	UNP P49327
A	-12	GLU	-	expression tag	UNP P49327
A	-11	ASN	-	expression tag	UNP P49327
A	-10	LEU	-	expression tag	UNP P49327
A	-9	TYR	-	expression tag	UNP P49327
A	-8	PHE	-	expression tag	UNP P49327
A	-7	GLN	-	expression tag	UNP P49327
A	-6	GLY	-	expression tag	UNP P49327

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	ALA	-	expression tag	UNP P49327
A	-4	MET	-	expression tag	UNP P49327
A	-3	GLY	-	expression tag	UNP P49327
A	-2	SER	-	expression tag	UNP P49327
A	-1	GLY	-	expression tag	UNP P49327
A	0	ILE	-	expression tag	UNP P49327
A	1	PRO	-	expression tag	UNP P49327
A	1151	THR	LYS	conflict	UNP P49327
A	2512	LEU	-	expression tag	UNP P49327
A	2513	GLU	-	expression tag	UNP P49327
A	2514	HIS	-	expression tag	UNP P49327
A	2515	HIS	-	expression tag	UNP P49327
A	2516	HIS	-	expression tag	UNP P49327
A	2517	HIS	-	expression tag	UNP P49327
A	2518	HIS	-	expression tag	UNP P49327
A	2519	HIS	-	expression tag	UNP P49327
A	2520	HIS	-	expression tag	UNP P49327
A	2521	HIS	-	expression tag	UNP P49327
B	-31	MET	-	expression tag	UNP P49327
B	-30	SER	-	expression tag	UNP P49327
B	-29	TYR	-	expression tag	UNP P49327
B	-28	TYR	-	expression tag	UNP P49327
B	-27	ASP	-	expression tag	UNP P49327
B	-26	TYR	-	expression tag	UNP P49327
B	-25	LYS	-	expression tag	UNP P49327
B	-24	ASP	-	expression tag	UNP P49327
B	-23	ASP	-	expression tag	UNP P49327
B	-22	ASP	-	expression tag	UNP P49327
B	-21	ASP	-	expression tag	UNP P49327
B	-20	LYS	-	expression tag	UNP P49327
B	-19	ASP	-	expression tag	UNP P49327
B	-18	TYR	-	expression tag	UNP P49327
B	-17	ASP	-	expression tag	UNP P49327
B	-16	ILE	-	expression tag	UNP P49327
B	-15	PRO	-	expression tag	UNP P49327
B	-14	THR	-	expression tag	UNP P49327
B	-13	THR	-	expression tag	UNP P49327
B	-12	GLU	-	expression tag	UNP P49327
B	-11	ASN	-	expression tag	UNP P49327
B	-10	LEU	-	expression tag	UNP P49327
B	-9	TYR	-	expression tag	UNP P49327
B	-8	PHE	-	expression tag	UNP P49327

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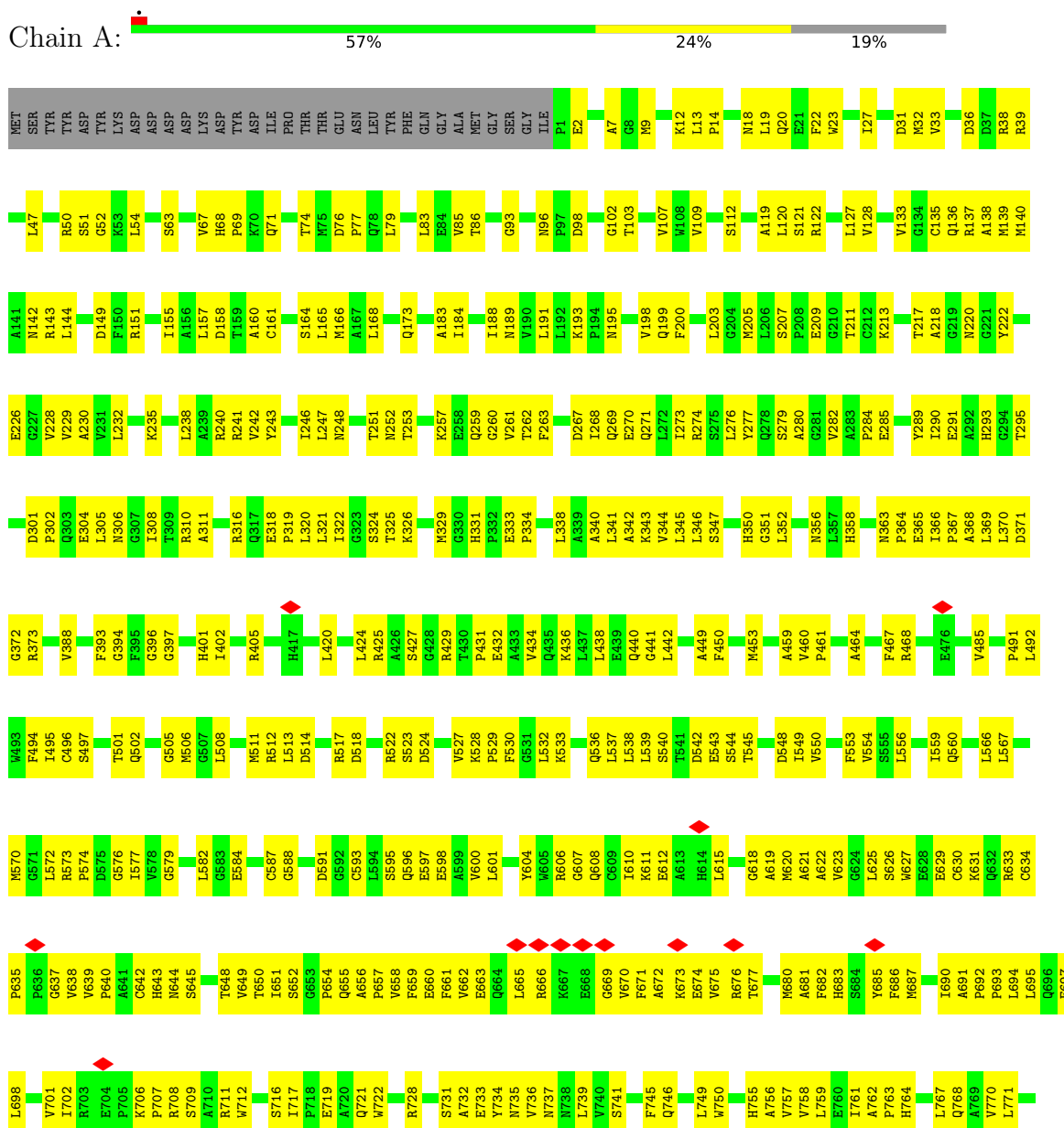


Mol	Chain	Residues	Atoms					AltConf	
2	A	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
2	A	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
2	B	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
2	B	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	

### 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: Fatty acid synthase





Q1374	Q1204	A1102	R652	L759	P693	E628	V550	E476	P367	A283	L206	P124	R38	MET
W1377	E1205	V1111	GLY	E760	L694	E629	H551	R477	A368	F284	L207	L127	R39	SER
R1387	R1206	V1112	SER	I761	L695	E630	V554		L369	E285	P208	L128	L47	TYR
L1388	P1207	T1120	GLY	A765	Q696	K631	S855	Q483	D371	T290	E209	Y130	R50	ASP
V1389	K1208	L1209	SER	L766	E697	Q632	L556	Q484	G372	E291	G210	E131	K63	LYS
G1390	L1209	E1126	PRO	L767	L698	R633	T557	V485	R373	A292	T211	M132		ASP
L1391	P1210	G1126	SER	Q768	K699	R634	I561	E489	L374	H293	C212	V133		ASP
K1392	E1211	L1128	ASP	A769	K700	C634	L562	R490	V376	G294	A214	C135	D56	ASP
Y1396	D865	S1129	D865	V770	I702	P636	L563	P491	Q375	T295	F215	C135	L57	ASP
F1401	S870	E1130	S870	K772	E704	V639	L566	W493	N391	V299	D216	A138	S58	LYS
V1417	D881	C1141	D881	G774	K706	A641	L567	F494	S392	M139	T217	M139	R59	ASP
V1424	L775	V1145	L775	K776	P707	A642	L568	I495	F393	R602	L217	M142	F60	TYR
K1429	L789	T898	L789	K776	R708	H643	S888	C642	V393	Q303	G221	M142		ASP
D1436	T898	T898	T898	K776	R708	H644	M570	C496	H401	L305	Y222	R143	P69	PRO
A1445	I924	T1150	I924	I781	W112	V649	G576	G498	Q409	G307	E226	F150	Q71	THR
I1446	V935	V1150	V935	I782	L713	T650	I577	M499	P412	I308	V228	A156	H73	GLU
V1457	R936	V1150	R936	P783	S714	I651	V578	M500	H417	R310	V228	L157	M75	GLU
C1471	L937	V1150	L937	L784	I717	S652	S581	T501	L420	R316	V231	L157	M75	GLU
L1474	L938	V1150	L938	K786	P718	G653	L582	F503	R429	S327	K236	S162	D76	LEU
E1485	L939	V1150	L939	K787	E719	P654	L583	M506	T430	L320	K236	S163	P77	TYR
V1486	E939	V1150	E939	K788	A720	Q655	E584	M506	L437	L322	S237	S164	P78	PHE
V1487	A940	V1150	A940	D788	E721	A656	E585	M506	L437	S327	A299	L165	Q78	GLN
C1471	S941	V1150	S941	H789	Q721	A656	E585	M506	L437	S327	A299	L165	L79	GLY
L1474	S941	V1150	S941	R790	W722	V657	V585	M506	L437	S327	A299	L165	R80	ALA
E1485	E948	V1150	E948	D791	H723	P657	V585	M506	L437	S327	A299	L165	R81	MET
V1486	N949	V1150	N949	N792	S724	F659	G588	M506	L437	S327	A299	L165	L82	GLY
L1493	R976	V1150	R976	F795	S725	E660	D591	M506	L437	S327	A299	L165	E84	GLY
L1497	P977	V1150	P977	L803	R727	V662	S595	M506	L437	S327	A299	L165	R85	ILE
Q1498	N978	V1150	N978	H804	E729	E663	Q596	M506	L437	S327	A299	L165	T86	ILE
L1501	E981	V1150	E981	L805	S730	Q664	E597	M506	L437	S327	A299	L165	Y87	PI
R1515	P982	V1150	P982	A810	A732	R666	E525	M506	L437	S327	A299	L165	Y88	V4
H1516	R997	V1150	R997	N811	E732	K667	A526	M506	L437	S327	A299	L165	A89	V6
F1517	E1014	V1150	E1014	A814	A732	E668	V527	M506	L437	S327	A299	L165	I90	I6
E1521	E1044	V1150	E1044	P817	L727	G669	K528	M506	L437	S327	A299	L165	G93	A7
R1552	K1043	V1150	K1043	L741	S741	F671	P529	M506	L437	S327	A299	L165	G94	M9
Q1555	L1046	V1150	L1046	P742	E742	G670	F530	M506	L437	S327	A299	L165	N96	K12
S1570	D1071	V1150	D1071	A823	L744	V670	G531	M506	L437	S327	A299	L165	P97	L13
I1588	K1072	V1150	K1072	E824	F745	E674	L532	M506	L437	S327	A299	L165	D98	P14
Q1595	D1072	V1150	D1072	K673	E746	B676	V534	M506	L437	S327	A299	L165	T105	E17
D1596	K1072	V1150	K1072	E674	E747	T677	S535	M506	L437	S327	A299	L165	W108	N16
E1602	H1093	V1150	H1093	I830	A748	M650	G618	M506	L437	S327	A299	L165	W109	L19
	L1202	V1150	L1202	L748	L748	A681	G619	M506	L437	S327	A299	L165	V110	F22
	A1203	V1150	A1203	L749	L749	F682	A619	M506	L437	S327	A299	L165	G110	W23
		V1150		L749	L749	H683	M620	M506	L437	S327	A299	L165	S111	D24
		V1150		L749	L749	S684	G621	M506	L437	S327	A299	L165	G113	N25
		V1150		L749	L749	F685	A622	M506	L437	S327	A299	L165	S114	L26
		V1150		L749	L749	F686	G623	M506	L437	S327	A299	L165	E115	L26
		V1150		L749	L749	M687	L625	M506	L437	S327	A299	L165	T116	L26
		V1150		L749	L749	E688	L625	M506	L437	S327	A299	L165	S117	M32
		V1150		L749	L749	A689	G626	M506	L437	S327	A299	L165	S117	V33
		V1150		L749	L749	P692	W627	M506	L437	S327	A299	L165	L120	D36
		V1150		L749	L749			M506	L437	S327	A299	L165	R202	D37



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	119577	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	52.4	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.790	Depositor
Minimum map value	-0.215	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.173	Depositor
Map size (Å)	384.84, 384.84, 384.84	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.069, 1.069, 1.069	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.16	0/16198	0.25	0/22023
1	B	0.22	0/16222	0.35	2/22055 (0.0%)
All	All	0.19	0/32420	0.31	2/44078 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	783	PRO	CB-CA-C	-6.75	103.13	111.64
1	B	1370	GLY	N-CA-C	-5.49	108.16	114.69

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	15833	9343	15809	554	0
1	B	15857	9380	15826	601	0
2	A	96	52	52	0	0
2	B	96	52	52	3	0
All	All	31882	18827	31739	1133	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 18.

All (1133) 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:B:1369:GLN:HA	1:B:1372:LEU:HD11	1.27	1.15
1:B:322:ILE:HD11	1:B:376:VAL:HG22	1.17	1.14
1:B:1372:LEU:HD22	1:B:1377:TRP:CZ2	1.81	1.14
1:B:1372:LEU:HD22	1:B:1377:TRP:CE2	1.82	1.13
1:A:155:ILE:CG2	1:B:157:LEU:HD22	1.83	1.08
1:B:322:ILE:CD1	1:B:376:VAL:HG22	1.86	1.06
1:B:1046:LEU:HD12	1:B:1046:LEU:O	1.56	1.05
1:B:322:ILE:HD11	1:B:376:VAL:CG2	1.88	1.04
1:B:1371:ILE:O	1:B:1372:LEU:HD12	1.57	1.02
1:B:768:GLN:HE22	1:B:781:ILE:HG22	1.22	1.02
1:A:468:ARG:HD2	1:A:485:VAL:HG21	1.43	1.01
1:B:556:LEU:HD23	1:B:582:LEU:HD23	1.39	1.01
1:B:768:GLN:CD	1:B:781:ILE:HG21	1.88	0.97
1:B:619:ALA:HB3	1:B:658:VAL:HG11	1.45	0.97
1:B:188:ILE:HG22	1:B:228:VAL:HG13	1.42	0.97
1:A:768:GLN:HG3	1:A:781:ILE:HG21	1.45	0.97
1:A:642:CYS:HB2	1:A:650:THR:HB	1.47	0.96
1:A:155:ILE:HG23	1:B:157:LEU:HD22	1.47	0.95
1:A:155:ILE:HG21	1:B:157:LEU:CD2	1.96	0.95
1:A:9:MET:HG2	1:A:19:LEU:HD11	1.47	0.94
1:B:654:PRO:HB2	1:B:657:PRO:HD2	1.48	0.94
1:B:499:MET:HG2	1:B:582:LEU:HB2	1.48	0.94
1:B:782:ILE:HG22	1:B:782:ILE:O	1.66	0.94
1:B:440:GLN:HG3	1:B:833:LEU:HD22	1.50	0.94
1:A:716:SER:HB2	1:A:741:SER:OG	1.68	0.92
1:A:155:ILE:HG21	1:B:157:LEU:HD22	1.52	0.91
1:A:549:ILE:HD11	1:A:611:LYS:HG3	1.53	0.91
1:B:768:GLN:NE2	1:B:781:ILE:HG22	1.86	0.91
1:B:768:GLN:NE2	1:B:781:ILE:CG2	2.33	0.91
1:B:333:GLU:HB2	1:B:334:PRO:HD3	1.53	0.90
1:B:768:GLN:OE1	1:B:781:ILE:HG21	1.71	0.90
1:A:155:ILE:CG2	1:B:157:LEU:CD2	2.50	0.87
1:A:191:LEU:HD13	1:A:226:GLU:HB3	1.57	0.86
1:A:621:ALA:HB3	1:A:651:ILE:HD11	1.55	0.86
1:B:322:ILE:HG12	1:B:375:GLN:O	1.75	0.86
1:B:707:PRO:HA	1:B:729:THR:HG22	1.60	0.84
1:B:1371:ILE:C	1:B:1372:LEU:HD12	2.03	0.84
1:B:491:PRO:HG3	1:B:753:PRO:HG2	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:683:HIS:H	1:A:687:MET:HG3	1.45	0.82
1:B:687:MET:HA	1:B:690:ILE:HD13	1.59	0.82
1:A:513:LEU:HD11	1:A:793:LEU:HD22	1.61	0.81
1:B:768:GLN:CD	1:B:781:ILE:CG2	2.53	0.81
1:A:363:ASN:HB3	1:A:366:ILE:HD13	1.61	0.81
1:A:1446:ILE:HG21	1:A:1486:VAL:HG21	1.62	0.81
1:B:654:PRO:HB2	1:B:657:PRO:CD	2.10	0.81
1:B:754:GLU:HG3	1:B:776:LYS:HE3	1.63	0.80
1:A:139:MET:HE2	1:A:139:MET:HA	1.63	0.80
1:B:1197:GLU:OE1	1:B:1197:GLU:N	2.16	0.79
1:B:654:PRO:HG3	1:B:686:PHE:HZ	1.45	0.79
1:B:429:ARG:NH1	1:B:464:ALA:O	2.15	0.79
1:A:759:LEU:HD21	1:A:803:LEU:HD13	1.65	0.79
1:B:654:PRO:HG3	1:B:686:PHE:CZ	2.17	0.78
1:B:235:LYS:HE3	1:B:238:LEU:HD13	1.65	0.78
1:B:644:ASN:ND2	1:B:650:THR:OG1	2.17	0.78
1:A:333:GLU:N	1:A:333:GLU:OE1	2.17	0.78
1:A:687:MET:HE2	1:A:739:LEU:HD11	1.65	0.77
1:A:138:ALA:HB3	1:B:160:ALA:HB2	1.66	0.77
1:A:189:ASN:HD22	1:A:334:PRO:HD2	1.50	0.77
1:B:60:PHE:CD1	1:B:80:ARG:HB3	2.21	0.76
1:A:615:LEU:HD12	1:A:680:MET:HE1	1.67	0.76
1:B:1145:VAL:HG21	1:B:1356:ILE:HG12	1.68	0.76
1:B:483:GLN:HG2	1:B:805:LEU:HD22	1.69	0.75
1:B:769:ALA:O	1:B:773:ARG:HG2	1.86	0.75
1:B:164:SER:HB3	1:B:338:LEU:HG	1.66	0.75
1:B:620:MET:O	1:B:675:VAL:HG22	1.87	0.75
1:B:881:ASP:CG	1:B:1046:LEU:HD21	2.11	0.75
1:A:304:GLU:HG3	1:A:393:PHE:HE2	1.51	0.75
1:B:1369:GLN:HA	1:B:1372:LEU:CD1	2.12	0.75
1:A:203:LEU:HD13	1:A:205:MET:HE3	1.69	0.75
1:A:14:PRO:HD2	1:A:329:MET:HE3	1.70	0.74
1:B:752:VAL:O	1:B:776:LYS:NZ	2.19	0.74
1:B:211:THR:HG22	1:B:213:LYS:HG3	1.69	0.74
1:A:1267:GLN:OE1	1:A:1267:GLN:N	2.21	0.74
1:A:1250:GLY:O	1:A:1316:ASN:ND2	2.21	0.74
1:A:1837:GLU:OE2	1:A:1841:ARG:NH2	2.21	0.74
1:A:164:SER:HB2	1:A:338:LEU:HD13	1.68	0.74
1:B:1195:GLN:O	1:B:1199:ALA:N	2.21	0.74
1:B:652:SER:HB2	1:B:681:ALA:HB1	1.70	0.74
1:B:1177:GLU:N	1:B:1177:GLU:OE1	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:ARG:NH1	1:A:464:ALA:O	2.18	0.73
1:B:254:ASP:HA	1:B:268:ILE:HG13	1.70	0.73
1:B:190:VAL:HG23	1:B:192:LEU:HD13	1.70	0.73
1:B:285:GLU:OE1	1:B:285:GLU:N	2.19	0.73
1:B:628:GLU:HA	1:B:631:LYS:HD2	1.70	0.73
1:B:423:LEU:HD13	1:B:472:VAL:HG22	1.70	0.73
1:A:697:GLU:O	1:A:701:VAL:HG23	1.89	0.73
1:A:285:GLU:OE1	1:A:285:GLU:N	2.20	0.73
1:A:1410:ASP:OD1	1:A:1411:SER:N	2.21	0.73
1:B:1457:VAL:HG21	1:B:1471:CYS:HB3	1.70	0.73
1:A:654:PRO:HB2	1:A:657:PRO:HD2	1.71	0.72
1:B:1372:LEU:CD2	1:B:1377:TRP:CE2	2.68	0.72
1:B:1485:GLU:N	1:B:1485:GLU:OE1	2.21	0.72
1:B:765:ALA:HB1	1:B:768:GLN:HG2	1.71	0.72
1:B:366:ILE:HG21	1:B:369:LEU:HD13	1.70	0.72
1:A:1085:ARG:NH2	1:A:1097:LEU:O	2.22	0.72
1:A:542:ASP:OD1	1:A:544:SER:N	2.18	0.72
1:B:633:ARG:NH2	1:B:668:GLU:OE2	2.22	0.72
1:B:736:VAL:O	1:B:740:VAL:HG22	1.90	0.72
1:A:161:CYS:HA	1:A:333:GLU:O	1.90	0.72
1:B:542:ASP:HB3	1:B:545:THR:OG1	1.88	0.72
1:A:396:GLY:HA3	1:B:142:ASN:HD22	1.55	0.71
1:A:692:PRO:O	1:A:695:LEU:HG	1.90	0.71
1:A:502:GLN:OE1	1:A:502:GLN:N	2.23	0.71
1:A:848:GLU:OE1	1:A:848:GLU:N	2.19	0.71
1:A:1278:GLN:OE1	1:A:1278:GLN:N	2.23	0.71
1:B:432:GLU:N	1:B:432:GLU:OE1	2.21	0.71
1:A:431:PRO:HG3	1:A:467:PHE:CE2	2.25	0.71
1:B:250:GLY:HA3	1:B:276:LEU:HD21	1.72	0.71
1:B:745:PHE:CE2	1:B:749:LEU:HD11	2.26	0.71
1:A:199:GLN:HG2	1:B:127:LEU:HD13	1.72	0.71
1:A:324:SER:H	1:A:356:ASN:HD21	1.39	0.71
1:A:1274:ASP:OD1	1:A:1275:ARG:N	2.23	0.71
1:A:366:ILE:HG21	1:A:369:LEU:HG	1.72	0.70
1:B:881:ASP:OD1	1:B:1046:LEU:CD2	2.39	0.70
1:A:168:LEU:HD22	1:A:402:ILE:HD11	1.72	0.70
1:B:768:GLN:OE1	1:B:781:ILE:CG2	2.39	0.70
1:A:248:ASN:HB2	1:A:280:ALA:HB2	1.74	0.70
1:A:550:VAL:HG21	1:A:611:LYS:HE2	1.72	0.70
1:A:1010:GLU:OE2	1:A:1019:ARG:NH2	2.24	0.70
1:B:581:SER:HA	1:B:738:ASN:HD21	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:642:CYS:HB2	1:B:650:THR:HB	1.74	0.70
1:A:139:MET:HE2	1:A:142:ASN:HB2	1.74	0.69
1:A:642:CYS:HB2	1:A:650:THR:CB	2.22	0.69
1:B:662:VAL:O	1:B:666:ARG:HG2	1.93	0.69
1:B:1602:GLU:OE2	1:B:1851:LYS:NZ	2.24	0.69
1:A:618:GLY:HA3	1:A:681:ALA:N	2.06	0.69
1:B:627:TRP:O	1:B:631:LYS:HG3	1.92	0.69
1:B:881:ASP:OD2	1:B:1046:LEU:HD21	1.92	0.69
1:B:536:GLN:O	1:B:540:SER:OG	2.11	0.69
1:B:391:ASN:OD1	1:B:391:ASN:O	2.11	0.69
1:B:569:CYS:SG	1:B:814:ALA:HB1	2.33	0.69
1:B:997:ARG:NH2	1:B:1043:LYS:O	2.26	0.69
1:B:1552:ARG:O	1:B:1555:GLN:NE2	2.26	0.69
1:A:325:THR:HB	1:A:343:LYS:HD2	1.75	0.69
1:A:619:ALA:HA	1:A:677:THR:HG22	1.74	0.69
1:B:747:GLU:N	1:B:747:GLU:OE1	2.26	0.69
1:B:333:GLU:OE1	1:B:333:GLU:N	2.26	0.68
1:B:524:ASP:OD1	1:B:534:VAL:HB	1.93	0.68
1:A:213:LYS:HG2	1:A:358:HIS:HB3	1.76	0.68
1:A:274:ARG:HA	1:A:277:TYR:CE2	2.28	0.68
1:A:570:MET:HE3	1:A:815:LEU:HD21	1.74	0.68
1:A:1489:GLY:O	1:A:1494:GLN:NE2	2.26	0.68
1:A:596:GLN:O	1:A:600:VAL:HG23	1.92	0.68
1:A:620:MET:HG2	1:A:652:SER:CB	2.24	0.68
1:B:332:PRO:HG2	1:B:336:SER:HA	1.75	0.68
1:B:468:ARG:HD2	1:B:485:VAL:HG21	1.74	0.68
1:A:203:LEU:HD12	1:B:132:MET:HE2	1.73	0.68
1:B:425:ARG:NH2	1:B:459:ALA:HB2	2.08	0.68
1:A:93:GLY:O	1:A:240:ARG:HB2	1.94	0.68
1:B:453:MET:HE2	1:B:830:ILE:HD12	1.76	0.68
1:A:209:GLU:OE1	1:A:209:GLU:N	2.27	0.67
1:A:539:LEU:HD23	1:A:539:LEU:O	1.94	0.67
1:A:1286:GLU:OE1	1:A:1286:GLU:N	2.27	0.67
1:A:644:ASN:HB3	1:A:770:VAL:HG11	1.74	0.67
1:B:460:VAL:HG11	1:B:465:MET:SD	2.34	0.67
1:B:477:ARG:HH12	1:B:790:ARG:HD2	1.57	0.67
1:A:508:LEU:HD11	1:A:538:LEU:O	1.94	0.67
1:B:412:PRO:HD3	1:B:824:PRO:HG2	1.75	0.67
1:B:765:ALA:HB1	1:B:768:GLN:CG	2.25	0.67
1:A:248:ASN:ND2	1:A:279:SER:OG	2.28	0.67
1:B:627:TRP:CD1	1:B:631:LYS:HE2	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:ARG:HG2	1:B:333:GLU:OE2	1.95	0.67
1:A:1176:GLN:N	1:A:1176:GLN:OE1	2.27	0.67
1:B:499:MET:HG2	1:B:582:LEU:CB	2.25	0.67
1:A:645:SER:N	1:A:648:THR:OG1	2.27	0.67
1:B:166:MET:HE1	1:B:251:THR:CG2	2.25	0.67
1:B:1446:ILE:HG23	1:B:1474:LEU:HD12	1.75	0.67
1:A:627:TRP:O	1:A:631:LYS:HG3	1.96	0.66
1:A:665:LEU:HB3	1:A:670:VAL:CG2	2.25	0.66
1:A:543:GLU:N	1:A:543:GLU:OE1	2.26	0.66
1:B:25:ASN:HB2	1:B:32:MET:HE2	1.77	0.66
1:B:705:PRO:HB3	1:B:730:SER:O	1.95	0.66
1:A:530:PHE:HB3	1:A:604:TYR:CZ	2.31	0.66
1:A:737:ASN:O	1:A:741:SER:N	2.21	0.66
1:B:440:GLN:HG3	1:B:833:LEU:CD2	2.24	0.66
1:B:1205:GLU:O	1:B:1209:LEU:N	2.29	0.66
1:B:291:GLU:HG2	1:B:340:ALA:HB1	1.76	0.66
1:B:322:ILE:CG1	1:B:376:VAL:HG22	2.25	0.66
1:A:14:PRO:O	1:A:32:MET:HE2	1.95	0.66
1:B:767:LEU:O	1:B:771:LEU:HD13	1.96	0.66
1:A:333:GLU:HB2	1:A:334:PRO:HD3	1.78	0.66
1:B:78:GLN:OE1	1:B:190:VAL:HG22	1.96	0.66
1:B:1300:ALA:O	1:B:1331:ASN:ND2	2.29	0.66
1:A:259:GLN:N	1:A:259:GLN:OE1	2.28	0.65
1:B:1274:ASP:OD1	1:B:1275:ARG:N	2.28	0.65
1:A:138:ALA:CB	1:B:160:ALA:HB2	2.26	0.65
1:A:549:ILE:HD12	1:A:550:VAL:N	2.12	0.65
1:A:1794:VAL:O	1:A:1795:LEU:HD23	1.97	0.65
1:B:661:PHE:CD2	1:B:665:LEU:HD11	2.31	0.65
1:B:591:ASP:OD2	1:B:712:TRP:HB2	1.97	0.65
1:B:1997:SER:O	1:B:2001:ASN:ND2	2.29	0.65
1:A:550:VAL:HG22	1:A:607:GLY:C	2.21	0.65
1:B:689:ALA:O	1:B:692:PRO:HD2	1.97	0.65
1:A:776:LYS:H	1:A:776:LYS:HD2	1.61	0.65
1:B:79:LEU:HD21	1:B:143:ARG:HG3	1.79	0.64
1:A:325:THR:HB	1:A:343:LYS:CD	2.28	0.64
1:B:548:ASP:OD1	1:B:550:VAL:HG12	1.97	0.64
1:A:716:SER:CB	1:A:741:SER:OG	2.44	0.64
1:B:621:ALA:CB	1:B:674:GLU:HA	2.28	0.64
1:B:627:TRP:CA	1:B:649:VAL:HG21	2.27	0.64
1:B:9:MET:HE3	1:B:19:LEU:HD13	1.80	0.64
1:B:116:THR:HG23	1:B:845:PRO:HG2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:SER:OG	1:B:335:ALA:HA	1.97	0.64
1:B:596:GLN:O	1:B:600:VAL:HG23	1.97	0.64
1:A:277:TYR:CE1	1:A:284:PRO:HG3	2.33	0.63
1:A:365:GLU:O	1:A:367:PRO:HD3	1.98	0.63
1:A:274:ARG:HA	1:A:277:TYR:CD2	2.33	0.63
1:B:1228:LEU:HD21	1:B:1256:ILE:HD12	1.78	0.63
1:A:136:GLN:HB3	1:A:139:MET:HG2	1.80	0.63
1:A:623:VAL:HG13	1:A:665:LEU:HD13	1.79	0.63
1:A:665:LEU:HD22	1:A:670:VAL:HG21	1.80	0.63
1:B:216:ASP:OD1	1:B:217:THR:N	2.30	0.63
1:B:333:GLU:CB	1:B:334:PRO:HD3	2.26	0.63
1:A:1418:ASP:OD1	1:A:1445:ALA:HB1	1.99	0.63
1:B:719:GLU:HA	1:B:722:TRP:NE1	2.14	0.63
1:B:620:MET:HE3	1:B:682:PHE:H	1.63	0.63
1:B:476:GLU:OE2	1:B:477:ARG:NH1	2.32	0.63
1:B:619:ALA:HB3	1:B:658:VAL:CG1	2.24	0.63
1:A:341:LEU:O	1:A:345:LEU:HG	1.99	0.63
1:A:997:ARG:NH1	1:A:1043:LYS:O	2.32	0.63
1:A:102:GLY:N	1:A:149:ASP:OD2	2.32	0.62
1:A:620:MET:HG2	1:A:652:SER:HB3	1.81	0.62
1:B:658:VAL:O	1:B:662:VAL:HG23	1.99	0.62
1:B:754:GLU:CG	1:B:776:LYS:HE3	2.28	0.62
1:A:852:ASN:O	1:A:852:ASN:ND2	2.32	0.62
1:A:633:ARG:HG3	1:A:661:PHE:CZ	2.35	0.62
1:B:624:GLY:N	1:B:671:PHE:O	2.26	0.62
1:A:492:LEU:HD13	1:A:808:ILE:CD1	2.30	0.62
1:B:881:ASP:OD1	1:B:1046:LEU:HD22	1.99	0.62
1:A:746:GLN:OE1	1:A:750:TRP:NE1	2.33	0.62
1:B:696:GLN:O	1:B:700:LYS:HG2	1.99	0.62
1:B:1417:VAL:HG12	1:B:1417:VAL:O	2.00	0.62
1:A:193:LYS:HE3	1:A:195:ASN:HB2	1.82	0.61
1:B:159:THR:CG2	1:B:163:SER:HA	2.29	0.61
1:A:608:GLN:O	1:A:612:GLU:HG3	1.99	0.61
1:A:1349:ARG:HB2	1:A:1371:ILE:HG22	1.82	0.61
1:B:1322:LEU:HD23	1:B:1369:GLN:HG3	1.82	0.61
1:A:1453:VAL:CG2	1:A:1471:CYS:SG	2.88	0.61
1:B:1214:LEU:O	1:B:1396:TYR:OH	2.14	0.61
1:A:1439:ARG:O	1:A:1468:ARG:NE	2.31	0.61
1:B:697:GLU:O	1:B:701:VAL:HG23	2.01	0.61
1:A:301:ASP:HB2	1:A:302:PRO:HD3	1.82	0.61
1:A:908:GLU:OE1	1:A:908:GLU:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:MET:HG3	1:B:79:LEU:HD23	1.83	0.61
1:B:267:ASP:O	1:B:271:GLN:HG3	2.01	0.61
1:B:417:HIS:HA	1:B:420:LEU:HD13	1.82	0.61
1:A:553:PHE:CD2	1:A:582:LEU:HD22	2.36	0.61
1:A:639:VAL:HG13	1:A:640:PRO:HD2	1.82	0.61
1:A:783:PRO:HD2	1:A:802:ARG:NH2	2.16	0.61
1:B:25:ASN:CB	1:B:32:MET:HE2	2.30	0.61
1:A:1337:ARG:NH1	1:A:1338:GLU:O	2.33	0.61
1:B:881:ASP:OD1	1:B:1046:LEU:HD21	2.00	0.61
1:A:22:PHE:HD1	1:A:32:MET:HE1	1.66	0.61
1:A:368:ALA:HA	1:A:371:ASP:OD2	2.01	0.61
1:B:542:ASP:OD1	1:B:544:SER:N	2.28	0.61
1:B:550:VAL:HG13	1:B:551:HIS:HD2	1.66	0.61
1:B:493:TRP:CE3	1:B:576:GLY:HA3	2.35	0.60
1:B:621:ALA:O	1:B:651:ILE:HG13	2.01	0.60
1:A:783:PRO:HD2	1:A:802:ARG:HH22	1.66	0.60
1:B:550:VAL:HG13	1:B:551:HIS:CD2	2.37	0.60
1:B:1324:ASP:OD1	1:B:1326:ALA:N	2.33	0.60
1:B:1879:THR:O	1:B:1907:ARG:NH1	2.33	0.60
1:A:1942:SER:O	1:A:1943:THR:OG1	2.13	0.60
1:B:476:GLU:OE2	1:B:790:ARG:NH1	2.34	0.60
1:B:745:PHE:CZ	1:B:749:LEU:HD21	2.37	0.60
1:A:188:ILE:HG22	1:A:228:VAL:HG13	1.83	0.60
1:A:241:ARG:HD2	1:A:453:MET:HE1	1.82	0.60
1:A:831:SER:OG	1:A:832:PRO:HD3	2.01	0.60
1:B:166:MET:HE1	1:B:251:THR:HG21	1.84	0.60
1:B:671:PHE:CZ	1:B:673:LYS:HD3	2.36	0.60
1:A:621:ALA:HA	1:A:675:VAL:H	1.67	0.60
1:A:1607:ASP:OD1	1:A:1608:ALA:N	2.33	0.60
1:B:22:PHE:O	1:B:26:LEU:HG	2.01	0.60
1:B:351:GLY:O	1:B:352:LEU:HD12	2.01	0.60
1:A:291:GLU:HG2	1:A:340:ALA:HB1	1.84	0.60
1:A:595:SER:HB3	1:A:598:GLU:HG3	1.84	0.60
1:B:1228:LEU:HD21	1:B:1256:ILE:CD1	2.31	0.60
1:A:522:ARG:NH1	1:A:596:GLN:OE1	2.35	0.60
1:A:556:LEU:O	1:A:560:GLN:HG3	2.01	0.60
1:A:1578:LEU:CD1	1:A:1583:LEU:HD23	2.32	0.60
1:A:1145:VAL:HG21	1:A:1356:ILE:HG12	1.84	0.59
1:B:661:PHE:CE2	1:B:665:LEU:HD11	2.37	0.59
1:A:514:ASP:HA	1:A:517:ARG:HH12	1.66	0.59
1:A:693:PRO:O	1:A:697:GLU:HG2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1571:LEU:O	1:A:1843:MET:HE1	2.01	0.59
1:B:782:ILE:HD13	1:B:803:LEU:HD23	1.83	0.59
1:A:656:ALA:HB3	1:A:657:PRO:HD3	1.84	0.59
1:B:639:VAL:HG13	1:B:640:PRO:HD2	1.83	0.59
1:B:939:GLU:OE1	1:B:939:GLU:N	2.34	0.59
1:B:1130:GLU:OE1	1:B:1130:GLU:N	2.33	0.59
1:B:506:MET:HE2	1:B:546:PHE:CE2	2.38	0.59
1:B:625:LEU:CD2	1:B:670:VAL:HG11	2.32	0.59
1:B:671:PHE:HZ	1:B:673:LYS:HD3	1.67	0.59
1:A:235:LYS:CG	1:A:238:LEU:HD13	2.33	0.59
1:A:440:GLN:HG3	1:A:833:LEU:HD22	1.85	0.59
1:A:566:LEU:HD22	1:A:815:LEU:HD22	1.85	0.59
1:A:737:ASN:OD1	1:A:741:SER:HB3	2.01	0.59
1:A:326:LYS:HE3	1:A:331:HIS:CD2	2.38	0.59
1:A:533:LYS:O	1:A:537:LEU:HG	2.03	0.59
1:A:618:GLY:O	1:A:677:THR:HB	2.03	0.59
1:B:366:ILE:CG2	1:B:369:LEU:HD13	2.31	0.59
1:B:515:ARG:HB2	1:B:566:LEU:CD2	2.32	0.59
1:B:782:ILE:O	1:B:782:ILE:CG2	2.39	0.59
1:A:621:ALA:O	1:A:651:ILE:HG13	2.03	0.59
1:A:692:PRO:HB2	1:A:693:PRO:HD3	1.84	0.59
1:B:621:ALA:HB1	1:B:673:LYS:O	2.03	0.59
1:B:737:ASN:HA	1:B:740:VAL:CG2	2.32	0.59
1:A:351:GLY:C	1:A:352:LEU:HD12	2.28	0.59
1:A:717:ILE:HG22	1:A:721:GLN:HB2	1.82	0.59
1:A:1616:LEU:HD13	1:A:1650:VAL:HG22	1.84	0.59
1:B:191:LEU:C	1:B:192:LEU:HD12	2.28	0.59
1:B:368:ALA:HB1	1:B:374:LEU:HB2	1.84	0.59
1:B:503:TRP:CH2	1:B:506:MET:HA	2.38	0.58
1:B:623:VAL:HG11	1:B:665:LEU:HD13	1.85	0.58
1:A:344:VAL:HG11	1:A:388:VAL:HG11	1.85	0.58
1:A:527:VAL:CG1	1:A:600:VAL:HG12	2.33	0.58
1:A:606:ARG:O	1:A:610:ILE:HG13	2.02	0.58
1:A:1417:VAL:CG1	1:A:1445:ALA:HB2	2.32	0.58
1:B:570:MET:HG2	1:B:811:ASN:O	2.03	0.58
1:A:1561:ALA:HB1	1:A:1627:LEU:HD11	1.85	0.58
1:A:205:MET:HB3	1:A:222:TYR:CE1	2.37	0.58
1:A:719:GLU:HA	1:A:722:TRP:CD1	2.39	0.58
1:A:784:LEU:O	1:A:785:MET:HG3	2.04	0.58
1:B:460:VAL:CG2	1:B:461:PRO:HD2	2.33	0.58
1:B:704:GLU:HG2	1:B:704:GLU:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:LEU:HD12	1:A:135:CYS:SG	2.44	0.58
1:A:694:LEU:HD23	1:A:698:LEU:HG	1.86	0.58
1:B:235:LYS:CE	1:B:238:LEU:HD13	2.34	0.58
1:B:351:GLY:C	1:B:352:LEU:HD12	2.28	0.58
1:B:719:GLU:HA	1:B:722:TRP:CD1	2.38	0.58
1:B:76:ASP:OD1	1:B:77:PRO:HD2	2.04	0.58
1:A:127:LEU:HD12	1:A:127:LEU:O	2.02	0.58
1:B:563:LEU:O	1:B:567:LEU:HD13	2.04	0.58
1:B:1014:GLU:N	1:B:1014:GLU:OE1	2.37	0.58
1:A:1417:VAL:HG13	1:A:1445:ALA:HB2	1.86	0.58
1:B:578:VAL:HG22	1:B:713:LEU:HB2	1.86	0.58
1:B:651:ILE:O	1:B:651:ILE:HD12	2.03	0.58
1:B:677:THR:O	1:B:680:MET:HG2	2.04	0.58
1:A:763:PRO:O	1:A:785:MET:HE2	2.04	0.58
1:B:81:LEU:O	1:B:85:VAL:HG23	2.03	0.58
1:A:661:PHE:O	1:A:665:LEU:HG	2.04	0.57
1:B:721:GLN:HB3	1:B:724:SER:OG	2.03	0.57
1:A:257:LYS:HE2	1:A:260:GLY:O	2.04	0.57
1:B:717:ILE:HD12	1:B:727:ALA:HB2	1.86	0.57
1:A:161:CYS:HB2	1:A:394:GLY:HA2	1.85	0.57
1:A:665:LEU:HB3	1:A:670:VAL:HG23	1.86	0.57
1:B:84:GLU:O	1:B:88:GLU:HG3	2.04	0.57
1:B:124:PRO:HA	1:B:127:LEU:HD23	1.86	0.57
1:B:623:VAL:CG1	1:B:665:LEU:HD13	2.34	0.57
1:A:137:ARG:O	1:A:140:MET:HG2	2.04	0.57
1:B:184:ILE:HD11	1:B:232:LEU:HD13	1.85	0.57
1:A:1453:VAL:HG22	1:A:1471:CYS:SG	2.45	0.57
1:A:1490:SER:O	1:A:1494:GLN:NE2	2.37	0.57
1:A:2034:TYR:O	1:A:2038:ASN:ND2	2.37	0.57
1:A:136:GLN:HB3	1:A:139:MET:CG	2.35	0.57
1:A:692:PRO:HA	1:A:695:LEU:CD2	2.34	0.57
1:A:621:ALA:HA	1:A:674:GLU:HA	1.86	0.57
1:B:499:MET:HG2	1:B:582:LEU:HD22	1.86	0.57
1:A:9:MET:HG2	1:A:19:LEU:CD1	2.27	0.57
1:A:112:SER:HA	1:A:137:ARG:HH12	1.69	0.57
1:A:166:MET:HE1	1:A:251:THR:OG1	2.05	0.57
1:A:556:LEU:HD13	1:A:763:PRO:HG3	1.87	0.57
1:A:759:LEU:HD21	1:A:803:LEU:CD1	2.33	0.57
1:B:719:GLU:HA	1:B:722:TRP:CE2	2.40	0.57
1:B:948:GLU:OE2	1:B:949:ASN:ND2	2.38	0.57
1:A:732:ALA:O	1:A:736:VAL:HG23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1275:ARG:NH2	1:A:1321:ALA:O	2.38	0.56
1:A:502:GLN:HB2	1:A:506:MET:HE1	1.86	0.56
1:A:306:ASN:O	1:A:310:ARG:HG3	2.06	0.56
1:A:1602:GLU:HB3	1:A:1650:VAL:HG23	1.87	0.56
1:B:57:LEU:HD23	1:B:81:LEU:HD11	1.87	0.56
1:B:1205:GLU:OE1	1:B:1209:LEU:HD12	2.06	0.56
1:A:293:HIS:N	1:A:304:GLU:OE2	2.24	0.56
1:B:627:TRP:N	1:B:649:VAL:HG21	2.21	0.56
1:A:513:LEU:HD12	1:A:513:LEU:H	1.70	0.56
1:A:683:HIS:N	1:A:687:MET:HG3	2.17	0.56
1:B:305:LEU:HD23	1:B:369:LEU:HD11	1.85	0.56
1:B:759:LEU:CD2	1:B:782:ILE:CG2	2.84	0.56
1:B:1212:ASP:OD1	1:B:1214:LEU:N	2.38	0.56
1:A:276:LEU:HD12	1:A:401:HIS:HB3	1.86	0.56
1:A:654:PRO:HB2	1:A:657:PRO:CD	2.35	0.56
1:B:86:THR:HG23	1:B:184:ILE:HG21	1.87	0.56
1:B:87:TYR:CE1	1:B:97:PRO:HG2	2.41	0.56
1:A:191:LEU:CD1	1:A:226:GLU:HB3	2.34	0.56
1:A:211:THR:HB	1:A:213:LYS:NZ	2.20	0.56
1:A:304:GLU:HG3	1:A:393:PHE:CE2	2.37	0.56
1:B:656:ALA:HB3	1:B:657:PRO:HD3	1.86	0.56
1:B:721:GLN:OE1	1:B:721:GLN:N	2.39	0.56
1:B:749:LEU:HB3	1:B:775:LEU:HD23	1.87	0.56
1:A:506:MET:O	1:A:538:LEU:HD22	2.06	0.55
1:A:68:HIS:HB3	1:A:71:GLN:OE1	2.05	0.55
1:A:656:ALA:O	1:A:660:GLU:HG3	2.06	0.55
1:B:515:ARG:HB2	1:B:566:LEU:HD23	1.88	0.55
1:A:1454:VAL:O	1:A:1458:ASN:ND2	2.39	0.55
1:B:499:MET:CG	1:B:582:LEU:HB2	2.27	0.55
1:A:1730:GLN:OE1	1:A:1730:GLN:N	2.39	0.55
1:B:1046:LEU:HD11	1:B:1102:ALA:HB3	1.87	0.55
1:A:316:ARG:NH1	1:A:320:LEU:HD13	2.20	0.55
1:B:503:TRP:CE2	1:B:506:MET:HB3	2.41	0.55
1:A:708:ARG:HG3	1:A:712:TRP:CE3	2.40	0.55
1:B:431:PRO:HG3	1:B:467:PHE:CE2	2.42	0.55
1:B:1343:LEU:HD12	1:B:1401:PHE:O	2.05	0.55
1:B:534:VAL:O	1:B:538:LEU:HD13	2.05	0.55
1:B:732:ALA:O	1:B:736:VAL:HG23	2.06	0.55
1:A:85:VAL:HG12	1:A:230:ALA:HB3	1.89	0.55
1:A:635:PRO:HD3	1:A:661:PHE:CD1	2.41	0.55
1:A:687:MET:CE	1:A:690:ILE:HD12	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:491:PRO:CG	1:B:753:PRO:HG2	2.34	0.55
1:B:674:GLU:N	1:B:674:GLU:OE1	2.40	0.55
1:B:720:ALA:HB3	1:B:721:GLN:OE1	2.06	0.55
1:B:783:PRO:O	1:B:795:PHE:HE1	1.89	0.55
1:A:514:ASP:HA	1:A:517:ARG:NH1	2.21	0.55
1:A:687:MET:HE2	1:A:739:LEU:CD1	2.35	0.55
1:A:990:VAL:HG13	1:A:1039:LEU:CD1	2.36	0.55
1:A:68:HIS:CG	1:A:69:PRO:HD2	2.41	0.55
1:A:290:ILE:HG23	1:A:322:ILE:HG13	1.88	0.55
1:A:497:SER:HB3	1:A:762:ALA:HB2	1.89	0.55
1:A:36:ASP:OD2	1:A:38:ARG:NE	2.40	0.54
1:A:811:ASN:OD1	1:A:813:ASN:HB2	2.06	0.54
1:B:322:ILE:HG21	1:B:374:LEU:HG	1.88	0.54
1:B:1178:LEU:CD1	1:B:1214:LEU:HD11	2.38	0.54
1:A:513:LEU:CD1	1:A:793:LEU:HD22	2.37	0.54
1:A:719:GLU:HA	1:A:722:TRP:NE1	2.22	0.54
1:B:189:ASN:HB2	1:B:334:PRO:HD2	1.89	0.54
1:B:1374:GLN:HE21	1:B:1391:LEU:HD11	1.71	0.54
1:B:1046:LEU:O	1:B:1046:LEU:CD1	2.45	0.54
1:B:9:MET:HG2	1:B:19:LEU:HD11	1.90	0.54
1:B:133:VAL:CG1	1:B:139:MET:HE2	2.37	0.54
1:B:225:SER:OG	1:B:330:GLY:HA3	2.07	0.54
1:A:261:VAL:HG23	1:A:262:THR:HG23	1.90	0.54
1:A:687:MET:CE	1:A:739:LEU:HD11	2.37	0.54
1:A:1974:VAL:HG12	1:A:1994:PRO:HG3	1.89	0.54
1:B:749:LEU:HD22	1:B:775:LEU:HD21	1.89	0.54
1:B:865:ASP:O	1:B:870:SER:OG	2.25	0.54
1:B:2042:GLU:OE2	1:B:2059:GLN:NE2	2.40	0.54
1:A:492:LEU:HD12	1:A:757:VAL:O	2.08	0.54
1:A:755:HIS:ND1	1:A:778:SER:HB2	2.23	0.54
1:B:115:GLU:OE1	1:B:193:LYS:N	2.40	0.54
1:B:198:VAL:O	1:B:202:ARG:HG2	2.07	0.54
1:B:304:GLU:HG3	1:B:393:PHE:HE2	1.73	0.54
1:B:848:GLU:N	1:B:848:GLU:OE1	2.40	0.54
1:B:1753:LEU:HD22	1:B:1754:GLN:HE22	1.73	0.54
1:A:625:LEU:HG	1:A:670:VAL:HG11	1.89	0.54
1:A:1234:ASN:OD1	1:A:1502:VAL:HG23	2.07	0.54
1:A:1077:ASP:OD1	1:A:1078:VAL:N	2.40	0.54
1:A:1446:ILE:HD12	1:A:1447:ASN:N	2.22	0.54
1:B:211:THR:CG2	1:B:213:LYS:HG3	2.38	0.54
1:B:293:HIS:HB3	1:B:304:GLU:OE1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:460:VAL:HG23	1:B:461:PRO:HD2	1.89	0.54
1:B:1080:VAL:HG22	1:B:1087:THR:HG23	1.89	0.54
1:A:14:PRO:CD	1:A:329:MET:HE3	2.38	0.54
1:A:23:TRP:O	1:A:27:ILE:HG22	2.08	0.54
1:A:366:ILE:HG22	1:A:369:LEU:H	1.72	0.54
1:A:523:SER:O	1:A:527:VAL:HG22	2.08	0.54
1:B:56:ASP:OD1	1:B:57:LEU:N	2.41	0.54
1:B:527:VAL:HG11	1:B:532:LEU:HD11	1.89	0.54
1:B:754:GLU:CG	1:B:776:LYS:CE	2.86	0.54
1:A:213:LYS:HE2	1:A:218:ALA:O	2.07	0.53
1:A:316:ARG:HH21	1:A:318:GLU:HG2	1.73	0.53
1:A:371:ASP:OD1	1:A:373:ARG:HG3	2.09	0.53
1:A:682:PHE:HB3	1:A:683:HIS:HD2	1.73	0.53
1:B:493:TRP:CZ3	1:B:576:GLY:HA3	2.43	0.53
1:B:708:ARG:NH2	1:B:714:SER:HB2	2.24	0.53
1:B:1141:CYS:O	1:B:1145:VAL:HG23	2.08	0.53
1:A:420:LEU:HD22	1:A:512:ARG:HE	1.73	0.53
1:A:460:VAL:HG13	1:A:461:PRO:HD2	1.89	0.53
1:B:528:LYS:HB3	1:B:529:PRO:HD3	1.91	0.53
1:B:1071:ASP:OD1	1:B:1072:LYS:N	2.37	0.53
1:A:366:ILE:O	1:A:370:LEU:HD13	2.08	0.53
1:B:159:THR:HG22	1:B:163:SER:HA	1.91	0.53
1:B:409:GLN:HB3	1:B:824:PRO:HA	1.91	0.53
1:B:617:PRO:HB2	1:B:655:GLN:CD	2.34	0.53
1:A:1535:THR:HG23	1:A:1535:THR:O	2.08	0.53
1:B:534:VAL:HG22	1:B:554:VAL:HG12	1.90	0.53
1:A:591:ASP:OD1	1:A:709:SER:HB3	2.09	0.53
1:A:86:THR:HG23	1:A:184:ILE:HG21	1.90	0.53
1:A:168:LEU:HD13	1:A:402:ILE:CD1	2.39	0.53
1:A:1118:CYS:SG	1:A:1119:PHE:N	2.80	0.53
1:B:7:ALA:HA	1:B:241:ARG:O	2.09	0.53
1:B:39:ARG:HD2	1:B:191:LEU:O	2.09	0.53
1:B:112:SER:HB3	1:B:334:PRO:HG3	1.90	0.53
1:B:209:GLU:N	1:B:209:GLU:OE1	2.41	0.53
1:B:691:ALA:O	1:B:695:LEU:N	2.31	0.53
1:B:754:GLU:HG2	1:B:776:LYS:CE	2.39	0.53
1:A:203:LEU:CD1	1:B:132:MET:HE2	2.39	0.53
1:A:13:LEU:HB3	1:A:14:PRO:HD2	1.91	0.53
1:A:47:LEU:HD21	1:A:198:VAL:HA	1.91	0.53
1:A:168:LEU:HD22	1:A:402:ILE:CD1	2.39	0.53
1:A:502:GLN:HB2	1:A:506:MET:CE	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1453:VAL:CG1	1:A:1471:CYS:SG	2.97	0.53
1:B:537:LEU:HB3	1:B:546:PHE:CE1	2.43	0.53
1:B:549:ILE:HD11	1:B:611:LYS:HG2	1.91	0.53
1:A:615:LEU:HD12	1:A:680:MET:CE	2.38	0.52
1:B:261:VAL:HG13	1:B:262:THR:HG23	1.91	0.52
1:B:328:ASN:OD1	1:B:357:LEU:HG	2.10	0.52
1:A:579:GLY:HA3	1:A:584:GLU:OE1	2.09	0.52
1:B:625:LEU:HB2	1:B:630:CYS:SG	2.49	0.52
1:B:1111:VAL:O	1:B:1111:VAL:HG13	2.10	0.52
1:A:633:ARG:HG3	1:A:661:PHE:HZ	1.72	0.52
1:A:891:TYR:OH	1:A:923:THR:HG22	2.09	0.52
1:A:1970:ASN:C	1:A:1971:LEU:HD12	2.34	0.52
1:B:306:ASN:O	1:B:310:ARG:HG3	2.09	0.52
1:B:1889:ILE:HD11	1:B:1912:LEU:HD11	1.91	0.52
1:A:270:GLU:HG3	1:A:311:ALA:HB2	1.91	0.52
1:B:759:LEU:CD2	1:B:782:ILE:HG22	2.39	0.52
1:A:63:SER:OG	1:A:429:ARG:NH2	2.43	0.52
1:A:468:ARG:CD	1:A:485:VAL:HG21	2.28	0.52
1:A:1457:VAL:HG21	1:A:1471:CYS:HB2	1.90	0.52
1:B:70:LYS:HE3	1:B:130:TYR:OH	2.09	0.52
1:B:695:LEU:O	1:B:699:LYS:HG2	2.10	0.52
1:A:550:VAL:CG2	1:A:611:LYS:HE2	2.38	0.52
1:A:767:LEU:O	1:A:771:LEU:HD13	2.10	0.52
1:A:1843:MET:HE3	1:A:1852:VAL:HB	1.92	0.52
1:B:537:LEU:HB3	1:B:546:PHE:HE1	1.73	0.52
1:B:640:PRO:HA	1:B:651:ILE:HG22	1.90	0.52
1:B:1336:LEU:HD12	1:B:1336:LEU:O	2.10	0.52
1:A:495:ILE:HD12	1:A:758:VAL:HG11	1.91	0.52
1:A:1975:LEU:HD12	1:A:1975:LEU:O	2.10	0.52
1:B:544:SER:OG	1:B:547:ASP:OD2	2.23	0.52
1:B:628:GLU:HA	1:B:631:LYS:CD	2.39	0.52
1:B:643:HIS:HD2	1:B:649:VAL:HG22	1.74	0.52
1:A:1219:LEU:HB3	1:A:1255:ARG:HE	1.74	0.52
1:A:1446:ILE:HG22	1:A:1474:LEU:CD1	2.40	0.52
1:B:527:VAL:HG12	1:B:527:VAL:O	2.09	0.52
1:B:1889:ILE:CD1	1:B:1912:LEU:HD11	2.40	0.52
1:A:491:PRO:HG2	1:A:756:ALA:CB	2.40	0.52
1:A:619:ALA:HA	1:A:677:THR:CG2	2.39	0.52
1:B:115:GLU:OE1	1:B:192:LEU:HB2	2.10	0.52
1:B:503:TRP:CZ2	1:B:506:MET:HA	2.45	0.52
1:A:639:VAL:CG1	1:A:640:PRO:HD2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:658:VAL:O	1:A:662:VAL:HG23	2.10	0.51
1:A:252:ASN:HD21	1:A:268:ILE:HG22	1.76	0.51
1:A:366:ILE:CG2	1:A:369:LEU:HG	2.40	0.51
1:A:442:LEU:HD23	1:A:442:LEU:O	2.10	0.51
1:B:110:GLY:CA	1:B:163:SER:HB2	2.39	0.51
1:B:608:GLN:O	1:B:611:LYS:HB2	2.09	0.51
1:B:718:PRO:HG3	1:B:744:LEU:HD11	1.91	0.51
1:A:79:LEU:HD21	1:A:143:ARG:HG3	1.92	0.51
1:A:625:LEU:CD2	1:A:670:VAL:HG11	2.40	0.51
1:B:274:ARG:HA	1:B:277:TYR:CD2	2.45	0.51
1:B:391:ASN:HB2	1:B:393:PHE:CZ	2.46	0.51
1:B:412:PRO:HD3	1:B:824:PRO:CG	2.40	0.51
1:B:437:LEU:HD22	1:B:454:LEU:HD22	1.93	0.51
1:B:511:MET:CE	1:B:520:ILE:HG21	2.40	0.51
1:A:121:SER:HB3	1:B:199:GLN:NE2	2.26	0.51
1:A:242:VAL:HG23	1:A:822:PRO:HB3	1.92	0.51
1:A:1336:LEU:HD11	1:A:1340:GLY:HA3	1.92	0.51
1:B:577:ILE:N	1:B:577:ILE:HD12	2.26	0.51
1:B:1128:LEU:HD12	1:B:1128:LEU:N	2.26	0.51
1:B:2020:SER:OG	1:B:2021:SER:N	2.43	0.51
1:A:654:PRO:O	1:A:657:PRO:HD2	2.11	0.51
1:A:745:PHE:O	1:A:749:LEU:HB2	2.11	0.51
1:B:50:ARG:HD3	1:B:209:GLU:O	2.10	0.51
1:B:2006:THR:HG21	1:B:2013:LEU:HD22	1.91	0.51
1:B:108:TRP:HB3	1:B:167:ALA:HB1	1.93	0.51
1:B:654:PRO:O	1:B:658:VAL:HG12	2.10	0.51
1:A:527:VAL:HG11	1:A:600:VAL:HG12	1.91	0.51
1:B:550:VAL:O	1:B:554:VAL:HG23	2.10	0.51
1:B:621:ALA:HB2	1:B:674:GLU:HA	1.93	0.51
1:B:702:ILE:HD12	1:B:702:ILE:N	2.25	0.51
1:A:1909:VAL:HG12	1:A:1911:LYS:H	1.75	0.51
1:B:206:LEU:HD21	1:B:224:ARG:HG3	1.93	0.51
1:A:316:ARG:HH12	1:A:320:LEU:HD13	1.75	0.51
1:A:623:VAL:HG22	1:A:665:LEU:CD1	2.41	0.51
1:B:105:THR:HG23	1:B:182:ALA:O	2.11	0.51
1:B:698:LEU:HD22	1:B:702:ILE:CD1	2.41	0.51
1:B:754:GLU:O	1:B:755:HIS:HB2	2.11	0.51
1:A:440:GLN:HG3	1:A:833:LEU:CD2	2.41	0.51
1:A:701:VAL:HG12	1:A:702:ILE:HG13	1.91	0.51
1:A:1942:SER:OG	1:A:1958:GLU:OE2	2.23	0.51
1:B:60:PHE:HB3	1:B:842:TRP:CD1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:VAL:HG23	1:B:822:PRO:HB3	1.93	0.51
1:A:1210:PRO:HB3	1:A:1319:VAL:HG11	1.92	0.50
1:B:615:LEU:HD12	1:B:615:LEU:O	2.11	0.50
1:B:654:PRO:HG2	1:B:657:PRO:HG2	1.91	0.50
1:B:713:LEU:HD22	1:B:722:TRP:CZ3	2.45	0.50
1:A:567:LEU:HD12	1:A:761:ILE:HD11	1.92	0.50
1:A:659:PHE:O	1:A:663:GLU:HG3	2.11	0.50
1:B:607:GLY:O	1:B:611:LYS:HG3	2.12	0.50
1:A:168:LEU:HD23	1:A:168:LEU:O	2.11	0.50
1:A:252:ASN:ND2	1:A:268:ILE:HG22	2.26	0.50
1:A:1432:LEU:HD22	1:A:1980:LEU:HD23	1.93	0.50
1:B:139:MET:HE3	1:B:143:ARG:CD	2.41	0.50
1:A:31:ASP:OD2	1:A:50:ARG:NH2	2.43	0.50
1:A:261:VAL:HG21	1:B:133:VAL:HG11	1.93	0.50
1:A:1130:GLU:OE1	1:A:1130:GLU:N	2.40	0.50
1:A:654:PRO:HG3	1:A:686:PHE:CZ	2.46	0.50
1:B:105:THR:O	1:B:150:PHE:HB3	2.10	0.50
1:B:1787:LYS:O	1:B:1789:VAL:HG23	2.12	0.50
1:A:597:GLU:O	1:A:601:LEU:HG	2.12	0.50
1:A:783:PRO:O	1:A:784:LEU:HB2	2.11	0.50
1:B:213:LYS:HG2	1:B:358:HIS:HB3	1.94	0.50
1:B:417:HIS:CD2	1:B:817:PRO:HG2	2.46	0.50
1:B:613:ALA:CB	1:B:690:ILE:HG13	2.42	0.50
1:A:542:ASP:O	1:A:545:THR:HG22	2.10	0.50
1:A:1415:LEU:HD21	1:A:1424:TRP:HB2	1.93	0.50
1:B:347:SER:HB2	1:B:352:LEU:O	2.12	0.50
1:B:661:PHE:O	1:B:665:LEU:HG	2.12	0.50
1:B:692:PRO:HB2	1:B:693:PRO:CD	2.41	0.50
1:A:662:VAL:O	1:A:666:ARG:HG3	2.11	0.50
1:A:1670:THR:C	1:A:1671:LEU:HD12	2.37	0.50
1:B:1233:GLU:OE1	1:B:1515:ARG:NH2	2.42	0.50
1:B:2097:LEU:O	1:B:2097:LEU:HD23	2.11	0.50
1:A:22:PHE:CD1	1:A:32:MET:HE1	2.45	0.49
1:A:122:ARG:NH1	1:A:849:ASP:HB3	2.27	0.49
1:A:158:ASP:HB2	1:B:156:ALA:HB3	1.93	0.49
1:A:567:LEU:CD1	1:A:761:ILE:HD11	2.42	0.49
1:A:733:GLU:OE1	1:A:733:GLU:N	2.35	0.49
1:A:775:LEU:HD12	1:A:781:ILE:HD11	1.93	0.49
1:A:1069:LEU:HD11	1:A:1075:VAL:HG11	1.93	0.49
1:B:105:THR:HG23	1:B:182:ALA:C	2.37	0.49
1:B:299:VAL:O	1:B:302:PRO:HD2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:759:LEU:HD23	1:B:782:ILE:CG2	2.42	0.49
1:B:1077:ASP:OD1	1:B:1078:VAL:N	2.44	0.49
1:A:635:PRO:HD3	1:A:661:PHE:CE1	2.47	0.49
1:A:52:GLY:O	1:A:226:GLU:HG2	2.12	0.49
1:A:83:LEU:HD23	1:A:144:LEU:CD2	2.42	0.49
1:A:536:GLN:O	1:A:540:SER:N	2.42	0.49
1:A:550:VAL:O	1:A:554:VAL:HG23	2.12	0.49
1:A:783:PRO:HB2	1:A:795:PHE:CE2	2.47	0.49
1:B:643:HIS:CD2	1:B:649:VAL:HG22	2.48	0.49
1:A:622:ALA:N	1:A:673:LYS:O	2.38	0.49
1:A:634:CYS:HA	1:A:661:PHE:CZ	2.48	0.49
1:B:93:GLY:O	1:B:240:ARG:HB2	2.11	0.49
1:B:1199:ALA:O	1:B:1203:ALA:N	2.42	0.49
1:A:13:LEU:HD22	1:A:329:MET:HE1	1.94	0.49
1:A:173:GLN:NE2	1:B:179:GLN:OE1	2.39	0.49
1:A:745:PHE:CE2	1:A:749:LEU:HD22	2.47	0.49
1:A:1243:VAL:HG12	1:A:1271:THR:CG2	2.43	0.49
1:B:47:LEU:HD23	1:B:201:LEU:HD22	1.94	0.49
1:A:620:MET:O	1:A:675:VAL:N	2.46	0.49
1:B:259:GLN:OE1	1:B:259:GLN:N	2.29	0.49
1:B:557:THR:O	1:B:561:ILE:HG13	2.12	0.49
1:A:83:LEU:HD23	1:A:144:LEU:HD23	1.95	0.49
1:A:211:THR:HB	1:A:213:LYS:HZ2	1.77	0.49
1:B:14:PRO:HD3	1:B:226:GLU:O	2.13	0.49
1:B:1369:GLN:CA	1:B:1372:LEU:HD11	2.19	0.49
1:A:692:PRO:HB2	1:A:693:PRO:CD	2.42	0.49
1:A:1391:LEU:HD23	1:A:1391:LEU:C	2.38	0.49
1:B:493:TRP:C	1:B:494:PHE:HD1	2.21	0.49
1:B:549:ILE:HD11	1:B:611:LYS:CG	2.42	0.49
1:B:1372:LEU:CD2	1:B:1377:TRP:CZ2	2.73	0.49
1:B:1429:LYS:NZ	1:B:1981:GLU:O	2.46	0.49
1:A:33:VAL:HG12	1:A:50:ARG:HB3	1.95	0.49
1:A:247:LEU:HD11	1:A:405:ARG:HB2	1.95	0.49
1:A:651:ILE:HD12	1:A:651:ILE:O	2.13	0.49
1:A:692:PRO:HA	1:A:695:LEU:HD21	1.94	0.49
1:B:425:ARG:NH1	1:B:810:ALA:O	2.46	0.49
1:B:620:MET:HE1	1:B:682:PHE:HB2	1.95	0.49
1:B:703:ARG:HB2	1:B:704:GLU:OE1	2.13	0.49
1:B:1120:THR:HG21	1:B:1517:PHE:CZ	2.47	0.49
1:B:1521:GLU:OE1	1:B:1521:GLU:N	2.42	0.49
1:A:107:VAL:HG12	1:A:109:VAL:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:881:ASP:CG	1:B:1046:LEU:CD2	2.82	0.49
1:A:997:ARG:NH2	1:A:1041:SER:O	2.46	0.48
1:A:1141:CYS:O	1:A:1145:VAL:HG23	2.13	0.48
1:B:492:LEU:HD12	1:B:757:VAL:O	2.13	0.48
1:B:768:GLN:NE2	1:B:783:PRO:HB3	2.27	0.48
1:A:139:MET:CE	1:A:142:ASN:HB2	2.40	0.48
1:A:247:LEU:HD23	1:A:282:VAL:HG21	1.95	0.48
1:A:432:GLU:OE1	1:A:432:GLU:N	2.40	0.48
1:B:4:VAL:HG22	1:B:175:ILE:HG22	1.94	0.48
1:B:14:PRO:HD2	1:B:329:MET:HE3	1.94	0.48
1:B:639:VAL:CG1	1:B:640:PRO:HD2	2.43	0.48
1:B:133:VAL:HG12	1:B:139:MET:HE2	1.95	0.48
1:A:68:HIS:CD2	1:A:69:PRO:HD2	2.48	0.48
1:B:627:TRP:CZ3	1:B:640:PRO:HB2	2.48	0.48
1:B:665:LEU:HD13	1:B:672:ALA:HB2	1.95	0.48
1:B:1898:LEU:HD11	1:B:1925:GLN:HG2	1.94	0.48
1:A:363:ASN:O	1:A:370:LEU:HD11	2.12	0.48
1:A:946:VAL:O	1:A:953:VAL:HG12	2.13	0.48
1:B:33:VAL:CG1	1:B:50:ARG:HB3	2.43	0.48
1:B:299:VAL:C	1:B:302:PRO:HD2	2.38	0.48
1:B:635:PRO:HD3	1:B:661:PHE:CD1	2.49	0.48
1:B:659:PHE:O	1:B:663:GLU:HG3	2.13	0.48
1:B:737:ASN:HA	1:B:740:VAL:HG22	1.95	0.48
1:A:654:PRO:C	1:A:657:PRO:HD2	2.39	0.48
1:A:716:SER:HB2	1:A:741:SER:CB	2.42	0.48
1:A:717:ILE:CG2	1:A:721:GLN:HB2	2.44	0.48
1:B:94:GLY:N	1:B:453:MET:HE3	2.28	0.48
1:B:1313:LEU:HD23	1:B:1314:VAL:N	2.28	0.48
1:A:638:VAL:HG13	1:A:652:SER:O	2.14	0.48
1:A:869:GLU:N	1:A:869:GLU:OE1	2.46	0.48
1:B:133:VAL:HG12	1:B:133:VAL:O	2.14	0.48
1:B:274:ARG:HA	1:B:277:TYR:CE2	2.49	0.48
1:A:606:ARG:HH21	1:A:739:LEU:HD13	1.79	0.48
1:A:1312:LEU:C	1:A:1313:LEU:HD12	2.38	0.48
1:A:1417:VAL:HG23	1:A:1424:TRP:CE2	2.48	0.48
1:B:740:VAL:HG23	1:B:741:SER:H	1.79	0.48
1:B:740:VAL:HG23	1:B:741:SER:N	2.29	0.48
1:B:1214:LEU:HD12	1:B:1214:LEU:C	2.38	0.48
1:A:1246:LEU:HD11	1:A:1299:PRO:HG2	1.96	0.48
1:B:117:SER:HB2	1:B:135:CYS:HB3	1.96	0.48
1:B:567:LEU:HD22	1:B:761:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:SER:OG	1:A:220:ASN:HB2	2.14	0.47
1:A:333:GLU:HB2	1:A:334:PRO:CD	2.42	0.47
1:A:496:CYS:HB2	1:A:587:CYS:SG	2.54	0.47
1:A:764:HIS:CD2	1:A:787:LYS:HD2	2.49	0.47
1:A:1606:ARG:NH2	1:A:1862:GLU:O	2.47	0.47
1:B:436:LYS:NZ	1:B:833:LEU:HD22	2.29	0.47
1:B:690:ILE:N	1:B:690:ILE:HD12	2.29	0.47
1:B:786:LYS:HE3	1:B:789:HIS:HD2	1.78	0.47
1:A:137:ARG:HB3	1:B:158:ASP:OD2	2.14	0.47
1:A:491:PRO:HG2	1:A:756:ALA:HA	1.95	0.47
1:A:513:LEU:HD11	1:A:793:LEU:CD2	2.36	0.47
1:B:532:LEU:C	1:B:532:LEU:HD12	2.39	0.47
1:A:505:GLY:C	1:A:508:LEU:HD13	2.39	0.47
1:A:763:PRO:HA	1:A:785:MET:CE	2.44	0.47
1:B:59:ARG:NH1	1:B:841:ALA:HB2	2.29	0.47
1:B:168:LEU:C	1:B:168:LEU:HD23	2.39	0.47
1:A:47:LEU:HD21	1:A:198:VAL:CA	2.45	0.47
1:A:532:LEU:HD12	1:A:604:TYR:HE2	1.78	0.47
1:B:12:LYS:NZ	1:B:17:GLU:OE2	2.43	0.47
1:B:36:ASP:OD2	1:B:38:ARG:HG3	2.14	0.47
1:B:491:PRO:HG3	1:B:753:PRO:CG	2.39	0.47
1:B:757:VAL:HG13	1:B:782:ILE:HD12	1.96	0.47
1:B:1046:LEU:HD12	1:B:1046:LEU:C	2.34	0.47
1:A:133:VAL:O	1:A:139:MET:HG3	2.14	0.47
1:B:4:VAL:HG22	1:B:175:ILE:CG2	2.45	0.47
1:B:222:TYR:HB3	1:B:295:THR:HG23	1.97	0.47
1:A:427:SER:OG	1:A:468:ARG:HG2	2.14	0.47
1:B:530:PHE:CE2	1:B:601:LEU:HD22	2.49	0.47
1:B:1445:ALA:O	1:B:1446:ILE:HD13	2.15	0.47
1:A:203:LEU:HD12	1:B:132:MET:CE	2.44	0.47
1:A:342:ALA:O	1:A:346:LEU:HG	2.15	0.47
1:A:460:VAL:CG1	1:A:461:PRO:HD2	2.45	0.47
1:A:542:ASP:HB3	1:A:545:THR:HB	1.97	0.47
1:A:1238:LEU:HD21	1:A:1265:LEU:HB3	1.96	0.47
1:A:1417:VAL:HG22	1:A:1417:VAL:O	2.15	0.47
1:A:1899:GLU:HB3	1:A:2088:MET:HE2	1.96	0.47
1:B:166:MET:HE2	1:B:400:VAL:CG2	2.45	0.47
1:B:332:PRO:O	1:B:336:SER:HB3	2.13	0.47
1:B:629:GLU:O	1:B:633:ARG:HG2	2.15	0.47
1:B:708:ARG:HD3	1:B:727:ALA:O	2.15	0.47
1:B:1730:GLN:OE1	1:B:1730:GLN:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:LEU:HD12	1:A:401:HIS:CD2	2.50	0.47
1:A:1020:LEU:HD22	1:A:1032:THR:HG22	1.97	0.47
1:A:1968:VAL:O	1:A:1968:VAL:HG23	2.14	0.47
1:B:451:LEU:HD13	1:B:473:LEU:HD12	1.96	0.47
1:B:462:ALA:CB	1:B:485:VAL:HG11	2.45	0.47
1:B:825:ARG:HG2	1:B:826:GLY:N	2.30	0.47
1:B:1246:LEU:N	1:B:1246:LEU:HD12	2.30	0.47
1:B:1391:LEU:C	1:B:1391:LEU:HD23	2.40	0.47
1:A:247:LEU:HD23	1:A:282:VAL:CG2	2.45	0.47
1:A:253:THR:HA	1:A:397:GLY:O	2.15	0.47
1:A:573:ARG:HH21	1:A:711:ARG:HH22	1.62	0.47
1:A:627:TRP:CE3	1:A:643:HIS:HB2	2.49	0.47
1:B:38:ARG:HH21	1:B:53:LYS:HE2	1.79	0.47
1:B:576:GLY:C	1:B:577:ILE:HD12	2.40	0.47
1:B:625:LEU:HD21	1:B:670:VAL:HG21	1.97	0.47
1:A:200:PHE:CE1	1:B:132:MET:HE1	2.50	0.47
1:A:431:PRO:HG3	1:A:467:PHE:CD2	2.50	0.47
1:A:945:GLU:OE2	1:B:941:SER:OG	2.19	0.47
1:B:577:ILE:HD13	1:B:591:ASP:OD1	2.14	0.47
1:B:651:ILE:HD12	1:B:651:ILE:C	2.40	0.47
1:A:193:LYS:HG3	1:A:850:PHE:CG	2.50	0.46
1:A:528:LYS:HB3	1:A:529:PRO:HD3	1.96	0.46
1:B:114:SER:OG	1:B:117:SER:HB3	2.15	0.46
1:B:453:MET:HE2	1:B:830:ILE:CD1	2.44	0.46
1:B:924:ILE:HD12	1:B:924:ILE:N	2.30	0.46
1:B:2006:THR:CG2	1:B:2013:LEU:HD22	2.45	0.46
1:A:13:LEU:HB3	1:A:14:PRO:CD	2.44	0.46
1:A:662:VAL:HG13	1:A:672:ALA:HB1	1.97	0.46
1:B:276:LEU:HD12	1:B:401:HIS:HB3	1.97	0.46
1:B:1973:VAL:HG12	2:B:2602:NDP:C5B	2.46	0.46
1:A:434:VAL:O	1:A:438:LEU:HG	2.15	0.46
1:A:1318:ALA:O	1:A:1367:TYR:OH	2.24	0.46
1:B:623:VAL:HG11	1:B:665:LEU:CD1	2.45	0.46
1:A:290:ILE:HG23	1:A:290:ILE:O	2.15	0.46
1:A:548:ASP:OD1	1:A:549:ILE:N	2.49	0.46
1:A:1578:LEU:HD12	1:A:1583:LEU:HD23	1.97	0.46
1:A:2018:VAL:HG11	1:A:2041:MET:HB3	1.97	0.46
1:A:235:LYS:HG2	1:A:238:LEU:HD13	1.97	0.46
1:A:450:PHE:HE1	1:A:830:ILE:HG12	1.80	0.46
1:A:912:VAL:HG22	1:A:913:VAL:H	1.78	0.46
1:A:1483:VAL:O	1:A:1483:VAL:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2033:ASN:OD1	1:A:2034:TYR:N	2.48	0.46
1:B:623:VAL:HA	1:B:671:PHE:O	2.15	0.46
1:B:1748:LEU:N	1:B:1748:LEU:HD23	2.30	0.46
1:A:707:PRO:HA	1:A:728:ARG:O	2.15	0.46
1:A:776:LYS:HD2	1:A:776:LYS:N	2.30	0.46
1:A:1453:VAL:HG13	1:A:1471:CYS:SG	2.56	0.46
1:A:1488:PRO:HA	1:A:1493:LEU:HD23	1.98	0.46
1:B:491:PRO:HG2	1:B:756:ALA:HA	1.98	0.46
1:B:511:MET:HE1	1:B:520:ILE:HG21	1.98	0.46
1:B:754:GLU:HG2	1:B:776:LYS:HD2	1.97	0.46
1:B:1196:LEU:C	1:B:1196:LEU:HD23	2.41	0.46
1:A:289:TYR:HA	1:A:321:LEU:O	2.16	0.46
1:A:511:MET:HE2	1:A:517:ARG:HG3	1.97	0.46
1:A:1925:GLN:O	1:A:1929:VAL:HG23	2.16	0.46
1:A:7:ALA:HA	1:A:241:ARG:O	2.15	0.46
1:A:160:ALA:O	1:A:161:CYS:HB2	2.16	0.46
1:A:363:ASN:CB	1:A:366:ILE:HD13	2.40	0.46
1:A:449:ALA:O	1:A:453:MET:HG3	2.16	0.46
1:A:513:LEU:HD12	1:A:513:LEU:N	2.31	0.46
1:B:327:SER:HB2	1:B:357:LEU:O	2.16	0.46
1:B:785:MET:HE3	1:B:792:ASN:ND2	2.31	0.46
1:A:1272:ALA:N	1:A:1293:ALA:O	2.46	0.46
1:B:1389:VAL:HG22	1:B:1501:LEU:HD11	1.96	0.46
1:A:103:THR:O	1:A:151:ARG:HB2	2.16	0.46
1:A:618:GLY:CA	1:A:681:ALA:HB2	2.46	0.46
1:B:47:LEU:HD21	1:B:198:VAL:HA	1.97	0.46
1:A:1125:GLU:N	1:A:1125:GLU:OE1	2.49	0.45
1:B:619:ALA:CB	1:B:658:VAL:HG11	2.33	0.45
1:B:1947:SER:O	1:B:2001:ASN:ND2	2.48	0.45
1:A:644:ASN:HB3	1:A:770:VAL:CG1	2.42	0.45
1:B:71:GLN:NE2	1:B:74:THR:OG1	2.49	0.45
1:B:450:PHE:HE1	1:B:830:ILE:HG12	1.81	0.45
1:B:622:ALA:HA	1:B:650:THR:HA	1.98	0.45
1:B:821:PHE:HA	1:B:822:PRO:C	2.40	0.45
1:B:1486:VAL:HG23	1:B:1493:LEU:HB2	1.98	0.45
1:A:644:ASN:HB2	1:A:648:THR:OG1	2.16	0.45
1:A:745:PHE:CE2	1:A:749:LEU:HD13	2.51	0.45
1:A:1578:LEU:HD11	1:A:1583:LEU:HD23	1.97	0.45
1:B:620:MET:HE3	1:B:682:PHE:N	2.30	0.45
1:A:74:THR:HG21	1:A:128:VAL:HG21	1.97	0.45
1:B:656:ALA:O	1:B:660:GLU:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:690:ILE:O	1:B:693:PRO:HG2	2.16	0.45
1:A:518:ASP:O	1:A:522:ARG:HG3	2.15	0.45
1:A:783:PRO:HB2	1:A:795:PHE:HE2	1.82	0.45
1:B:14:PRO:CD	1:B:329:MET:HE3	2.46	0.45
1:B:242:VAL:CG2	1:B:822:PRO:HB3	2.46	0.45
1:B:615:LEU:HD12	1:B:615:LEU:C	2.42	0.45
1:A:157:LEU:N	1:A:157:LEU:HD12	2.31	0.45
1:A:276:LEU:CD1	1:A:401:HIS:HB3	2.46	0.45
1:A:316:ARG:HH21	1:A:318:GLU:CG	2.30	0.45
1:A:420:LEU:CD2	1:A:512:ARG:HE	2.28	0.45
1:A:425:ARG:HH22	1:A:459:ALA:HB2	1.81	0.45
1:A:637:GLY:O	1:A:685:TYR:HE2	2.00	0.45
1:A:676:ARG:HH22	1:A:787:LYS:HZ1	1.63	0.45
1:B:702:ILE:HD12	1:B:702:ILE:H	1.81	0.45
1:B:1190:LEU:O	1:B:1195:GLN:NE2	2.49	0.45
1:A:47:LEU:HD21	1:A:198:VAL:CG2	2.47	0.45
1:A:347:SER:HB3	1:A:352:LEU:O	2.17	0.45
1:A:1971:LEU:HD12	1:A:1971:LEU:N	2.31	0.45
1:B:116:THR:O	1:B:120:LEU:HD13	2.16	0.45
1:B:501:THR:HG23	1:B:501:THR:O	2.17	0.45
1:B:526:ALA:O	1:B:601:LEU:HD21	2.16	0.45
1:B:1088:VAL:HG22	1:B:1093:HIS:CD2	2.52	0.45
1:B:1387:ARG:NE	1:B:1498:GLN:OE1	2.50	0.45
1:B:1837:GLU:OE1	1:B:1837:GLU:N	2.45	0.45
1:A:257:LYS:HE3	1:A:263:PHE:O	2.17	0.45
1:A:524:ASP:OD1	1:A:533:LYS:HA	2.16	0.45
1:A:606:ARG:HH21	1:A:739:LEU:CD1	2.30	0.45
1:B:6:ILE:HG23	1:B:231:VAL:CG1	2.47	0.45
1:B:23:TRP:HB2	1:B:346:LEU:HD13	1.99	0.45
1:B:191:LEU:HD22	1:B:224:ARG:HH21	1.82	0.45
1:B:211:THR:HG23	1:B:358:HIS:CD2	2.52	0.45
1:B:494:PHE:CZ	1:B:567:LEU:HD23	2.52	0.45
1:A:183:ALA:O	1:A:232:LEU:HD12	2.16	0.45
1:A:625:LEU:CD1	1:A:633:ARG:HG2	2.47	0.45
1:A:1232:VAL:HG22	1:A:1240:MET:SD	2.56	0.45
1:B:241:ARG:NH2	1:B:830:ILE:HG13	2.32	0.45
1:B:282:VAL:HG12	1:B:283:ALA:N	2.31	0.45
1:B:462:ALA:HB1	1:B:485:VAL:HG11	1.99	0.45
1:B:1249:HIS:O	1:B:1251:HIS:ND1	2.49	0.45
1:A:1019:ARG:CD	1:A:1075:VAL:HG21	2.47	0.44
1:B:110:GLY:HA3	1:B:163:SER:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:497:SER:OG	1:B:501:THR:HG21	2.17	0.44
1:B:623:VAL:HG21	1:B:665:LEU:CD1	2.47	0.44
1:B:187:GLY:O	1:B:228:VAL:HA	2.18	0.44
1:B:423:LEU:CD1	1:B:472:VAL:HG22	2.43	0.44
1:B:739:LEU:HD12	1:B:739:LEU:O	2.17	0.44
1:B:759:LEU:HD11	1:B:803:LEU:HD11	1.99	0.44
1:B:1909:VAL:HG11	1:B:1912:LEU:HD13	2.00	0.44
1:B:2088:MET:HE3	1:B:2091:CYS:HB2	1.98	0.44
1:A:494:PHE:CD2	1:A:574:PRO:HB3	2.52	0.44
1:A:665:LEU:O	1:A:669:GLY:N	2.51	0.44
1:A:1974:VAL:O	1:A:1974:VAL:HG13	2.18	0.44
1:B:93:GLY:C	1:B:453:MET:HE3	2.43	0.44
1:B:340:ALA:O	1:B:344:VAL:HG23	2.17	0.44
1:B:515:ARG:HB2	1:B:566:LEU:HD21	1.99	0.44
1:B:527:VAL:CG2	1:B:600:VAL:HG12	2.48	0.44
1:B:1391:LEU:HD23	1:B:1392:LYS:N	2.32	0.44
1:A:698:LEU:HB3	1:A:732:ALA:HB1	2.00	0.44
1:A:1346:THR:HG22	1:A:1347:LEU:N	2.33	0.44
1:B:717:ILE:HD11	1:B:726:LEU:CD2	2.47	0.44
1:B:757:VAL:CG1	1:B:782:ILE:HD12	2.47	0.44
1:A:876:VAL:HG12	1:A:876:VAL:O	2.18	0.44
1:A:1196:LEU:C	1:A:1196:LEU:HD23	2.43	0.44
1:A:1245:VAL:HG21	1:A:1332:MET:HE2	1.98	0.44
1:B:191:LEU:HD22	1:B:224:ARG:HE	1.83	0.44
1:B:692:PRO:HB2	1:B:693:PRO:HD3	1.99	0.44
1:A:694:LEU:HD23	1:A:694:LEU:O	2.16	0.44
1:A:1020:LEU:HD22	1:A:1032:THR:CG2	2.47	0.44
1:B:371:ASP:OD1	1:B:372:GLY:N	2.42	0.44
1:B:489:GLU:HA	1:B:489:GLU:OE1	2.18	0.44
1:B:698:LEU:HB3	1:B:732:ALA:CB	2.48	0.44
1:B:1371:ILE:C	1:B:1372:LEU:CD1	2.85	0.44
1:A:1319:VAL:HG23	1:A:1320:ALA:N	2.33	0.44
1:B:584:GLU:O	1:B:585:VAL:C	2.60	0.44
1:B:597:GLU:OE1	1:B:597:GLU:N	2.32	0.44
1:B:670:VAL:HG12	1:B:671:PHE:N	2.33	0.44
1:B:697:GLU:HA	1:B:697:GLU:OE1	2.18	0.44
1:A:325:THR:HG21	1:A:340:ALA:HA	2.00	0.44
1:A:436:LYS:O	1:A:440:GLN:HG2	2.18	0.44
1:A:491:PRO:HG2	1:A:756:ALA:HB2	1.99	0.44
1:A:761:ILE:HD13	1:A:784:LEU:HD12	2.00	0.44
1:B:95:ILE:HD12	1:B:95:ILE:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:PRO:HG2	1:B:370:LEU:CD2	2.48	0.44
1:B:717:ILE:HD11	1:B:726:LEU:HD23	2.00	0.44
1:B:1968:VAL:CG1	1:B:2002:LEU:HD13	2.48	0.44
1:A:305:LEU:HD11	1:A:322:ILE:HD11	2.00	0.43
1:A:319:PRO:HB3	1:A:372:GLY:O	2.17	0.43
1:A:934:GLU:OE1	1:A:936:ARG:NH2	2.51	0.43
1:A:1088:VAL:HG22	1:A:1093:HIS:CD2	2.53	0.43
1:A:1453:VAL:HG21	1:A:1471:CYS:SG	2.57	0.43
1:B:139:MET:HA	1:B:142:ASN:HB2	1.99	0.43
1:B:190:VAL:CG2	1:B:192:LEU:HD13	2.43	0.43
1:B:530:PHE:HE2	1:B:601:LEU:HD22	1.83	0.43
1:B:556:LEU:CD2	1:B:582:LEU:HD23	2.28	0.43
1:B:619:ALA:O	1:B:658:VAL:HG21	2.18	0.43
1:B:1246:LEU:HD23	1:B:1320:ALA:HB1	2.00	0.43
1:A:606:ARG:NH2	1:A:739:LEU:HA	2.33	0.43
1:A:627:TRP:HA	1:A:630:CYS:SG	2.58	0.43
1:A:1887:TYR:CD1	1:A:1909:VAL:HG13	2.53	0.43
1:B:588:GLY:HA2	1:B:712:TRP:CZ3	2.53	0.43
1:B:627:TRP:NE1	1:B:631:LYS:HE2	2.33	0.43
1:A:211:THR:HG22	1:A:213:LYS:HG3	2.00	0.43
1:A:1899:GLU:CB	1:A:2088:MET:HE2	2.48	0.43
1:B:127:LEU:C	1:B:127:LEU:HD12	2.42	0.43
1:B:627:TRP:HA	1:B:649:VAL:HG21	1.99	0.43
1:B:728:ARG:C	1:B:729:THR:HG23	2.42	0.43
1:A:1021:LEU:HD23	1:A:1075:VAL:HG12	2.00	0.43
1:B:139:MET:HE3	1:B:143:ARG:HD3	2.00	0.43
1:B:757:VAL:HG13	1:B:782:ILE:CD1	2.48	0.43
1:A:165:LEU:HD12	1:A:165:LEU:HA	1.87	0.43
1:A:293:HIS:CD2	1:A:295:THR:HG23	2.53	0.43
1:B:581:SER:HB3	1:B:683:HIS:NE2	2.33	0.43
1:B:655:GLN:HA	1:B:658:VAL:HG12	1.99	0.43
1:B:1127:CYS:HB3	1:B:1128:LEU:HD12	1.99	0.43
1:A:54:LEU:HG	1:A:226:GLU:HG3	2.01	0.43
1:A:247:LEU:CD1	1:A:405:ARG:HB2	2.49	0.43
1:A:325:THR:HB	1:A:343:LYS:HD3	2.00	0.43
1:B:618:GLY:HA2	1:B:655:GLN:N	2.34	0.43
1:B:654:PRO:C	1:B:657:PRO:HD2	2.43	0.43
1:B:759:LEU:CD2	1:B:782:ILE:HG21	2.49	0.43
1:A:217:THR:HG22	1:A:364:PRO:HD3	2.01	0.43
1:A:618:GLY:HA3	1:A:681:ALA:HB2	2.00	0.43
1:A:1247:ALA:N	1:A:1273:THR:O	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1519:LEU:HD21	1:A:2101:GLN:OE1	2.18	0.43
1:B:509:SER:HB2	1:B:792:ASN:HB2	2.01	0.43
1:B:627:TRP:HE3	1:B:649:VAL:HG13	1.83	0.43
1:B:693:PRO:O	1:B:697:GLU:HG2	2.18	0.43
1:B:1367:TYR:CD2	1:B:1367:TYR:C	2.96	0.43
1:B:493:TRP:NE1	1:B:753:PRO:HD2	2.34	0.43
1:B:542:ASP:OD1	1:B:543:GLU:N	2.51	0.43
1:B:642:CYS:HA	1:B:743:VAL:HB	2.01	0.43
1:B:790:ARG:HG3	1:B:791:ASP:N	2.33	0.43
1:B:1896:PHE:CE1	1:B:2088:MET:HE1	2.54	0.43
1:A:366:ILE:HD12	1:A:366:ILE:N	2.34	0.43
1:B:160:ALA:O	1:B:161:CYS:HB3	2.18	0.43
1:B:248:ASN:HB2	1:B:280:ALA:HB2	1.99	0.43
1:A:33:VAL:HG13	1:A:51:SER:C	2.44	0.43
1:A:76:ASP:OD1	1:A:77:PRO:HD2	2.19	0.43
1:A:1019:ARG:HD2	1:A:1075:VAL:HG21	2.01	0.43
1:A:2042:GLU:OE2	1:A:2059:GLN:NE2	2.51	0.43
1:B:212:CYS:SG	1:B:222:TYR:HA	2.59	0.43
1:B:222:TYR:CD2	1:B:331:HIS:HB3	2.54	0.43
1:A:18:ASN:OD1	1:A:20:GLN:HB3	2.19	0.42
1:A:205:MET:HB3	1:A:222:TYR:HE1	1.81	0.42
1:A:536:GLN:O	1:A:540:SER:OG	2.26	0.42
1:A:548:ASP:OD1	1:A:611:LYS:HD3	2.19	0.42
1:A:593:CYS:O	1:A:706:LYS:HE2	2.19	0.42
1:A:1555:GLN:N	1:A:1555:GLN:OE1	2.52	0.42
1:B:545:THR:HG22	1:B:546:PHE:HD1	1.84	0.42
1:B:1445:ALA:C	1:B:1446:ILE:HD13	2.43	0.42
1:A:691:ALA:O	1:A:695:LEU:N	2.31	0.42
1:A:1616:LEU:HD13	1:A:1650:VAL:CG2	2.49	0.42
1:B:133:VAL:HG13	1:B:139:MET:HE2	2.00	0.42
1:B:362:PRO:HG2	1:B:370:LEU:HD23	2.00	0.42
1:B:706:LYS:HB3	1:B:707:PRO:HD2	2.01	0.42
1:B:759:LEU:HD21	1:B:782:ILE:HG21	2.00	0.42
1:A:1526:GLU:OE2	1:A:1552:ARG:NH1	2.49	0.42
1:B:86:THR:CG2	1:B:184:ILE:HG21	2.47	0.42
1:B:235:LYS:HE3	1:B:237:SER:OG	2.19	0.42
1:B:685:TYR:HA	1:B:688:GLU:HG3	2.01	0.42
1:B:1198:LEU:O	1:B:1202:LEU:N	2.36	0.42
1:A:731:SER:O	1:A:734:TYR:N	2.53	0.42
1:A:759:LEU:CD2	1:A:782:ILE:HD12	2.49	0.42
1:A:1493:LEU:HA	1:A:1496:VAL:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1826:LEU:HD12	1:A:1826:LEU:N	2.34	0.42
1:B:188:ILE:CG2	1:B:228:VAL:HG13	2.30	0.42
1:B:322:ILE:CG2	1:B:374:LEU:HG	2.49	0.42
1:B:627:TRP:HB2	1:B:643:HIS:CD2	2.54	0.42
1:B:628:GLU:O	1:B:631:LYS:HB2	2.19	0.42
1:B:898:THR:OG1	1:B:935:VAL:HG11	2.20	0.42
1:B:1971:LEU:N	1:B:1971:LEU:HD12	2.34	0.42
1:A:112:SER:CA	1:A:137:ARG:HH12	2.31	0.42
1:A:189:ASN:ND2	1:A:334:PRO:HD2	2.27	0.42
1:A:640:PRO:HA	1:A:650:THR:O	2.19	0.42
1:A:991:TYR:CZ	1:A:1006:GLN:HA	2.54	0.42
1:B:139:MET:HB3	1:B:143:ARG:HG2	2.00	0.42
1:B:787:LYS:HE3	1:B:788:ASP:OD2	2.19	0.42
1:B:1046:LEU:CD1	1:B:1102:ALA:HB3	2.49	0.42
1:A:763:PRO:HA	1:A:785:MET:HE2	2.00	0.42
1:A:1699:VAL:HG21	1:A:1705:ARG:HB2	2.01	0.42
1:B:494:PHE:O	1:B:495:ILE:HD13	2.19	0.42
1:B:1078:VAL:HG23	1:B:1089:ALA:HB2	2.01	0.42
1:A:2020:SER:OG	1:A:2021:SER:N	2.53	0.42
1:B:69:PRO:O	1:B:73:HIS:HD2	2.03	0.42
1:B:78:GLN:HG2	1:B:190:VAL:HG13	2.02	0.42
1:B:215:PHE:N	1:B:215:PHE:CD1	2.84	0.42
1:B:581:SER:CB	1:B:683:HIS:NE2	2.83	0.42
1:B:597:GLU:H	1:B:597:GLU:CD	2.21	0.42
1:B:628:GLU:H	1:B:628:GLU:CD	2.27	0.42
1:B:654:PRO:CG	1:B:657:PRO:HG2	2.49	0.42
1:B:1973:VAL:HG12	2:B:2602:NDP:H52A	2.01	0.42
1:A:23:TRP:NE1	1:A:350:HIS:HD2	2.16	0.42
1:A:267:ASP:O	1:A:271:GLN:HG3	2.20	0.42
1:A:424:LEU:CD2	1:A:441:GLY:HA3	2.50	0.42
1:A:532:LEU:HD12	1:A:604:TYR:CE2	2.55	0.42
1:A:556:LEU:HD11	1:A:560:GLN:HE21	1.85	0.42
1:B:291:GLU:CG	1:B:340:ALA:HB1	2.48	0.42
1:B:316:ARG:HH12	1:B:320:LEU:HD13	1.85	0.42
1:B:1417:VAL:HG13	1:B:1424:TRP:CE2	2.55	0.42
1:A:243:TYR:OH	1:A:829:LEU:HD22	2.20	0.42
1:A:440:GLN:HG3	1:A:833:LEU:HD13	2.01	0.42
1:A:625:LEU:CG	1:A:670:VAL:HG11	2.49	0.42
1:A:793:LEU:HD12	1:A:793:LEU:O	2.20	0.42
1:A:1148:LEU:HD12	1:A:1148:LEU:N	2.35	0.42
1:B:83:LEU:HA	1:B:144:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:ILE:O	1:B:290:ILE:HG23	2.19	0.42
1:B:674:GLU:H	1:B:674:GLU:CD	2.28	0.42
1:A:695:LEU:HD12	1:A:695:LEU:C	2.44	0.42
1:B:96:ASN:OD1	1:B:98:ASP:HB2	2.20	0.42
1:B:207:SER:HB3	1:B:221:GLY:O	2.20	0.42
1:B:620:MET:HG3	1:B:652:SER:HB3	2.01	0.42
1:B:1120:THR:HG21	1:B:1517:PHE:HZ	1.84	0.42
1:A:13:LEU:HD21	1:A:229:VAL:CG2	2.50	0.41
1:A:501:THR:OG1	1:A:763:PRO:HG2	2.20	0.41
1:A:549:ILE:O	1:A:553:PHE:HD1	2.02	0.41
1:A:990:VAL:HG13	1:A:1039:LEU:HD12	2.02	0.41
1:A:1351:HIS:O	1:A:1352:PRO:C	2.63	0.41
1:B:322:ILE:HG12	1:B:375:GLN:C	2.42	0.41
1:B:364:PRO:HA	1:B:370:LEU:HD11	2.01	0.41
1:B:1125:GLU:N	1:B:1125:GLU:OE1	2.53	0.41
1:A:261:VAL:HG21	1:B:133:VAL:CG1	2.49	0.41
1:A:937:LEU:C	1:A:938:LEU:HD12	2.45	0.41
1:A:1379:SER:O	1:A:1382:SER:OG	2.34	0.41
1:A:1617:VAL:HG12	1:A:1628:LEU:HD13	2.01	0.41
1:A:1640:TRP:CZ3	1:A:1648:VAL:HG21	2.56	0.41
1:B:47:LEU:HD21	1:B:198:VAL:HG22	2.02	0.41
1:B:595:SER:OG	1:B:598:GLU:HG3	2.20	0.41
1:B:1348:LEU:HD22	1:B:1374:GLN:HB2	2.01	0.41
1:B:1372:LEU:HB2	1:B:1377:TRP:NE1	2.35	0.41
1:A:2:GLU:OE1	1:A:2:GLU:HA	2.21	0.41
1:A:83:LEU:CD2	1:A:144:LEU:HD23	2.50	0.41
1:A:158:ASP:O	1:B:138:ALA:HB2	2.19	0.41
1:A:485:VAL:HG22	1:A:805:LEU:O	2.20	0.41
1:A:497:SER:HB3	1:A:762:ALA:CB	2.50	0.41
1:A:626:SER:OG	1:A:629:GLU:HG3	2.20	0.41
1:A:1446:ILE:HD12	1:A:1446:ILE:C	2.45	0.41
1:A:1533:VAL:HG13	1:A:1544:ILE:HG23	2.01	0.41
1:B:193:LYS:HE2	1:B:195:ASN:HB2	2.01	0.41
1:B:462:ALA:HB1	1:B:485:VAL:CG1	2.50	0.41
1:A:12:LYS:O	1:A:13:LEU:HD23	2.21	0.41
1:A:143:ARG:HA	1:A:143:ARG:HD2	1.81	0.41
1:A:199:GLN:HG2	1:B:127:LEU:CD1	2.47	0.41
1:A:290:ILE:HG12	1:A:308:ILE:HD13	2.01	0.41
1:A:576:GLY:C	1:A:577:ILE:HG13	2.45	0.41
1:B:83:LEU:HD12	1:B:144:LEU:CD2	2.50	0.41
1:B:981:GLU:N	1:B:982:PRO:HD3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1588:ILE:N	1:B:1588:ILE:HD12	2.34	0.41
1:A:588:GLY:HA2	1:A:712:TRP:CZ3	2.56	0.41
1:B:545:THR:HG22	1:B:546:PHE:CD1	2.54	0.41
1:B:623:VAL:HG11	1:B:665:LEU:HD22	2.02	0.41
1:B:759:LEU:HD23	1:B:782:ILE:HG22	2.02	0.41
1:A:96:ASN:HD22	1:A:98:ASP:HB2	1.84	0.41
1:A:502:GLN:HA	1:A:506:MET:SD	2.61	0.41
1:A:506:MET:HG3	1:A:559:ILE:CD1	2.51	0.41
1:B:158:ASP:O	1:B:159:THR:HG22	2.19	0.41
1:B:159:THR:HG21	1:B:163:SER:HA	2.00	0.41
1:B:1261:SER:N	1:B:1262:PRO:CD	2.84	0.41
1:A:995:ARG:HA	1:A:999:TYR:O	2.21	0.41
1:B:158:ASP:O	1:B:163:SER:HB3	2.20	0.41
1:B:766:LEU:C	1:B:766:LEU:HD23	2.45	0.41
1:B:936:ARG:C	1:B:937:LEU:HD12	2.45	0.41
1:A:606:ARG:HH21	1:A:739:LEU:HA	1.86	0.41
1:A:655:GLN:HG2	1:A:656:ALA:N	2.36	0.41
1:A:168:LEU:HD21	1:A:246:ILE:CD1	2.51	0.41
1:A:191:LEU:HD12	1:A:191:LEU:N	2.36	0.41
1:A:570:MET:HE2	1:A:815:LEU:HG	2.02	0.41
1:A:630:CYS:SG	1:A:649:VAL:HG21	2.61	0.41
1:A:1652:TYR:OH	1:A:1824:ARG:O	2.31	0.41
1:A:1864:VAL:O	1:A:1864:VAL:HG13	2.21	0.41
1:A:1913:VAL:C	1:A:1914:LEU:HD12	2.46	0.41
1:B:167:ALA:CB	1:B:185:VAL:HG13	2.50	0.41
1:B:171:ALA:HB1	1:B:183:ALA:HB3	2.03	0.41
1:B:655:GLN:HA	1:B:658:VAL:CG1	2.50	0.41
1:B:706:LYS:O	1:B:729:THR:HB	2.21	0.41
1:B:708:ARG:HG3	1:B:729:THR:HA	2.02	0.41
1:B:1570:SER:OG	1:B:1646:ALA:O	2.33	0.41
1:B:1651:VAL:HG23	1:B:1652:TYR:N	2.36	0.41
1:A:269:GLN:O	1:A:273:ILE:HG13	2.20	0.41
1:A:698:LEU:HB3	1:A:732:ALA:CB	2.51	0.41
1:A:698:LEU:HD13	1:A:735:ASN:HB2	2.03	0.41
1:A:1228:LEU:HD11	1:A:1256:ILE:HD12	2.03	0.41
1:B:39:ARG:HA	1:B:39:ARG:HD3	1.89	0.41
1:B:627:TRP:HB2	1:B:649:VAL:HG21	2.02	0.41
1:B:768:GLN:HE22	1:B:783:PRO:HD3	1.86	0.41
1:A:623:VAL:HA	1:A:671:PHE:O	2.20	0.40
1:A:1973:VAL:HG23	1:A:2034:TYR:HE1	1.85	0.40
1:B:86:THR:O	1:B:90:ILE:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:728:ARG:O	1:B:729:THR:CG2	2.69	0.40
1:B:1497:LEU:HD12	1:B:1497:LEU:C	2.46	0.40
1:A:67:VAL:HG22	1:A:143:ARG:NH2	2.36	0.40
1:A:211:THR:CG2	1:A:213:LYS:HG3	2.51	0.40
1:A:1243:VAL:O	1:A:1243:VAL:HG23	2.21	0.40
1:B:25:ASN:HB3	1:B:32:MET:HE2	2.03	0.40
1:B:1896:PHE:HB3	2:B:2602:NDP:H52N	2.02	0.40
1:A:39:ARG:HD2	1:A:191:LEU:O	2.20	0.40
1:A:238:LEU:N	1:A:238:LEU:HD12	2.37	0.40
1:A:651:ILE:HD12	1:A:651:ILE:C	2.46	0.40
1:A:1052:VAL:HG11	1:A:1055:ILE:HD11	2.03	0.40
1:B:304:GLU:O	1:B:308:ILE:HG13	2.22	0.40
1:A:291:GLU:OE2	1:A:325:THR:HG22	2.20	0.40
1:A:1580:THR:HG22	1:A:1580:THR:O	2.22	0.40
1:A:1657:TYR:OH	1:A:1662:ARG:NH1	2.52	0.40
1:B:608:GLN:O	1:B:611:LYS:N	2.55	0.40
1:B:617:PRO:HB2	1:B:655:GLN:OE1	2.21	0.40
1:B:627:TRP:HE3	1:B:649:VAL:CG1	2.34	0.40
1:A:119:ALA:O	1:A:122:ARG:NH1	2.55	0.40
1:A:567:LEU:HD22	1:A:572:LEU:HD12	2.03	0.40
1:A:625:LEU:HD21	1:A:670:VAL:HG11	2.03	0.40
1:A:655:GLN:H	1:A:655:GLN:CD	2.29	0.40
1:A:1312:LEU:O	1:A:1313:LEU:HD12	2.22	0.40
1:A:1893:LEU:HD12	1:A:1916:SER:OG	2.21	0.40
1:B:424:LEU:HD12	1:B:455:ASN:OD1	2.21	0.40
1:B:440:GLN:CB	1:B:833:LEU:HD13	2.51	0.40
1:B:495:ILE:HA	1:B:578:VAL:O	2.22	0.40
1:B:848:GLU:CD	1:B:848:GLU:H	2.29	0.40
1:B:1209:LEU:N	1:B:1210:PRO:HD2	2.36	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	2060/2553 (81%)	2004 (97%)	56 (3%)	0	100	100
1	B	2063/2553 (81%)	2003 (97%)	60 (3%)	0	100	100
All	All	4123/5106 (81%)	4007 (97%)	116 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1705/2117 (80%)	1705 (100%)	0	100	100
1	B	1708/2117 (81%)	1705 (100%)	3 (0%)	87	88
All	All	3413/4234 (81%)	3410 (100%)	3 (0%)	87	90

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	277	TYR
1	B	1671	LEU
1	B	1748	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	HIS
1	A	96	ASN
1	A	169	GLN
1	A	195	ASN
1	A	248	ASN
1	A	328	ASN
1	A	331	HIS
1	A	350	HIS
1	A	356	ASN
1	A	358	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	379	GLN
1	A	387	ASN
1	A	399	ASN
1	A	446	GLN
1	A	560	GLN
1	A	614	HIS
1	A	643	HIS
1	A	683	HIS
1	A	804	HIS
1	A	863	ASN
1	A	949	ASN
1	A	971	HIS
1	A	1056	HIS
1	A	1110	GLN
1	A	1193	ASN
1	A	1263	HIS
1	A	1290	HIS
1	A	1458	ASN
1	A	1494	GLN
1	A	1504	ASN
1	A	1763	HIS
1	A	1815	GLN
1	A	1906	GLN
1	A	1945	ASN
1	A	2103	HIS
1	B	71	GLN
1	B	73	HIS
1	B	173	GLN
1	B	358	HIS
1	B	375	GLN
1	B	399	ASN
1	B	446	GLN
1	B	502	GLN
1	B	551	HIS
1	B	644	ASN
1	B	746	GLN
1	B	764	HIS
1	B	768	GLN
1	B	949	ASN
1	B	971	HIS
1	B	1006	GLN
1	B	1093	HIS

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Mol	Chain	Res	Type
1	B	1098	HIS
1	B	1267	GLN
1	B	1284	GLN
1	B	1516	HIS
1	B	1572	ASN
1	B	1595	GLN
1	B	1682	GLN
1	B	1731	HIS
1	B	1754	GLN
1	B	1763	HIS
1	B	1788	ASN
1	B	1815	GLN
1	B	1845	GLN
1	B	1983	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

4 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
2	NDP	A	2602	-	51,52,52	0.52	0	71,80,80	0.67	1 (1%)
2	NDP	B	2601	-	51,52,52	0.48	0	71,80,80	0.78	1 (1%)
2	NDP	A	2601	-	51,52,52	0.50	0	71,80,80	0.75	2 (2%)
2	NDP	B	2602	-	51,52,52	0.52	0	71,80,80	0.66	1 (1%)

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
2	NDP	A	2602	-	-	13/34/77/77	0/5/5/5
2	NDP	B	2601	-	-	14/34/77/77	0/5/5/5
2	NDP	A	2601	-	-	13/34/77/77	0/5/5/5
2	NDP	B	2602	-	-	12/34/77/77	0/5/5/5

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2601	NDP	P2B-O2B-C2B	-5.03	110.00	123.43
2	B	2602	NDP	P2B-O2B-C2B	-3.74	113.44	123.43
2	A	2602	NDP	P2B-O2B-C2B	-3.41	114.33	123.43
2	A	2601	NDP	O2B-C2B-C3B	2.08	119.13	111.68
2	A	2601	NDP	O3B-C3B-C2B	2.03	116.86	111.19

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2601	NDP	C5D-O5D-PN-O3
2	A	2601	NDP	C5D-O5D-PN-O1N
2	A	2601	NDP	C5D-O5D-PN-O2N
2	A	2601	NDP	O4D-C1D-N1N-C2N
2	A	2601	NDP	C2N-C3N-C7N-O7N
2	A	2602	NDP	C5B-O5B-PA-O2A
2	A	2602	NDP	C5B-O5B-PA-O3
2	A	2602	NDP	O4B-C4B-C5B-O5B
2	A	2602	NDP	C5D-O5D-PN-O3

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Mol	Chain	Res	Type	Atoms
2	A	2602	NDP	C5D-O5D-PN-O1N
2	B	2601	NDP	C5D-O5D-PN-O3
2	B	2601	NDP	C5D-O5D-PN-O1N
2	B	2601	NDP	O4D-C1D-N1N-C2N
2	B	2601	NDP	C2N-C3N-C7N-N7N
2	B	2602	NDP	C5B-O5B-PA-O2A
2	B	2602	NDP	C4B-C5B-O5B-PA
2	B	2602	NDP	C2N-C3N-C7N-N7N
2	A	2602	NDP	C3B-C4B-C5B-O5B
2	B	2601	NDP	O4B-C4B-C5B-O5B
2	B	2601	NDP	C3B-C4B-C5B-O5B
2	A	2601	NDP	C3B-C2B-O2B-P2B
2	A	2602	NDP	O4D-C1D-N1N-C6N
2	A	2601	NDP	C1B-C2B-O2B-P2B
2	A	2601	NDP	C3B-C4B-C5B-O5B
2	B	2602	NDP	O4D-C4D-C5D-O5D
2	A	2601	NDP	O4B-C4B-C5B-O5B
2	A	2601	NDP	O4D-C4D-C5D-O5D
2	A	2601	NDP	C2N-C3N-C7N-N7N
2	B	2602	NDP	O4B-C4B-C5B-O5B
2	B	2602	NDP	O4D-C1D-N1N-C6N
2	A	2601	NDP	C3D-C4D-C5D-O5D
2	A	2602	NDP	C5D-O5D-PN-O2N
2	B	2601	NDP	C5D-O5D-PN-O2N
2	B	2602	NDP	C5B-O5B-PA-O1A
2	B	2602	NDP	C5B-O5B-PA-O3
2	B	2602	NDP	C5D-O5D-PN-O1N
2	A	2602	NDP	PA-O3-PN-O1N
2	B	2601	NDP	C2B-O2B-P2B-O2X
2	A	2602	NDP	C2N-C3N-C7N-N7N
2	A	2601	NDP	C2B-O2B-P2B-O1X
2	B	2601	NDP	C2B-O2B-P2B-O1X
2	B	2601	NDP	O4B-C1B-N9A-C4A
2	B	2601	NDP	PA-O3-PN-O1N
2	B	2602	NDP	PN-O3-PA-O1A
2	B	2601	NDP	O4B-C1B-N9A-C8A
2	A	2602	NDP	C4B-C5B-O5B-PA
2	B	2602	NDP	C4D-C5D-O5D-PN
2	A	2602	NDP	C2N-C3N-C7N-O7N
2	A	2602	NDP	PA-O3-PN-O2N
2	B	2601	NDP	PN-O3-PA-O2A
2	B	2601	NDP	PA-O3-PN-O2N

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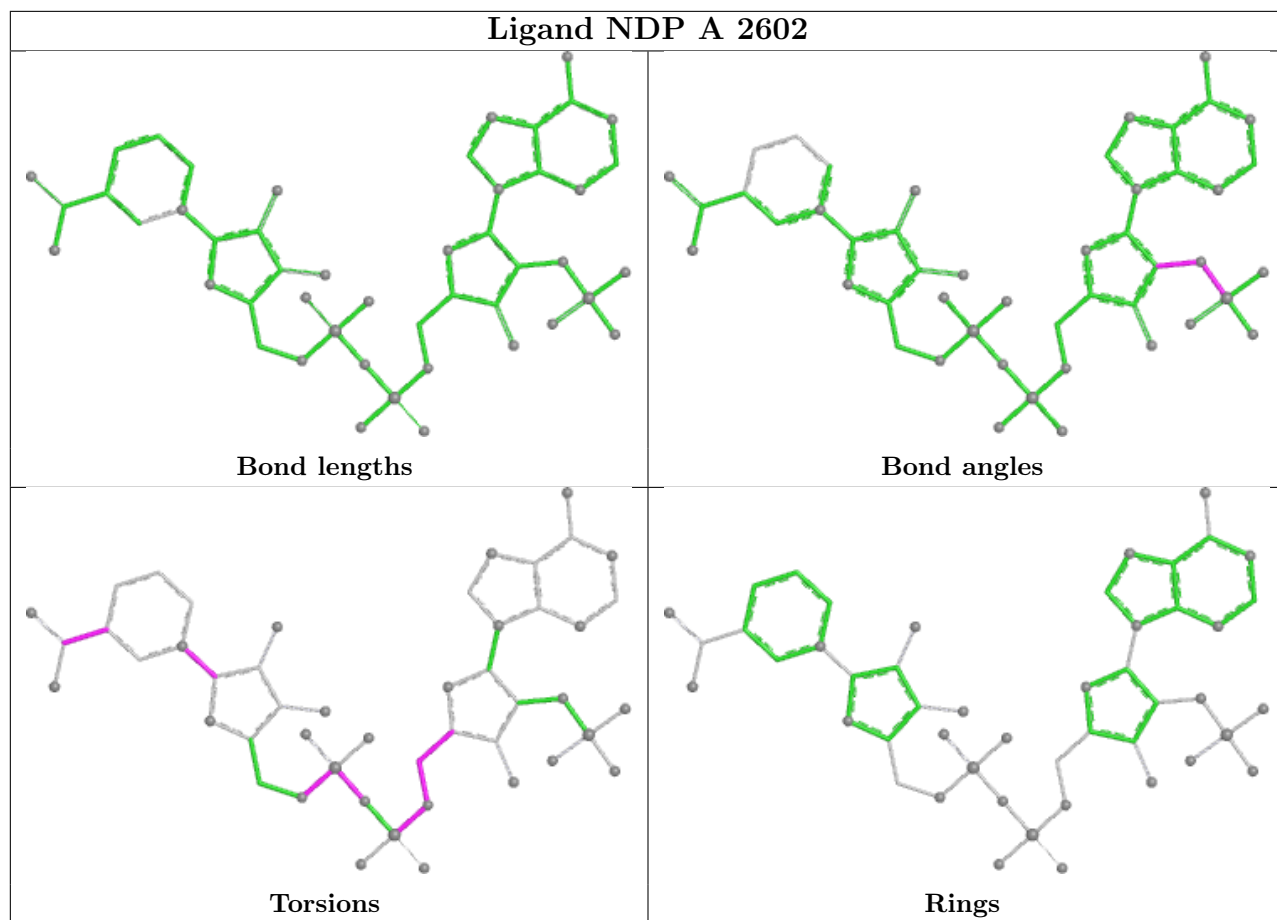
Mol	Chain	Res	Type	Atoms
2	B	2602	NDP	PN-O3-PA-O2A

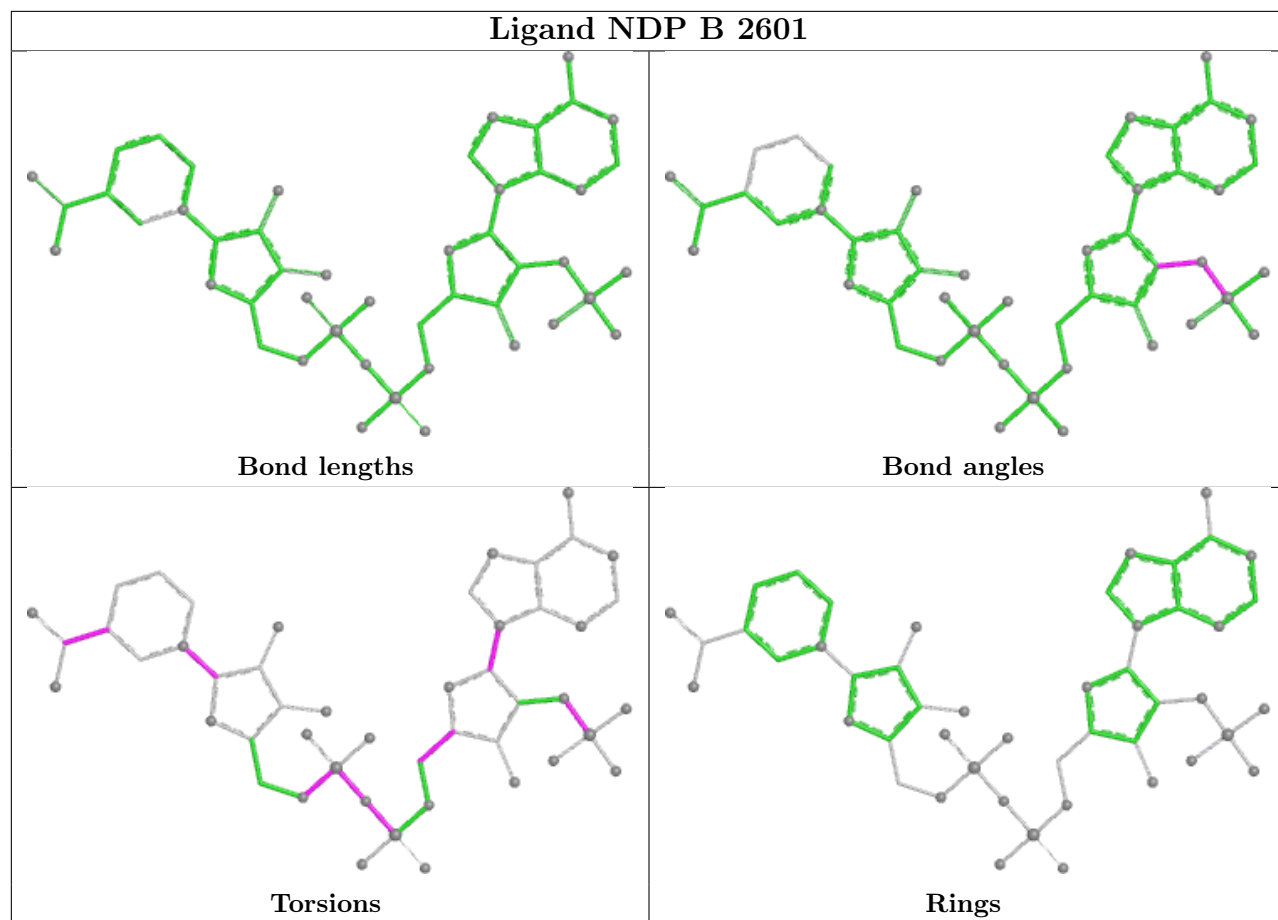
There are no ring outliers.

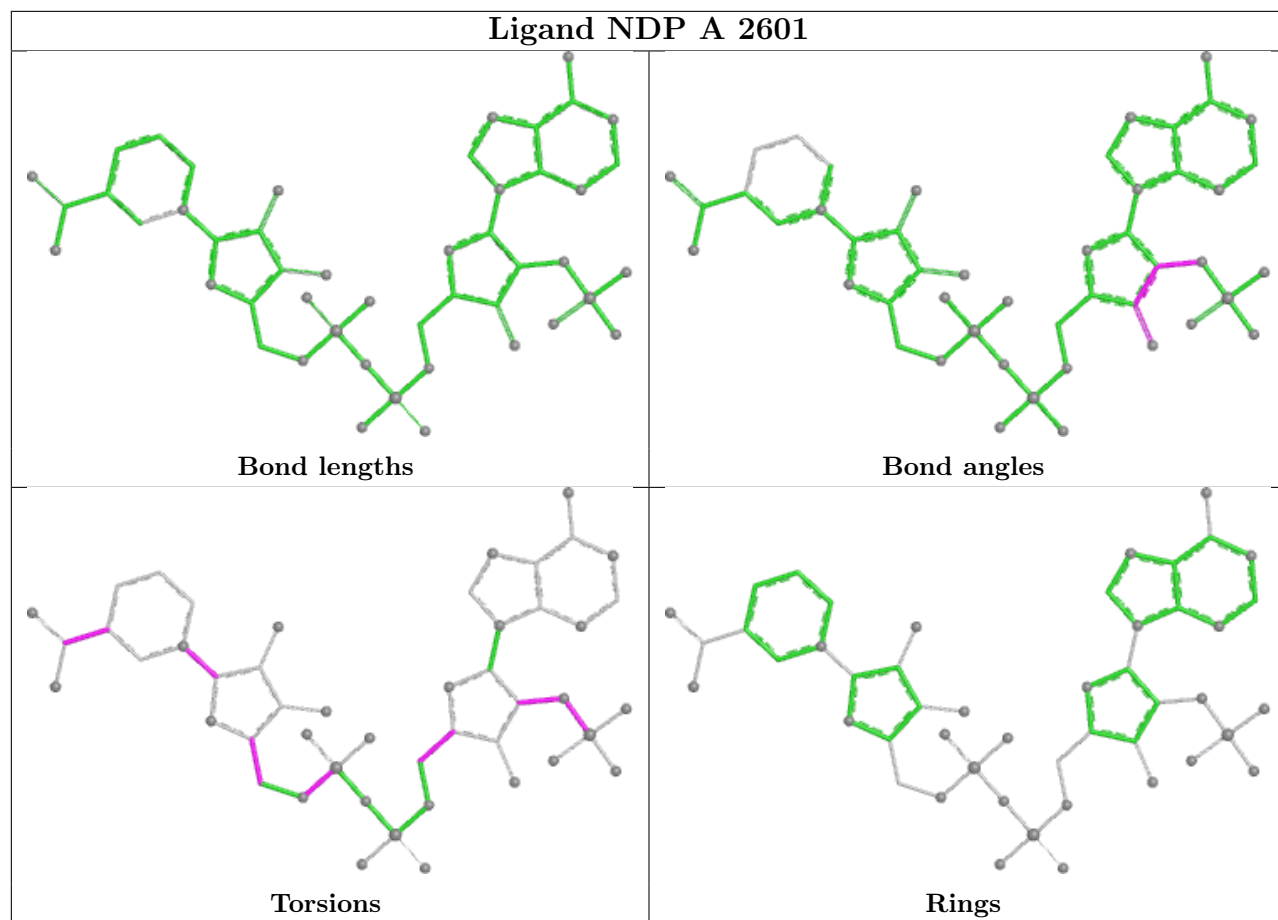
1 monomer is involved in 3 short contacts:

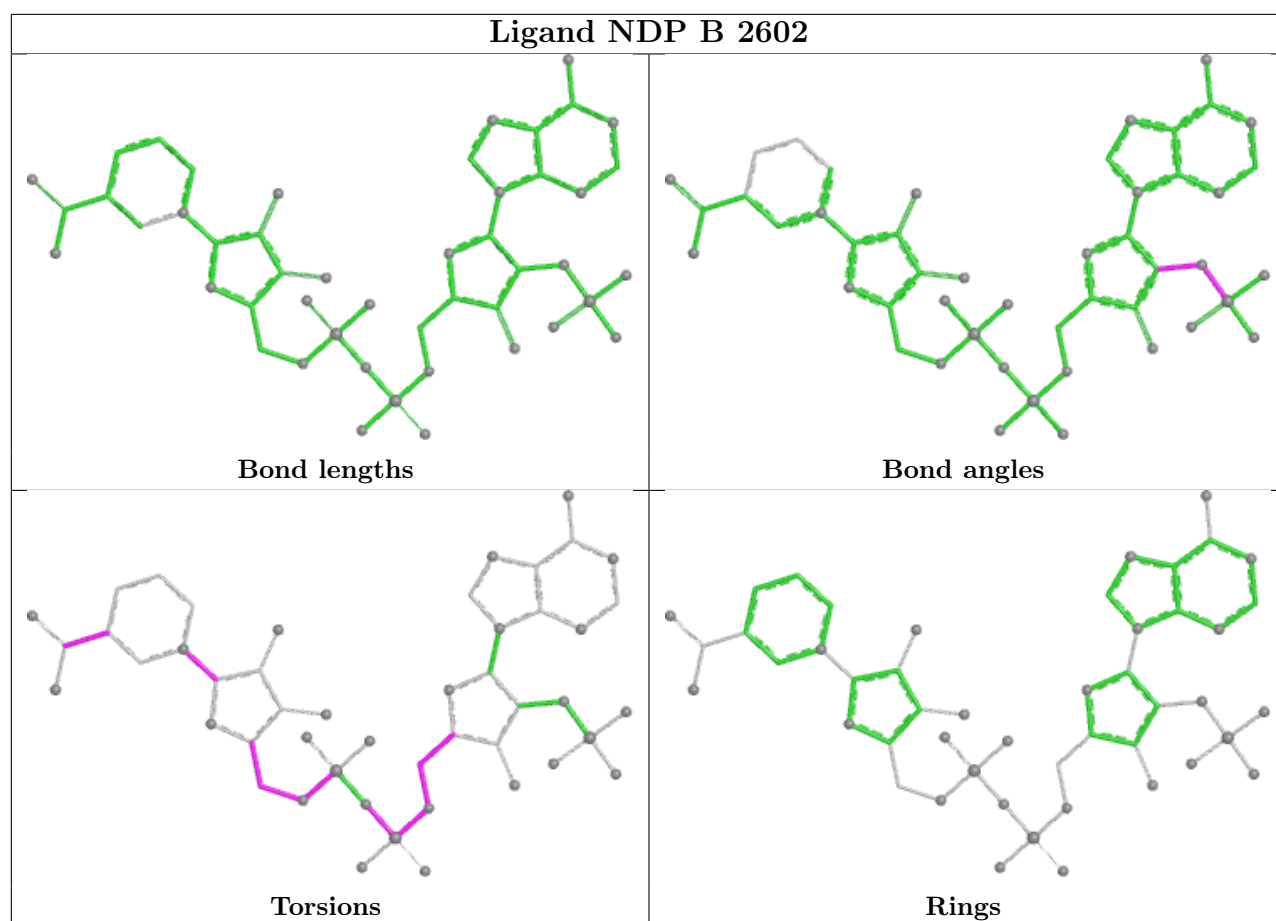
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2602	NDP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









## 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.

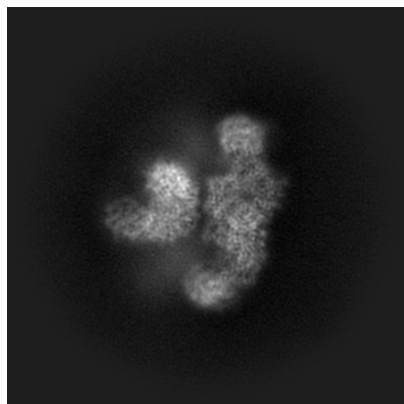
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43355. These allow visual inspection of the internal detail of the map and identification of artifacts.

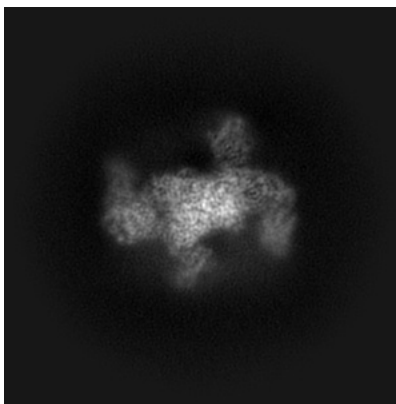
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

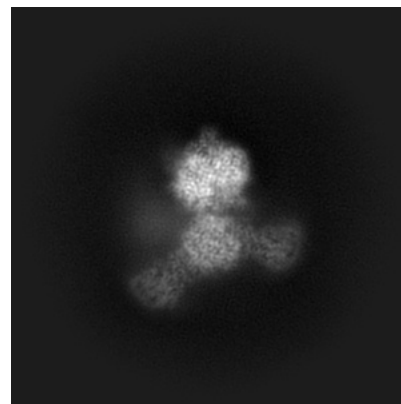
#### 6.1.1 Primary map



X

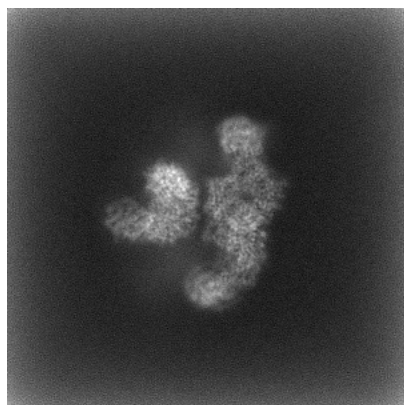


Y

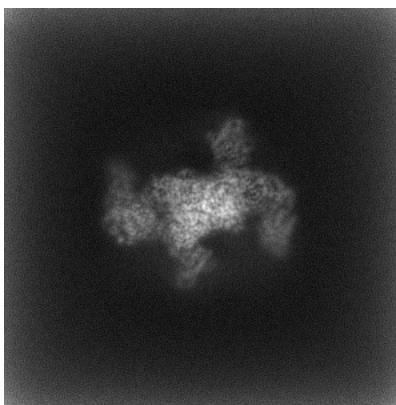


Z

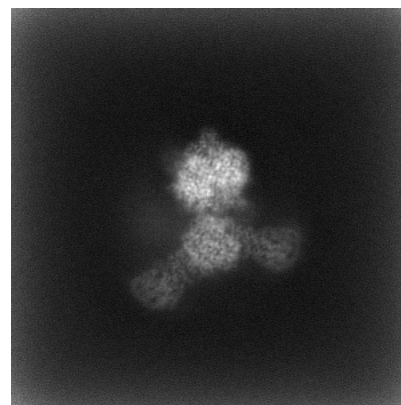
#### 6.1.2 Raw map



X



Y

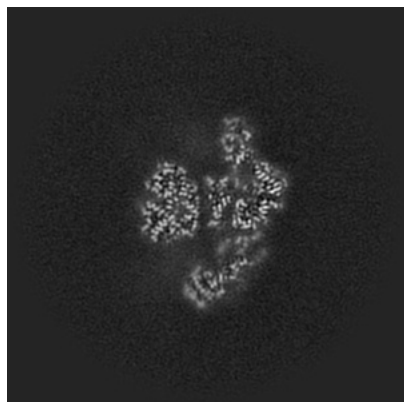


Z

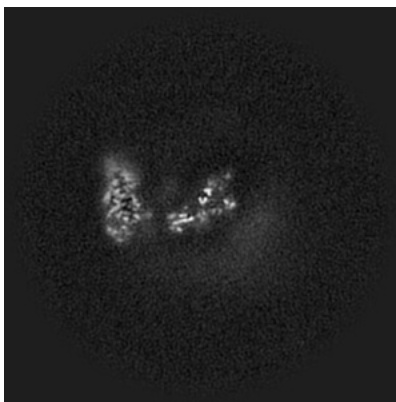
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

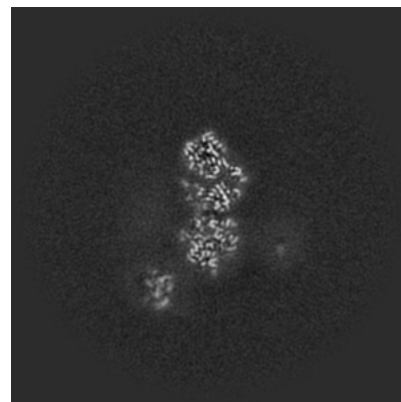
### 6.2.1 Primary map



X Index: 180



Y Index: 180



Z Index: 180

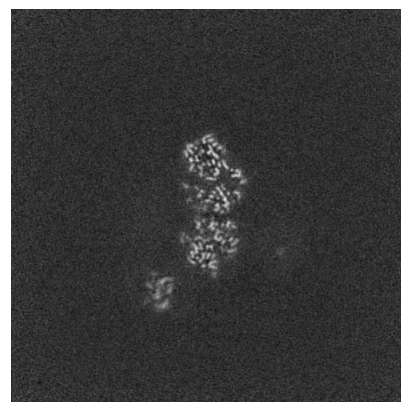
### 6.2.2 Raw map



X Index: 180



Y Index: 180

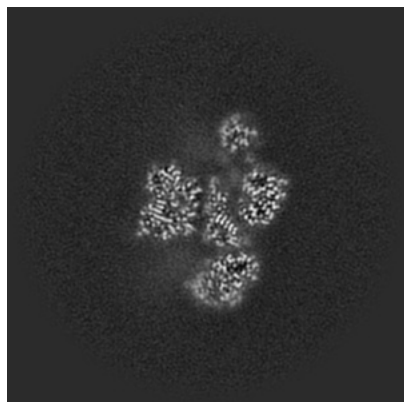


Z Index: 180

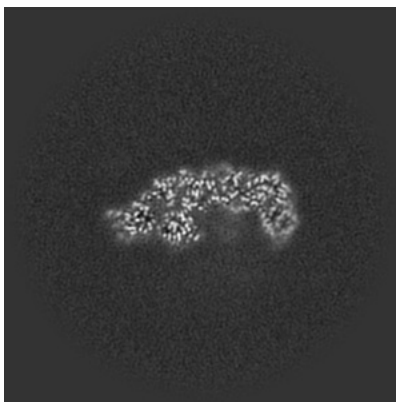
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

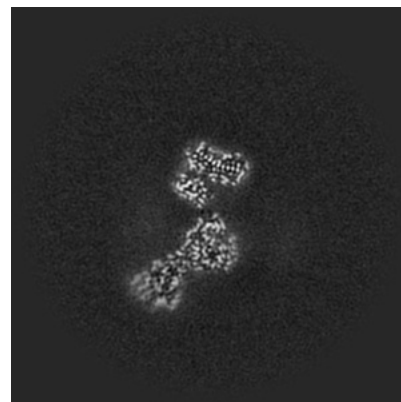
### 6.3.1 Primary map



X Index: 173

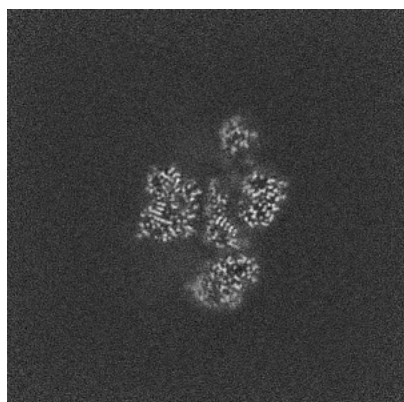


Y Index: 205

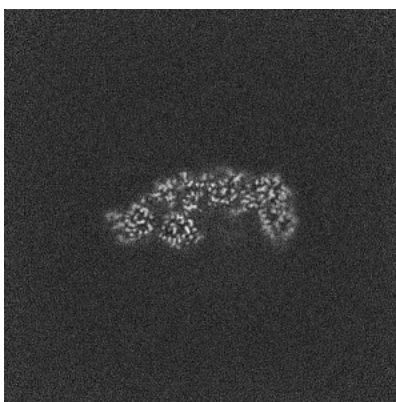


Z Index: 169

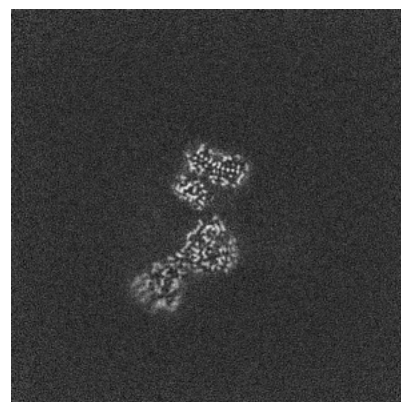
### 6.3.2 Raw map



X Index: 173



Y Index: 204

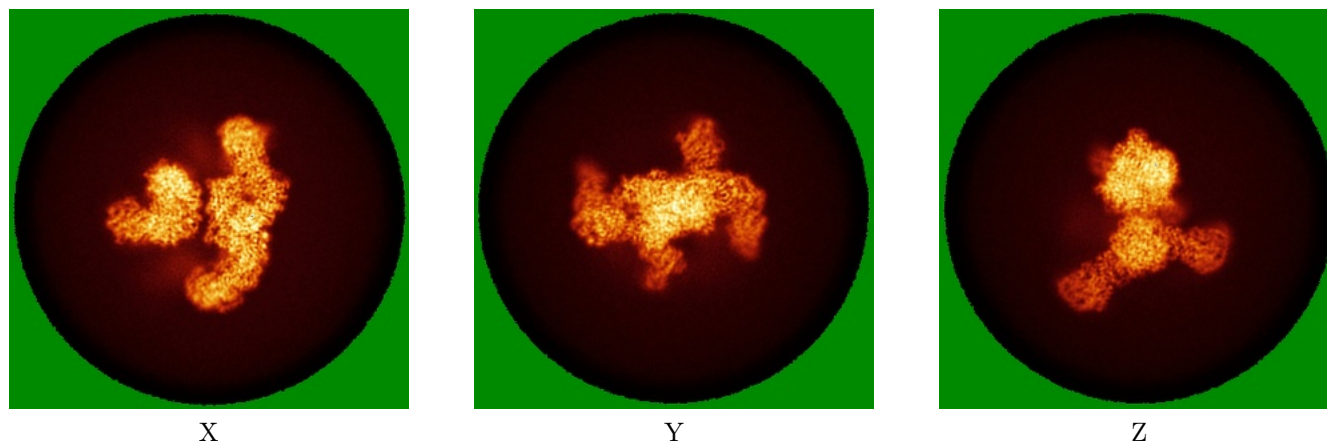


Z Index: 169

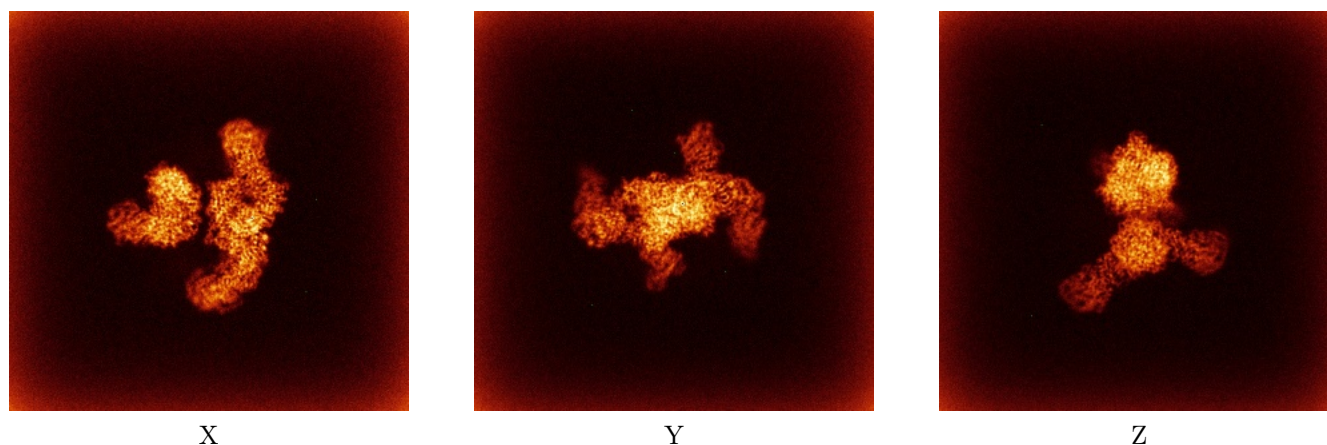
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



### 6.4.2 Raw map



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](#)

This section was not generated.

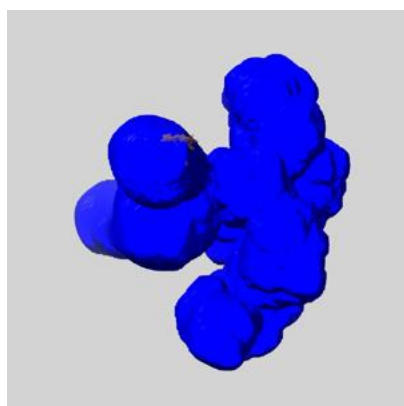
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

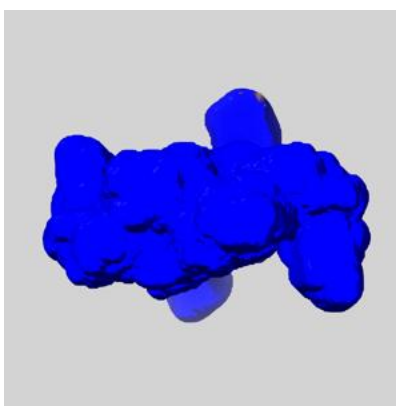
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

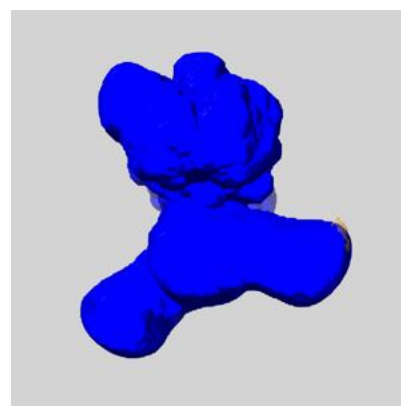
### 6.6.1 emd\_43355\_msk\_1.map [i](#)



X



Y

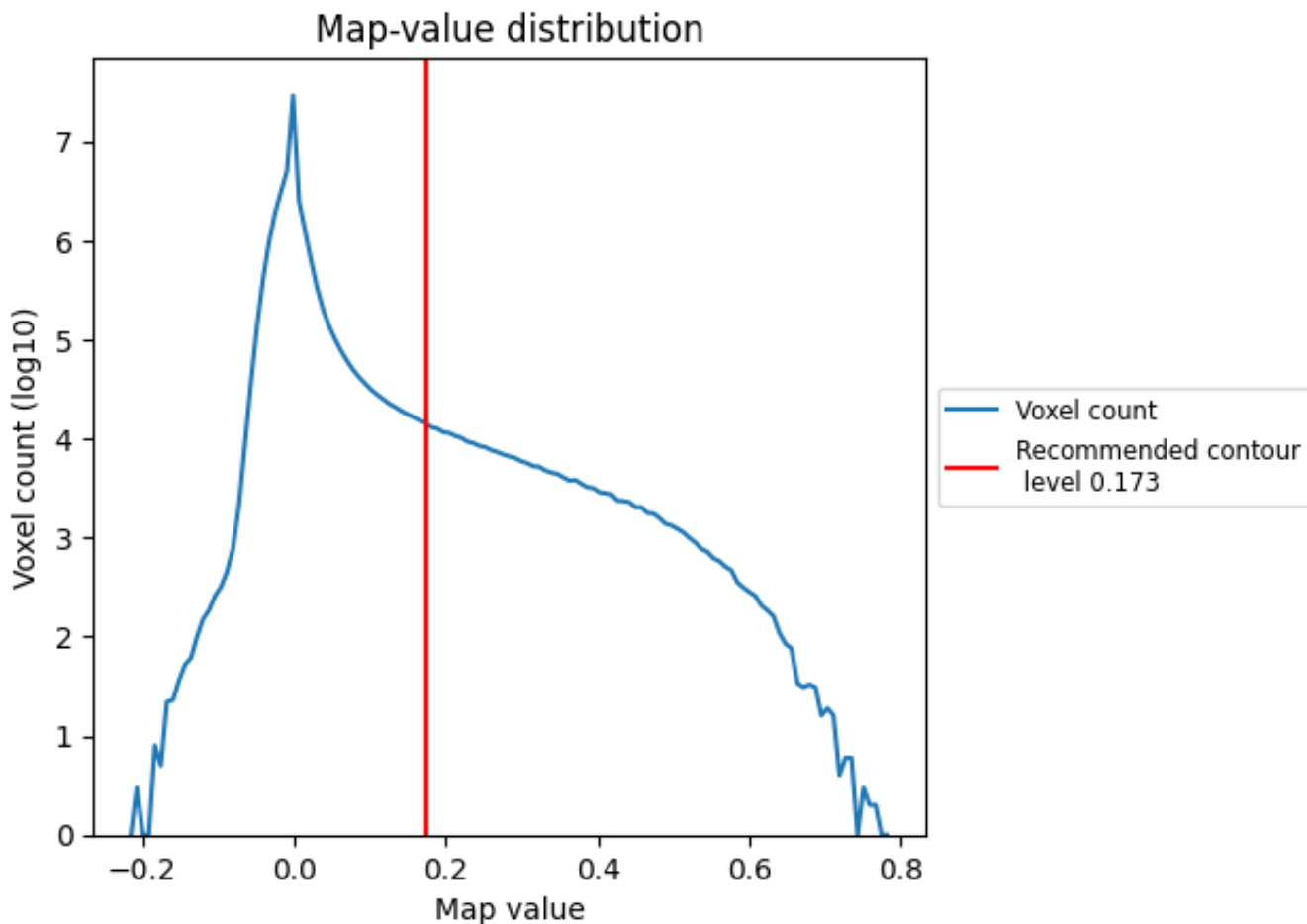


Z

## 7 Map analysis [i](#)

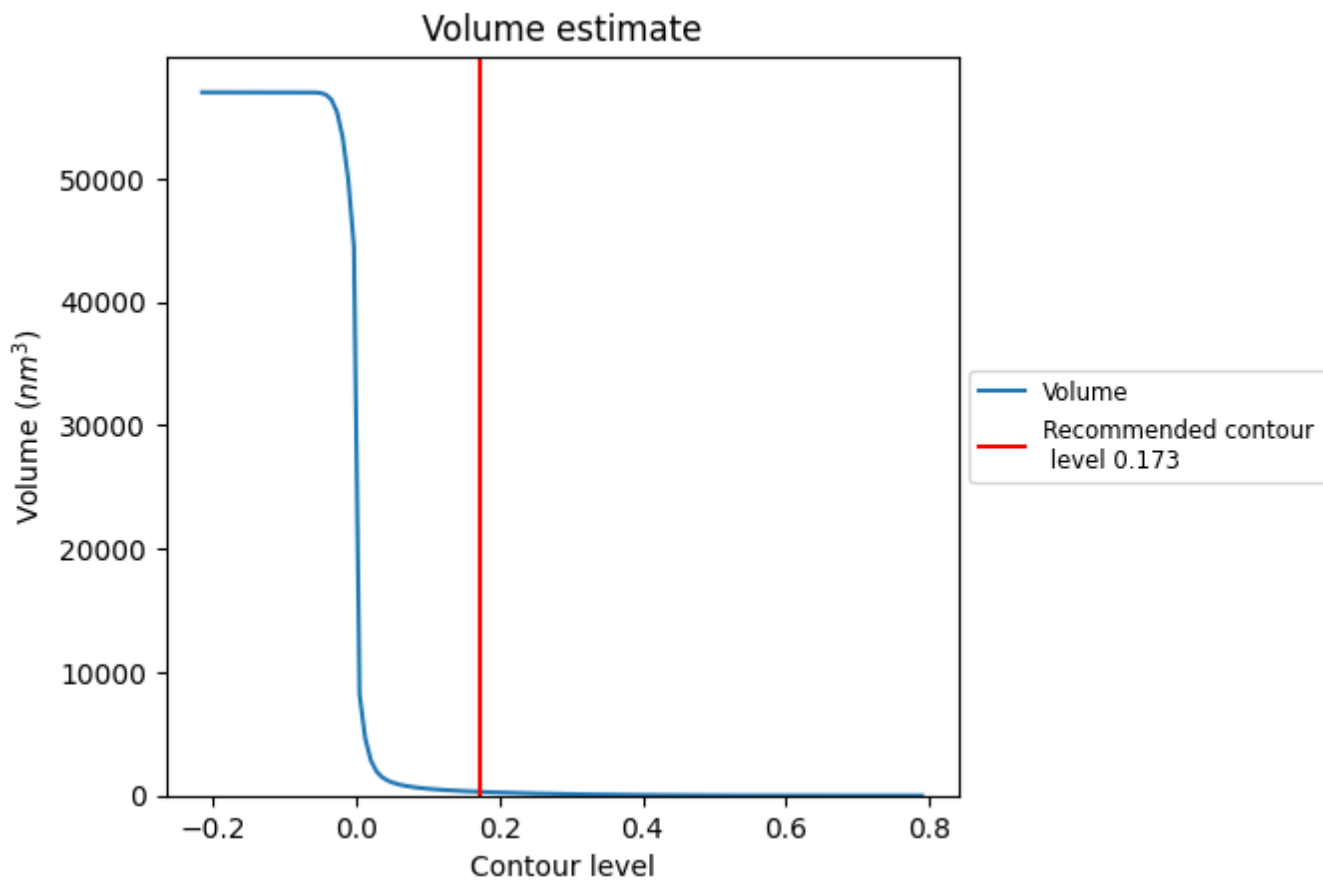
This section contains the results of statistical analysis of the map.

### 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.

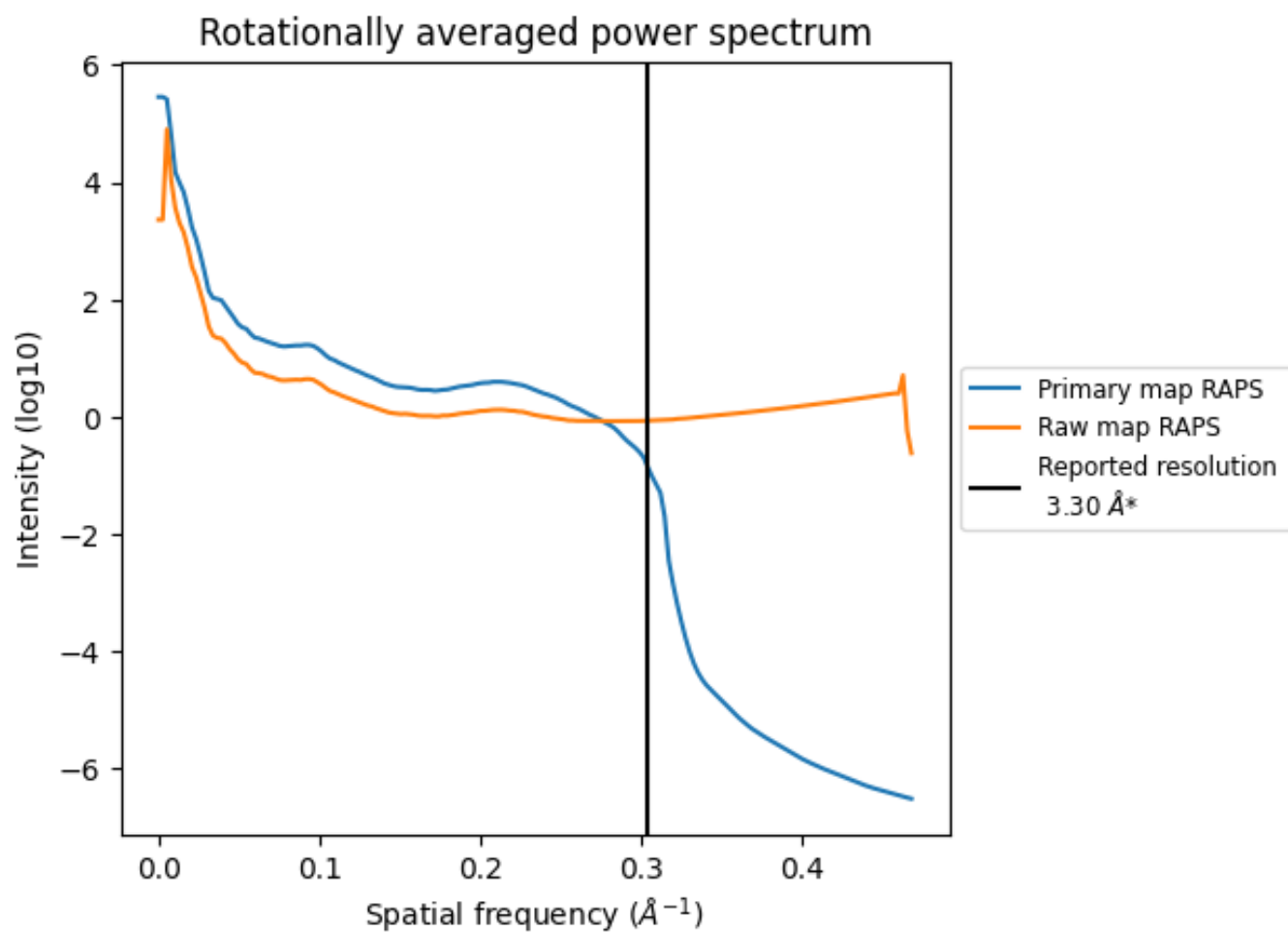
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 304 nm<sup>3</sup>; this corresponds to an approximate mass of 275 kDa.

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

### 7.3 Rotationally averaged power spectrum i

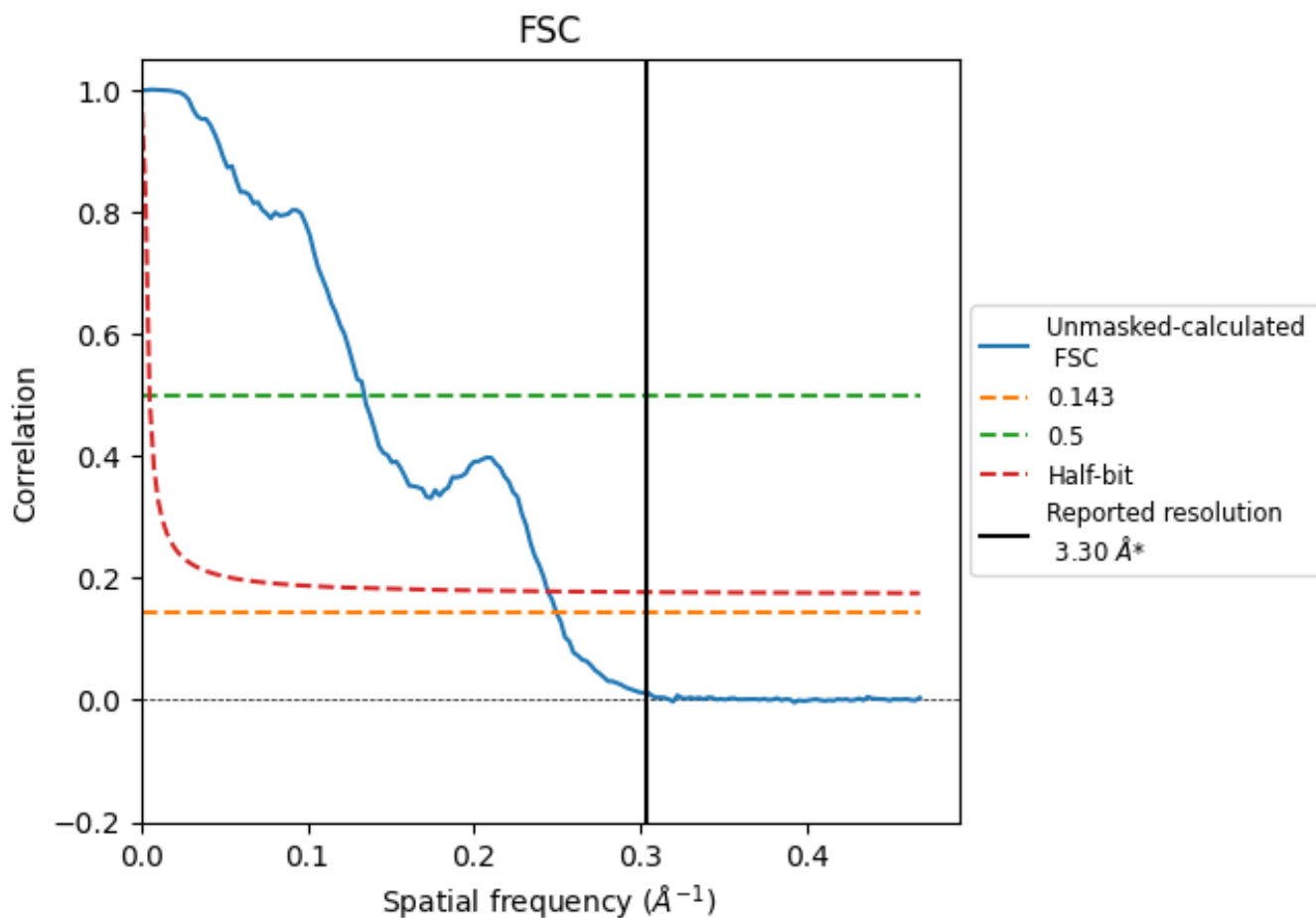


\*Reported resolution corresponds to spatial frequency of  $0.303 \text{ \AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

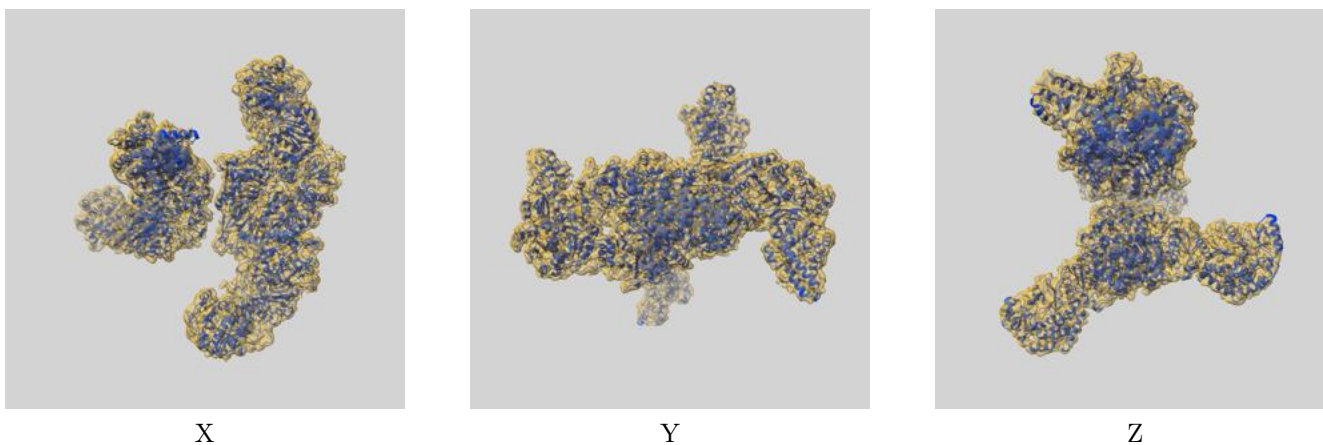
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.01	7.46	4.10

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.01 differs from the reported value 3.3 by more than 10 %

## 9 Map-model fit [i](#)

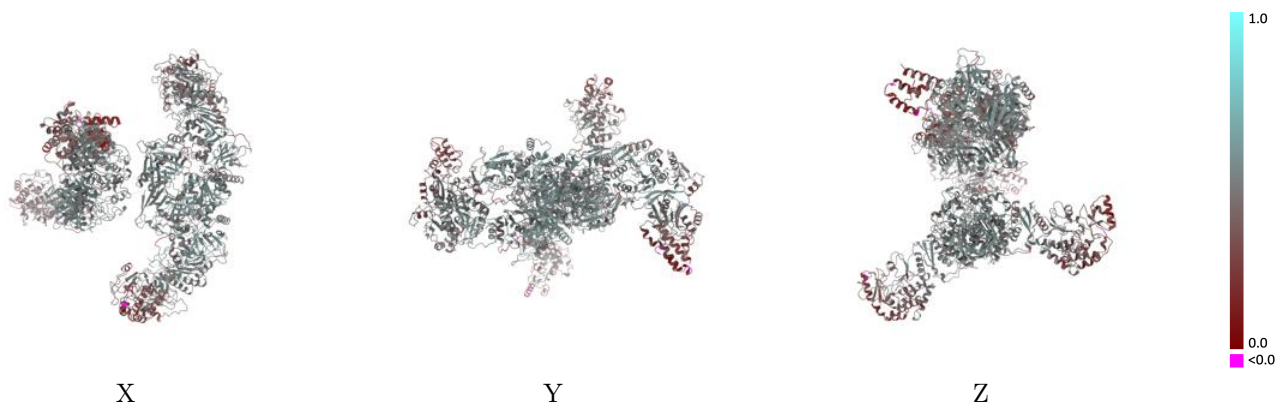
This section contains information regarding the fit between EMDB map EMD-43355 and PDB model 8VMC. Per-residue inclusion information can be found in section [3](#) on page [7](#).

### 9.1 Map-model overlay [i](#)



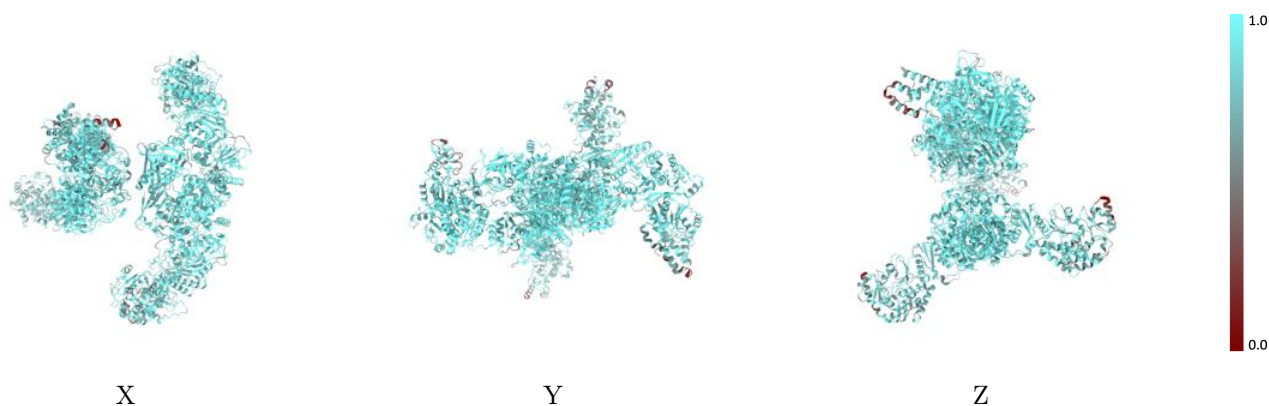
The images above show the 3D surface view of the map at the recommended contour level 0.173 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



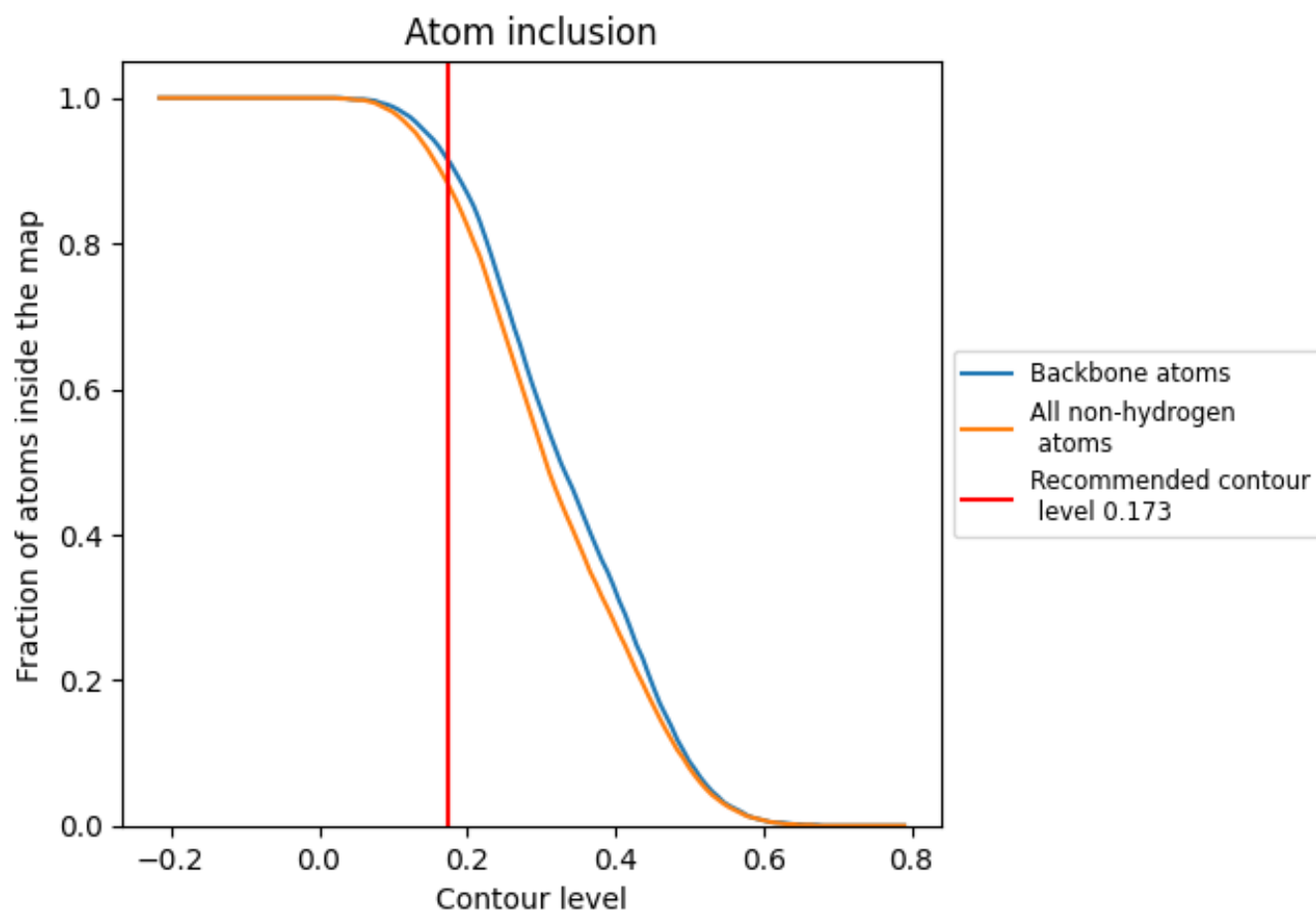
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.173).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.173) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8840	 0.4640
A	 0.8830	 0.4640
B	 0.8860	 0.4640

