



## Full wwPDB EM Validation Report ⓘ

May 8, 2025 – 02:22 PM EDT

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.dev118  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

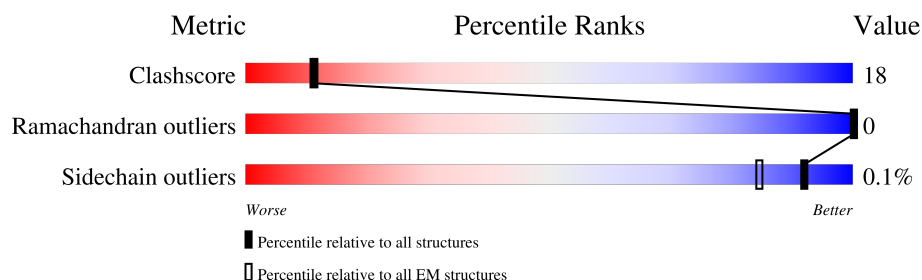
# 1 Overall quality at a glance

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	
1	B	2553	

## 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
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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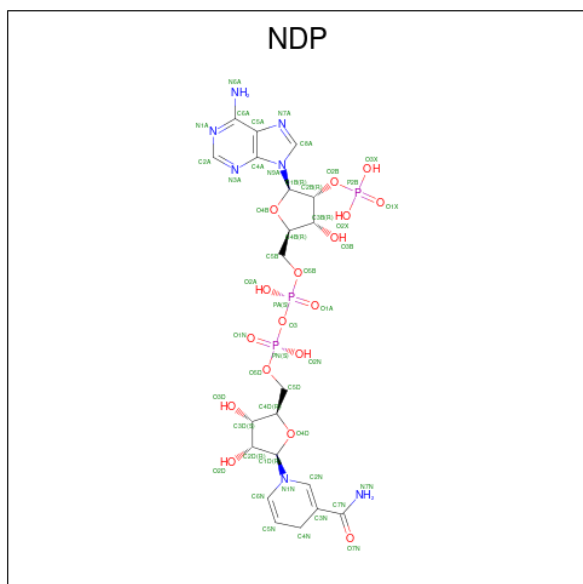
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	ALA	-	expression tag	UNP P49327
A	-4	MET	-	expression tag	UNP P49327
A	-3	GLY	-	expression tag	UNP P49327
A	-2	SER	-	expression tag	UNP P49327
A	-1	GLY	-	expression tag	UNP P49327
A	0	ILE	-	expression tag	UNP P49327
A	1	PRO	-	expression tag	UNP P49327
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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Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	GLN	-	expression tag	UNP P49327
B	-6	GLY	-	expression tag	UNP P49327
B	-5	ALA	-	expression tag	UNP P49327
B	-4	MET	-	expression tag	UNP P49327
B	-3	GLY	-	expression tag	UNP P49327
B	-2	SER	-	expression tag	UNP P49327
B	-1	GLY	-	expression tag	UNP P49327
B	0	ILE	-	expression tag	UNP P49327
B	1	PRO	-	expression tag	UNP P49327
B	1151	THR	LYS	conflict	UNP P49327
B	2512	LEU	-	expression tag	UNP P49327
B	2513	GLU	-	expression tag	UNP P49327
B	2514	HIS	-	expression tag	UNP P49327
B	2515	HIS	-	expression tag	UNP P49327
B	2516	HIS	-	expression tag	UNP P49327
B	2517	HIS	-	expression tag	UNP P49327
B	2518	HIS	-	expression tag	UNP P49327
B	2519	HIS	-	expression tag	UNP P49327
B	2520	HIS	-	expression tag	UNP P49327
B	2521	HIS	-	expression tag	UNP P49327

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ) (labeled as "Ligand of Interest" by depositor).

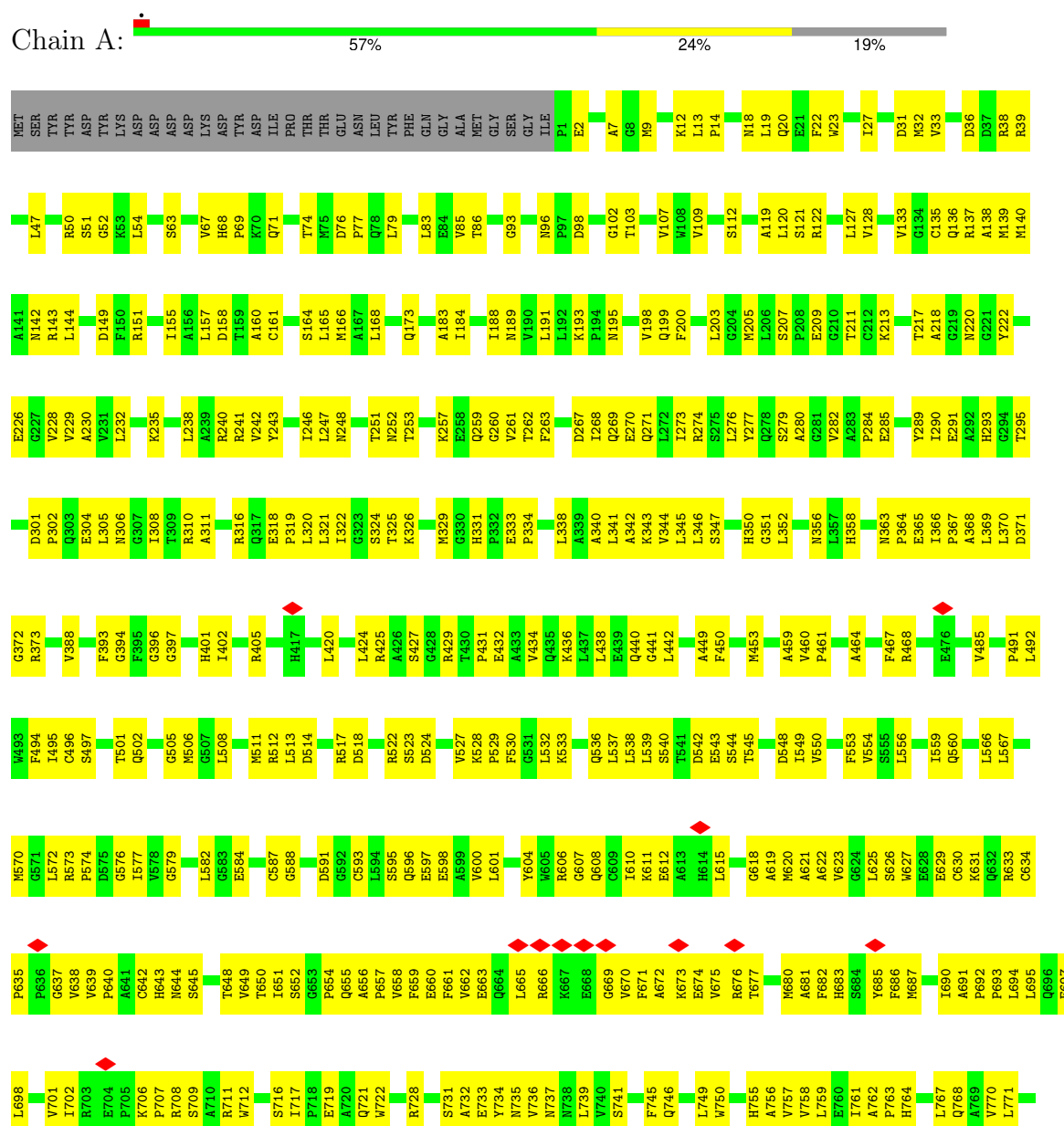


Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
2	A	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
2	B	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
2	B	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	

### 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.

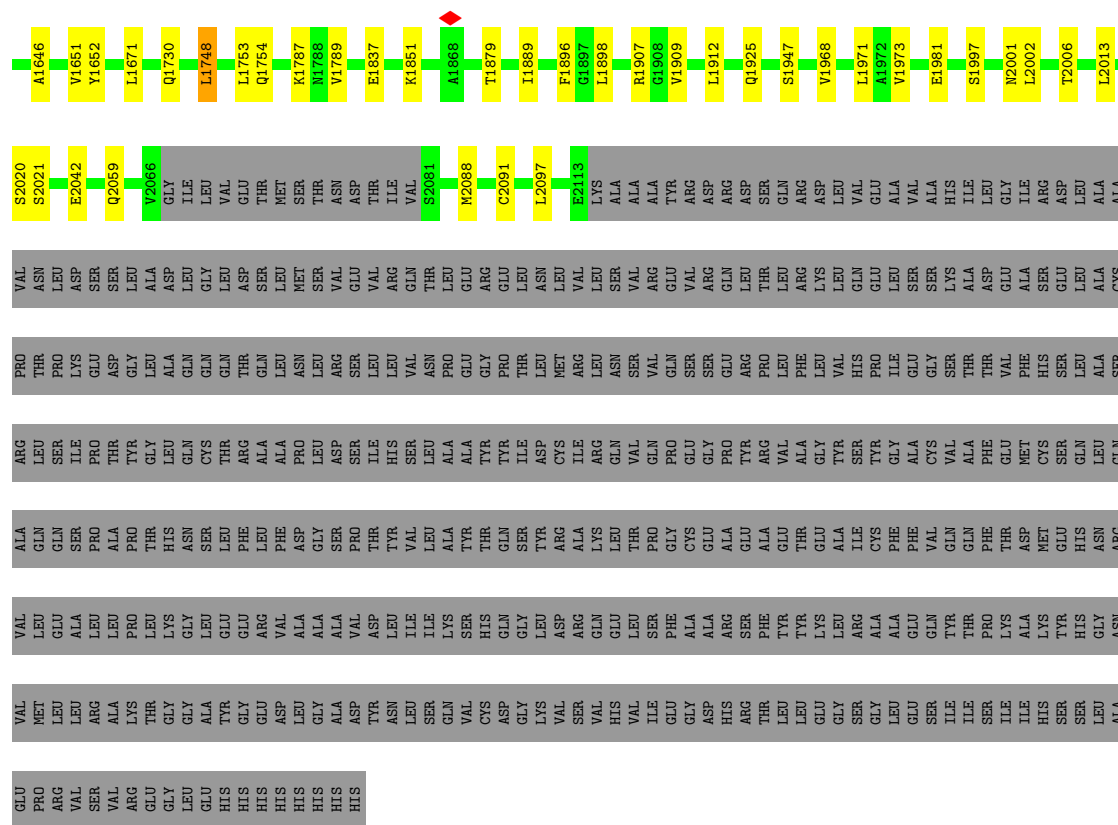
#### • Molecule 1: Fatty acid synthase







Q1374	Q1204	A1102	L759	P693	V550	P367	A283	L206	P124	R38	MET
W1377	E1205	V1111	E760	L694	H551	A368	F284	L207	L127	R39	SER
R1387	R1206	T1120	I761	L695	V554	L369	E285	P208	L127	L47	TYR
L1388	P1207	T1120	A765	L696	S555	D371	I290	G210	Y130	R50	ASP
V1389	K1208	E1126	L766	L697	L556	G372	E291	G210	S131	K63	LYS
G1390	L1209	G1126	L767	L698	T557	E373	A292	T211	M132		ASP
L1391	P1210	G1127	Q768	L699		L374	H293	C212	V133		ASP
K1392	E1211	C1127	A769	K700	T561	V376	G294	K213	G134	D56	ASP
Y1396	D1212	L1128	L770	V701	L563		T295	A214	C135	L57	ASP
F1401	P1213	S1129	L771	R702	L567	N391	V299	F215	A138	S58	LYS
V1417	S870	E1130	R772	E704	L567	S392		D216	M139	R59	LYS
V1424	D881	C1141	R773	P705	L567	F393	P302	T217	M139	F60	TYR
K1429	T898	V1145	G774	K706	L567	V400	Q303	G221	N142	P69	ASP
D1436	L1228	E1233	L775	P707	S568	H401	Q303	Y222	R143	K70	PRO
A1445	L1246	L1246	K776	R708	C569	Q409	I308	C223	L144	Q71	THR
I1446	H1249	H1249	L781	W712	M570	P412	R310	R224	F150	H73	GLU
V1457	G1250	G1250	L782	L713	G576	H417	R316	E226	A156	M75	ASN
C1471	H1251	H1251	P783	S714	I577	L420	L320	V228	L157	D76	LEU
L1474	R935	R935	L784	I717	V578	L423	L321	G227	D158	P77	PHE
E1485	L937	L937	K785	P718	S581	E432	I322	L232	T159	Q78	GLN
V1486	L937	L937	K786	L582	G583	L430	L424	L232	A160	L79	GLY
L1493	L938	L938	L787	E719	E584	E436	L425	L232	C161	R80	ALA
L1313	E939	E939	L788	A720	V585	L437	S327	A239	S162	L82	GLY
V1314	L940	L940	H789	Q721	G588	L437	S327	A239	S164	E84	SER
A1300	S941	S941	R790	W722	D591	L437	S327	A239	M166	V85	GLY
L1320	E948	E948	L791	H723	S595	L437	S327	A239	A167	T86	ILE
L1322	N949	N949	W724	G725	I520	L437	S327	A239	L168	Y87	P1
D1324	E981	E981	L792	S725	S595	L437	S327	A239	A171	E88	V4
F1325	P977	P977	L793	L726	S595	L437	S327	A239	I175	A89	V5
A1326	H978	H978	L794	A727	Q596	L437	S327	A239	I175	I90	I6
N1331	E981	E981	L795	L727	E597	L437	S327	A239	Q179	G93	G8
L1336	P982	P982	L796	A727	E598	L437	S327	A239	A182	G94	A7
L1343	R997	R997	L797	L728	A599	L437	S327	A239	A183	N95	M9
L1348	E1014	E1014	L798	E729	V600	L437	S327	A239	I184	K12	K12
L1356	L1043	L1043	L799	P671	L601	L437	S327	A239	V185	P97	L13
Y1367	L1046	L1046	L801	A672	K611	L437	S327	A239	G186	D98	P14
Q1368	D1071	D1071	L802	K673	E612	L437	S327	A239	G187	T105	E17
Q1369	K1072	K1072	L803	E674	A613	L437	S327	A239	I188	W108	N18
G1370	D1077	D1077	L804	E674	H614	L437	S327	A239	N189	V109	L19
I1371	K1072	K1072	L805	E674	L615	L437	S327	A239	V190	G110	F22
L1372	H1093	H1093	L806	E674	P616	L437	S327	A239	L191	V111	W23
S1373	L1202	L1202	L807	E674	P616	L437	S327	A239	L192	G111	D24
E1602	A1203	A1203	L808	E674	P616	L437	S327	A239	K193	S112	N25
			L809	E674	P616	L437	S327	A239	N195	G113	L26
			L810	E674	P616	L437	S327	A239	V198	E115	M32
			L811	E674	P616	L437	S327	A239	Q199	S117	V33
			L812	E674	P616	L437	S327	A239	F200	L120	D36
			L813	E674	P616	L437	S327	A239	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 ⓘ

### 5.3.1 Protein backbone ⓘ

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

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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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 ⓘ

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%)	92	95
All	All	3413/4234 (81%)	3410 (100%)	3 (0%)	92	96

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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Mol	Chain	Res	Type
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	B	2601	-	47,52,52	0.63	0	61,80,80	0.90	2 (3%)
2	NDP	B	2602	-	47,52,52	0.66	0	61,80,80	0.79	2 (3%)
2	NDP	A	2601	-	47,52,52	0.65	0	61,80,80	0.94	4 (6%)
2	NDP	A	2602	-	47,52,52	0.67	0	61,80,80	0.79	2 (3%)

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	B	2601	-	-	12/30/77/77	0/5/5/5
2	NDP	B	2602	-	-	12/30/77/77	0/5/5/5
2	NDP	A	2601	-	-	13/30/77/77	0/5/5/5
2	NDP	A	2602	-	-	13/30/77/77	0/5/5/5

There are no bond length outliers.

All (10) 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	C4B-O4B-C1B	-3.08	107.11	109.92
2	A	2602	NDP	C5A-C6A-N6A	2.25	123.73	120.31
2	B	2602	NDP	C5A-C6A-N6A	2.21	123.68	120.31
2	A	2601	NDP	C5A-C6A-N6A	2.21	123.68	120.31
2	B	2601	NDP	C5A-C6A-N6A	2.17	123.62	120.31
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 (50) 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

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Mol	Chain	Res	Type	Atoms
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
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	PA-O3-PN-O1N
2	B	2602	NDP	PN-O3-PA-O1A
2	A	2602	NDP	C4B-C5B-O5B-PA
2	B	2602	NDP	C4D-C5D-O5D-PN
2	A	2602	NDP	C2N-C3N-C7N-O7N

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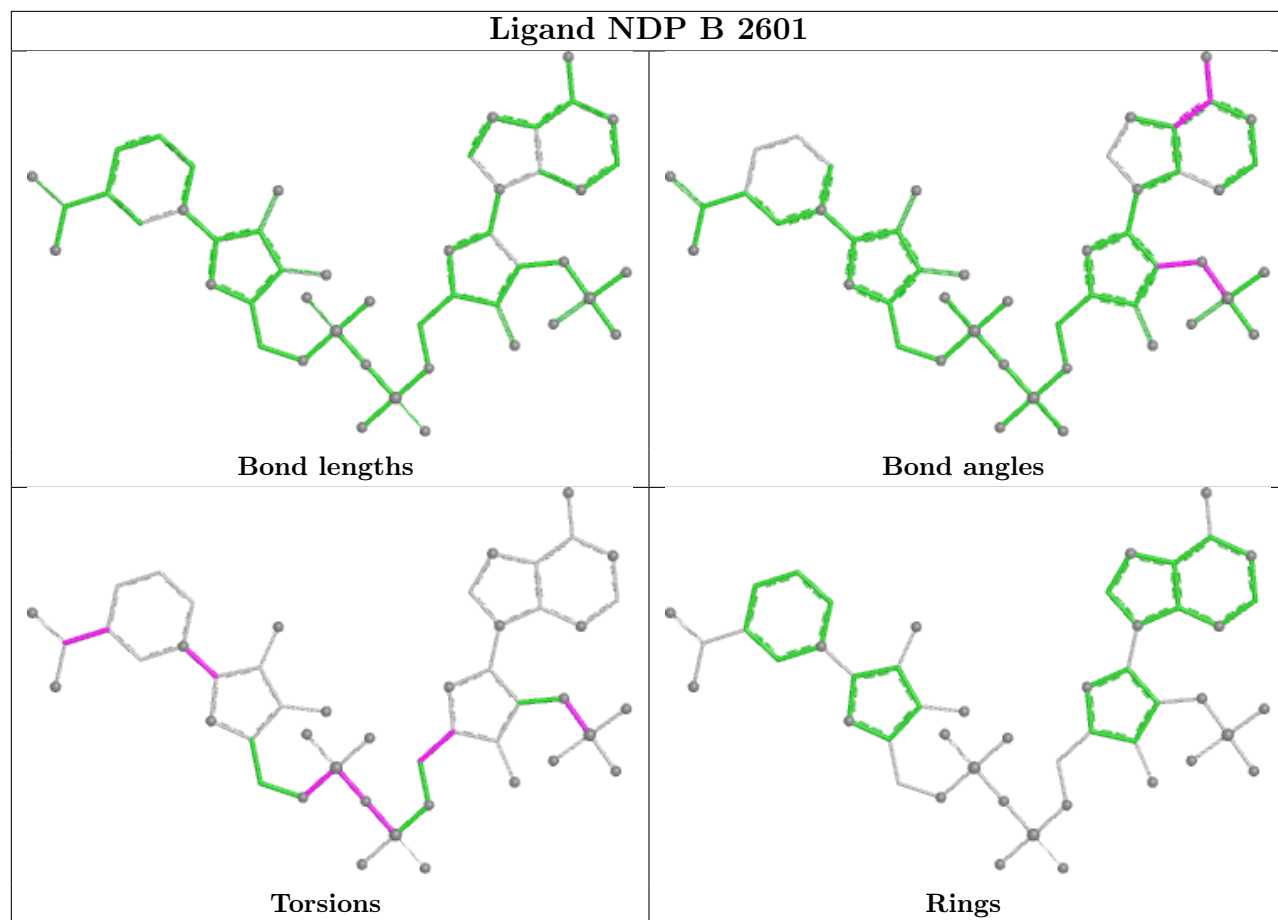
Mol	Chain	Res	Type	Atoms
2	A	2602	NDP	PA-O3-PN-O2N
2	B	2601	NDP	PN-O3-PA-O2A
2	B	2601	NDP	PA-O3-PN-O2N
2	B	2602	NDP	PN-O3-PA-O2A

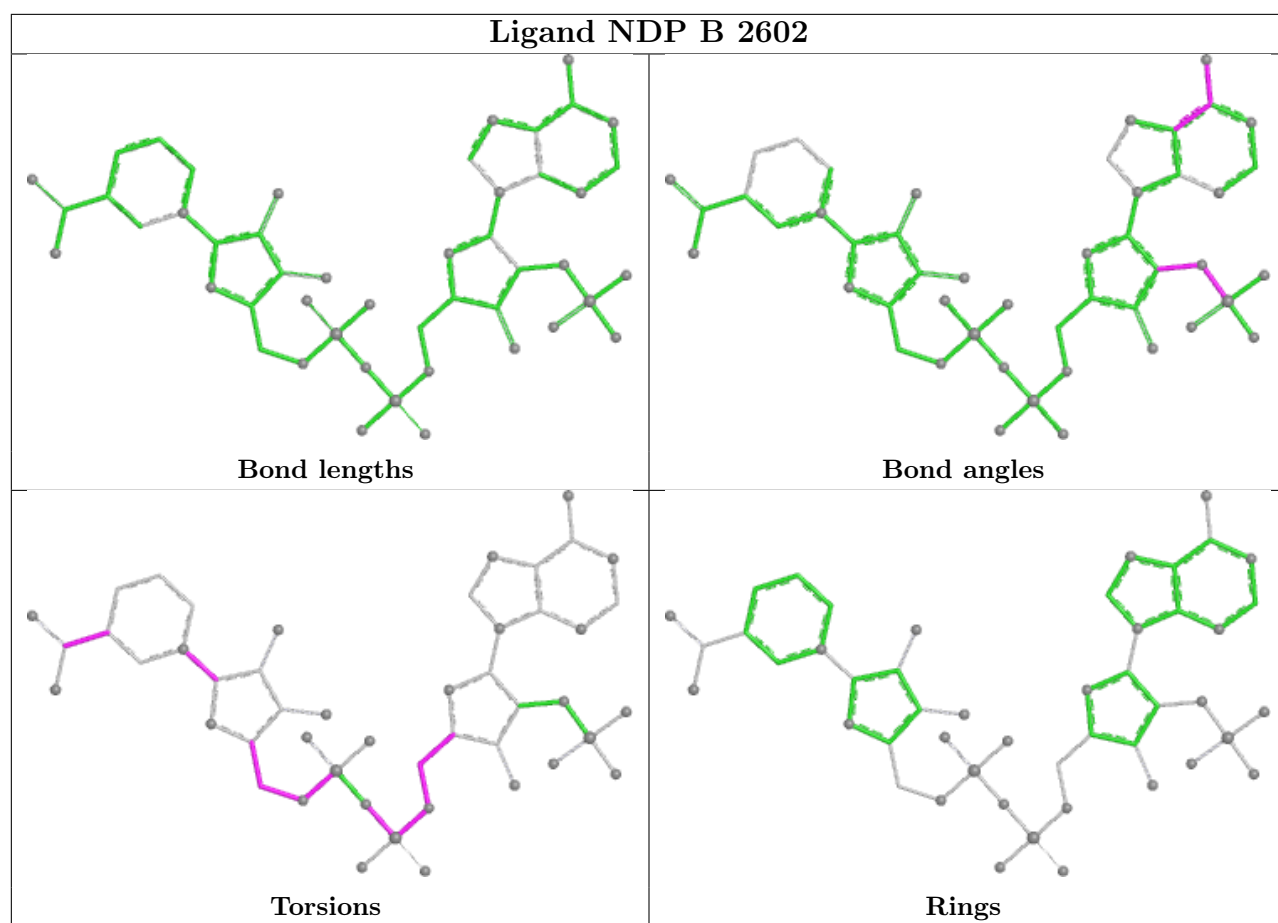
There are no ring outliers.

1 monomer is involved in 3 short contacts:

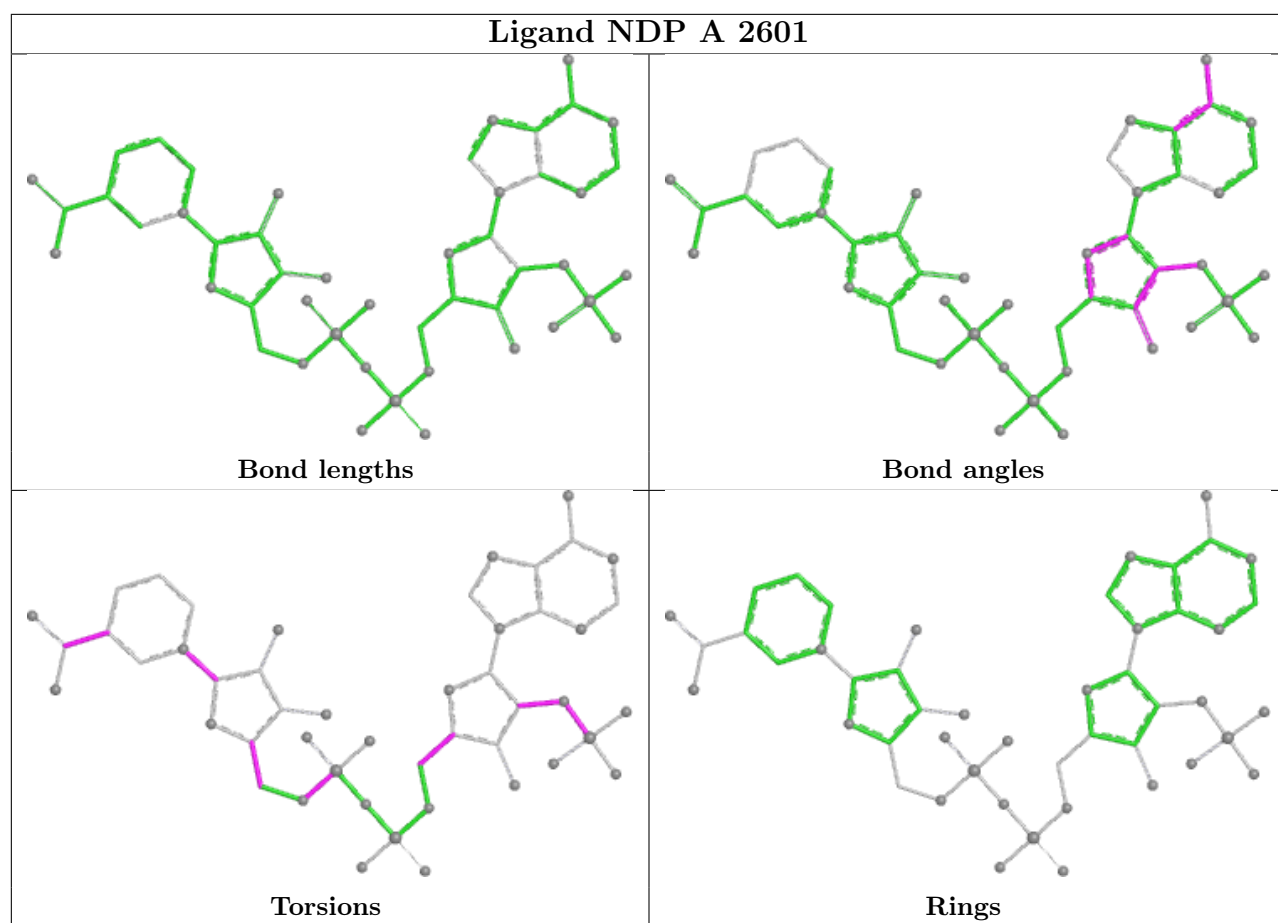
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2602	NDP	3	0

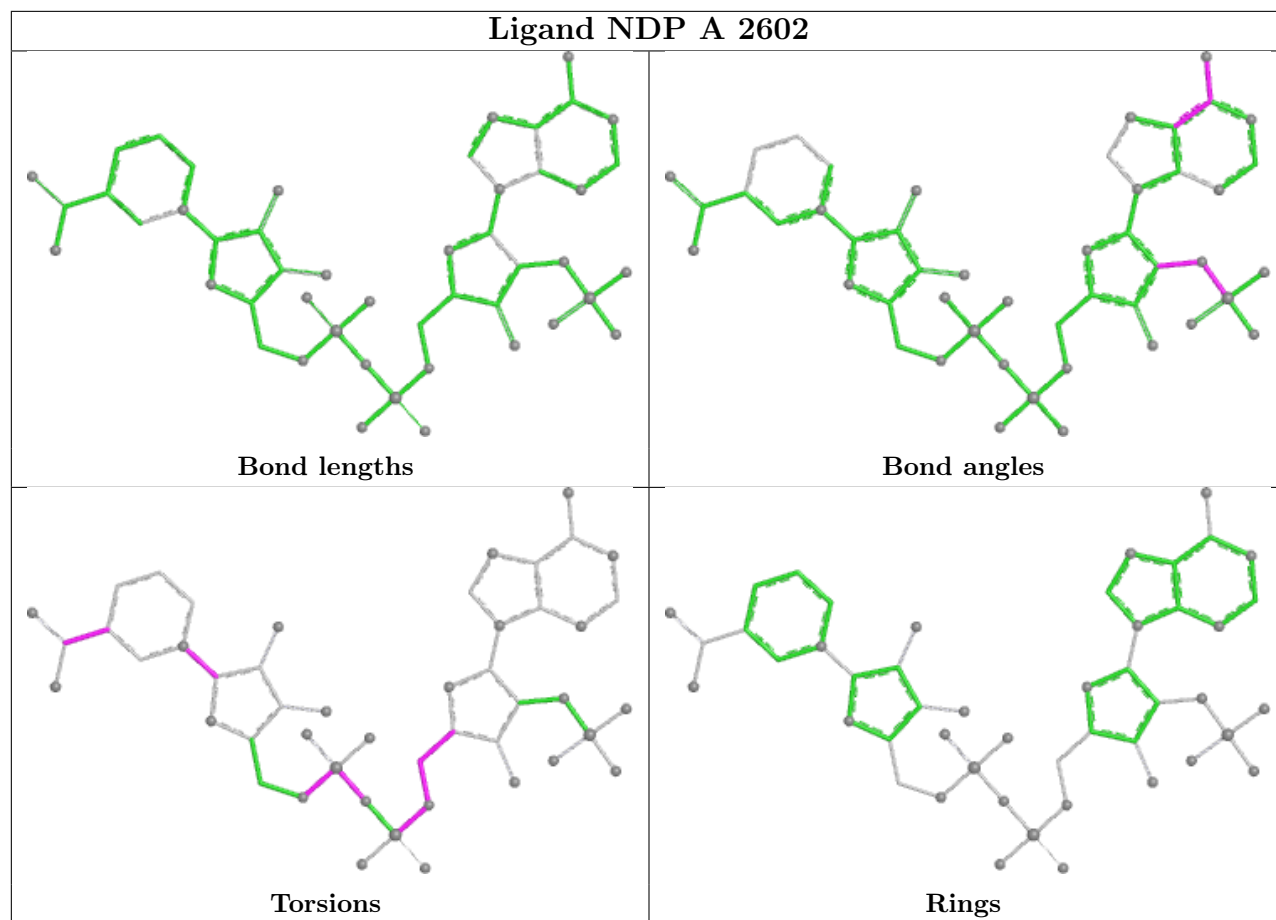
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

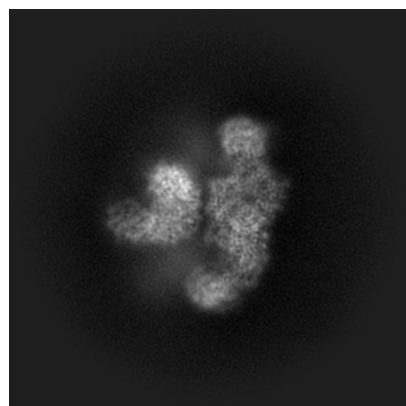
## 6 Map visualisation [i](#)

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.

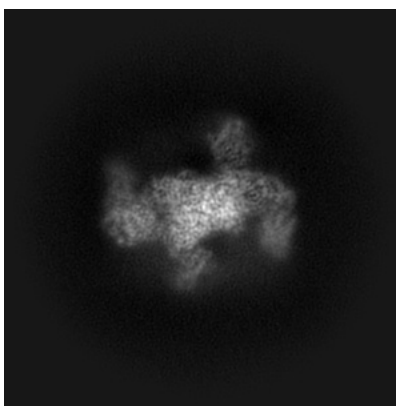
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

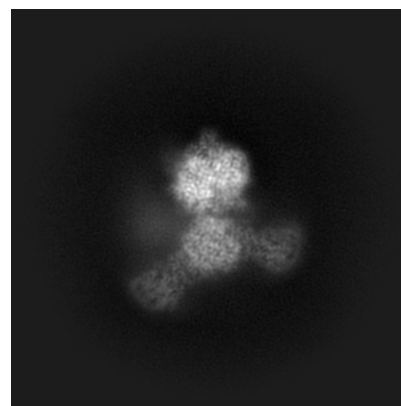
#### 6.1.1 Primary map



X

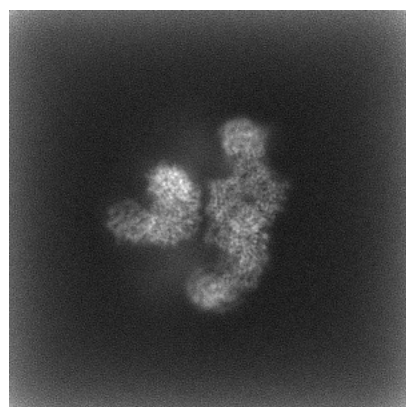


Y

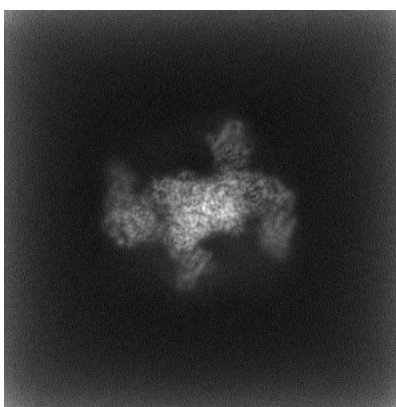


Z

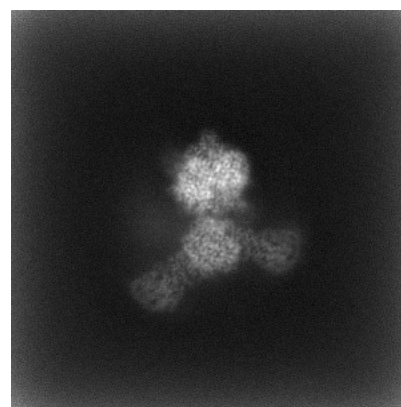
#### 6.1.2 Raw map



X



Y

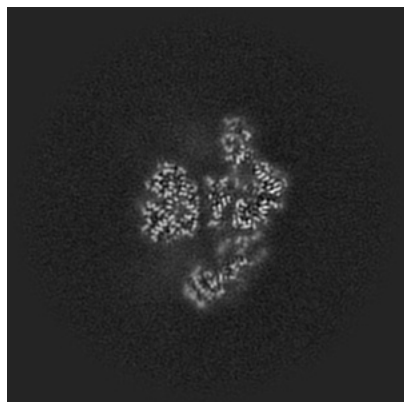


Z

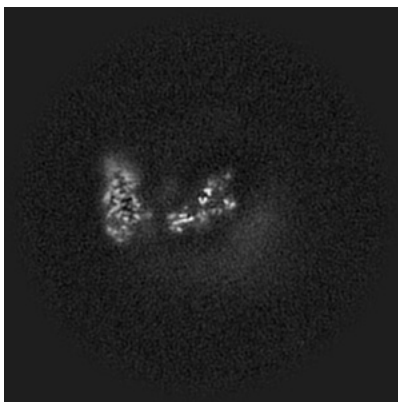
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

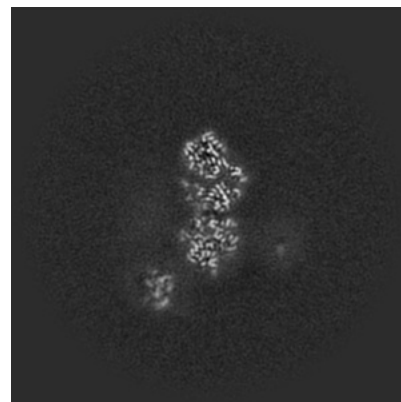
### 6.2.1 Primary map



X Index: 180

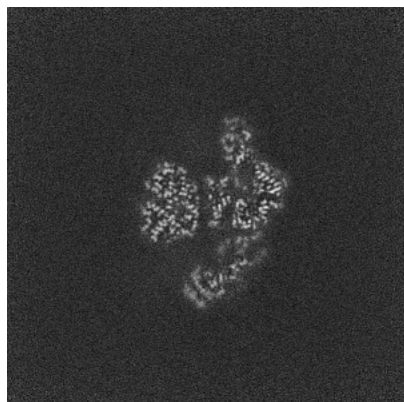


Y Index: 180



Z Index: 180

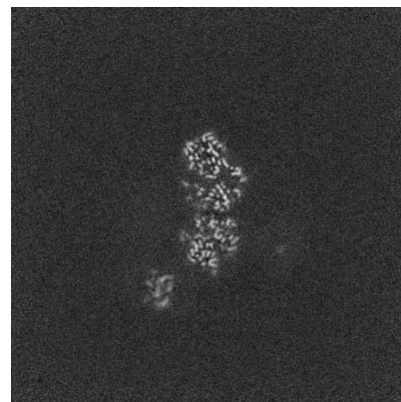
### 6.2.2 Raw map



X Index: 180



Y Index: 180

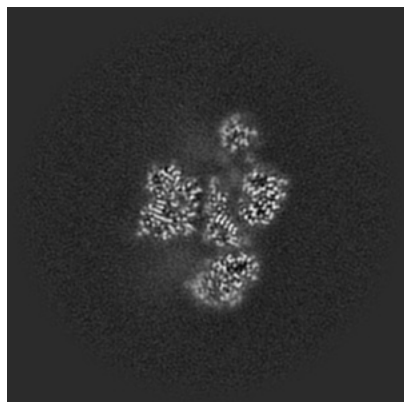


Z Index: 180

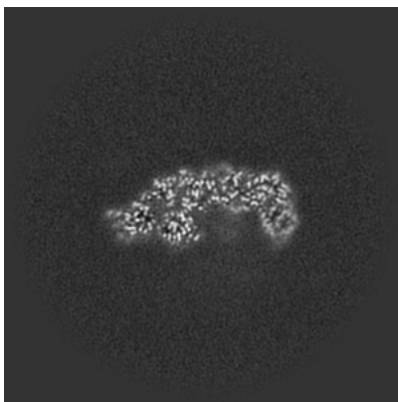
The images above show central slices of the map in three orthogonal directions.

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

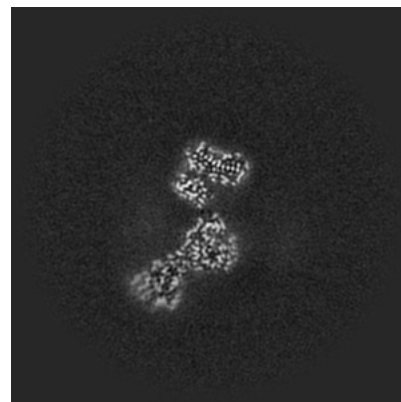
### 6.3.1 Primary map



X Index: 173

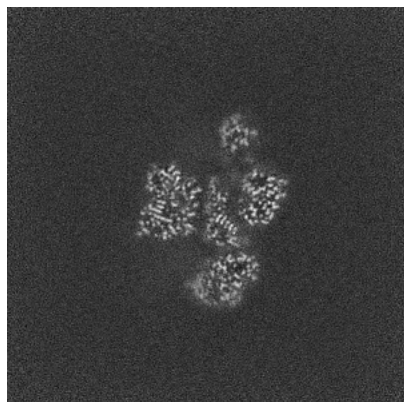


Y Index: 205

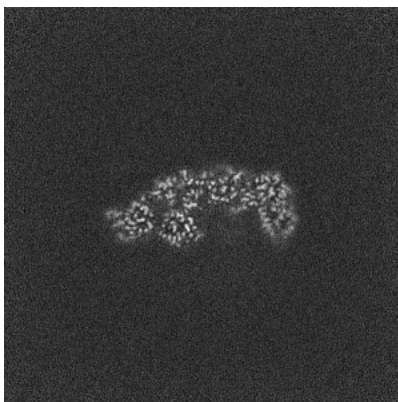


Z Index: 169

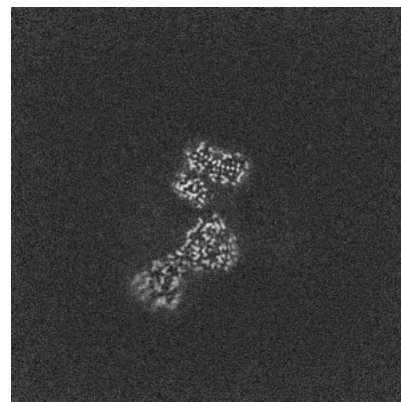
### 6.3.2 Raw map



X Index: 173



Y Index: 204



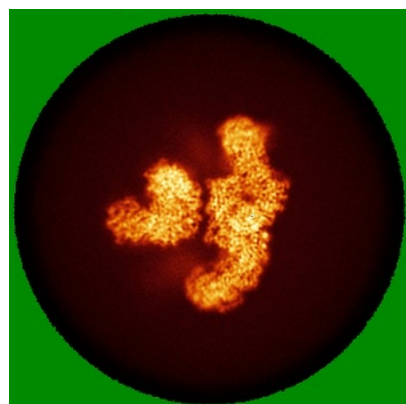
Z Index: 169

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

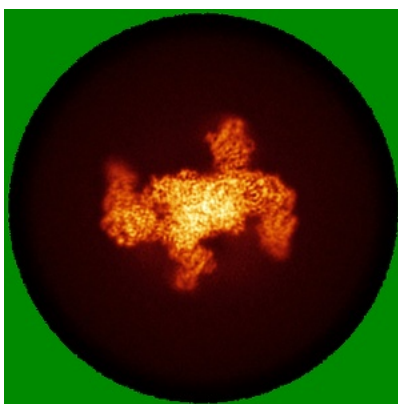


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

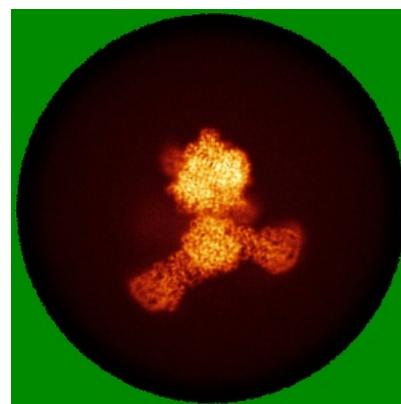
### 6.4.1 Primary map



X

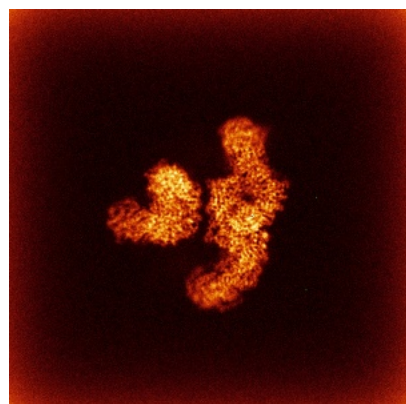


Y

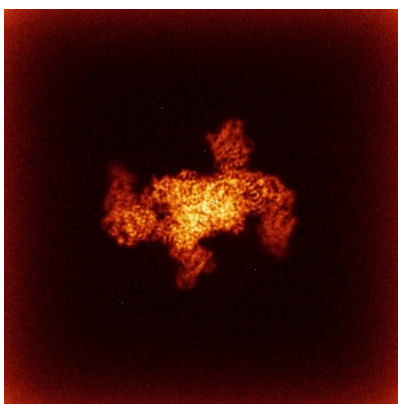


Z

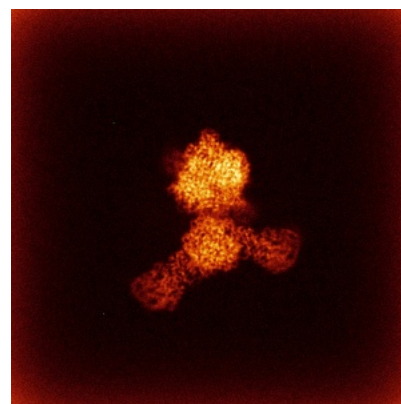
### 6.4.2 Raw map



X



Y

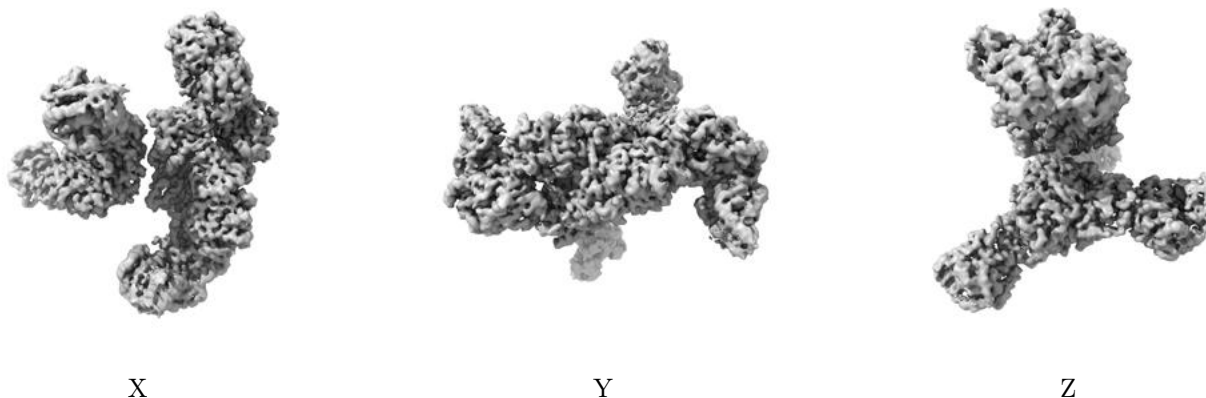


Z

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

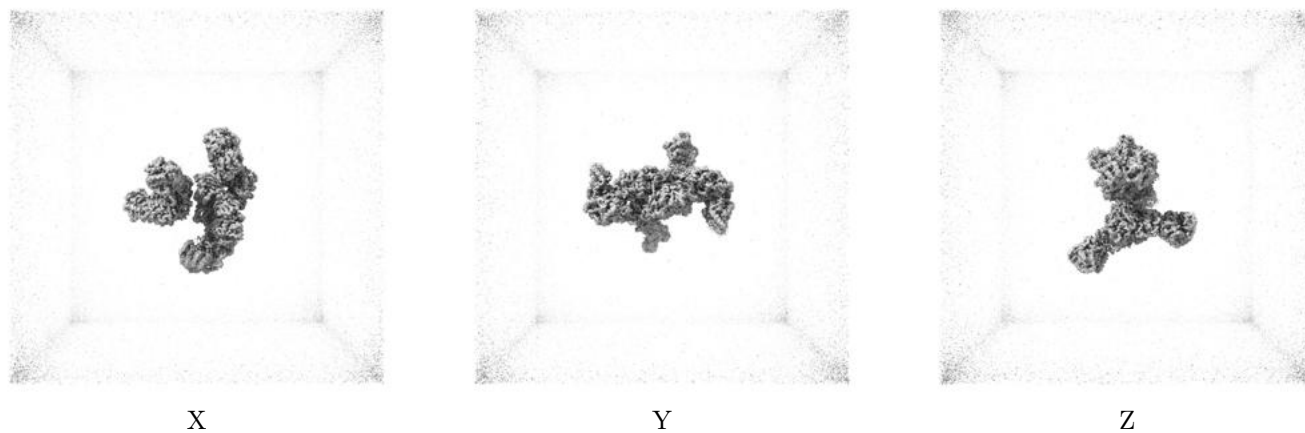
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.173. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

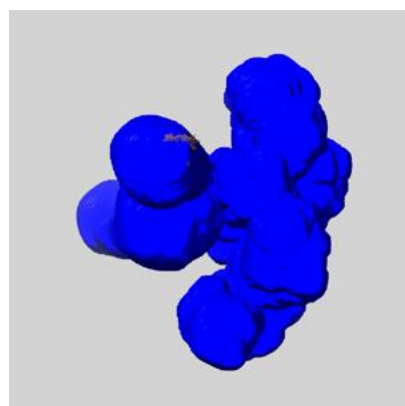
## 6.6 Mask visualisation [i](#)

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

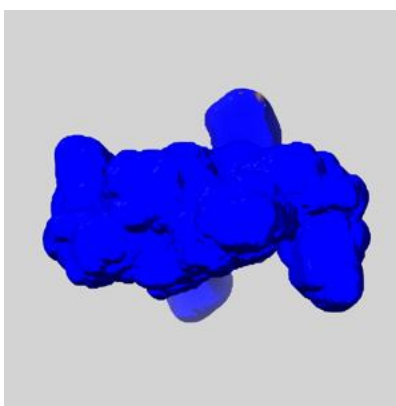
A mask typically either:

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

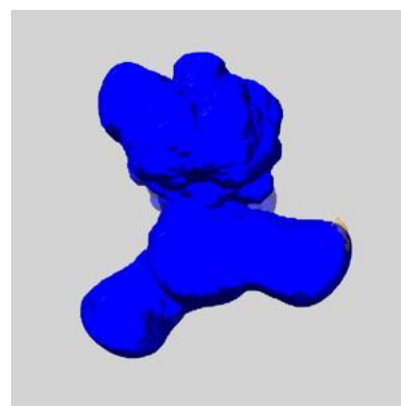
### 6.6.1 emd\_43355\_msk\_1.map [i](#)



X



Y



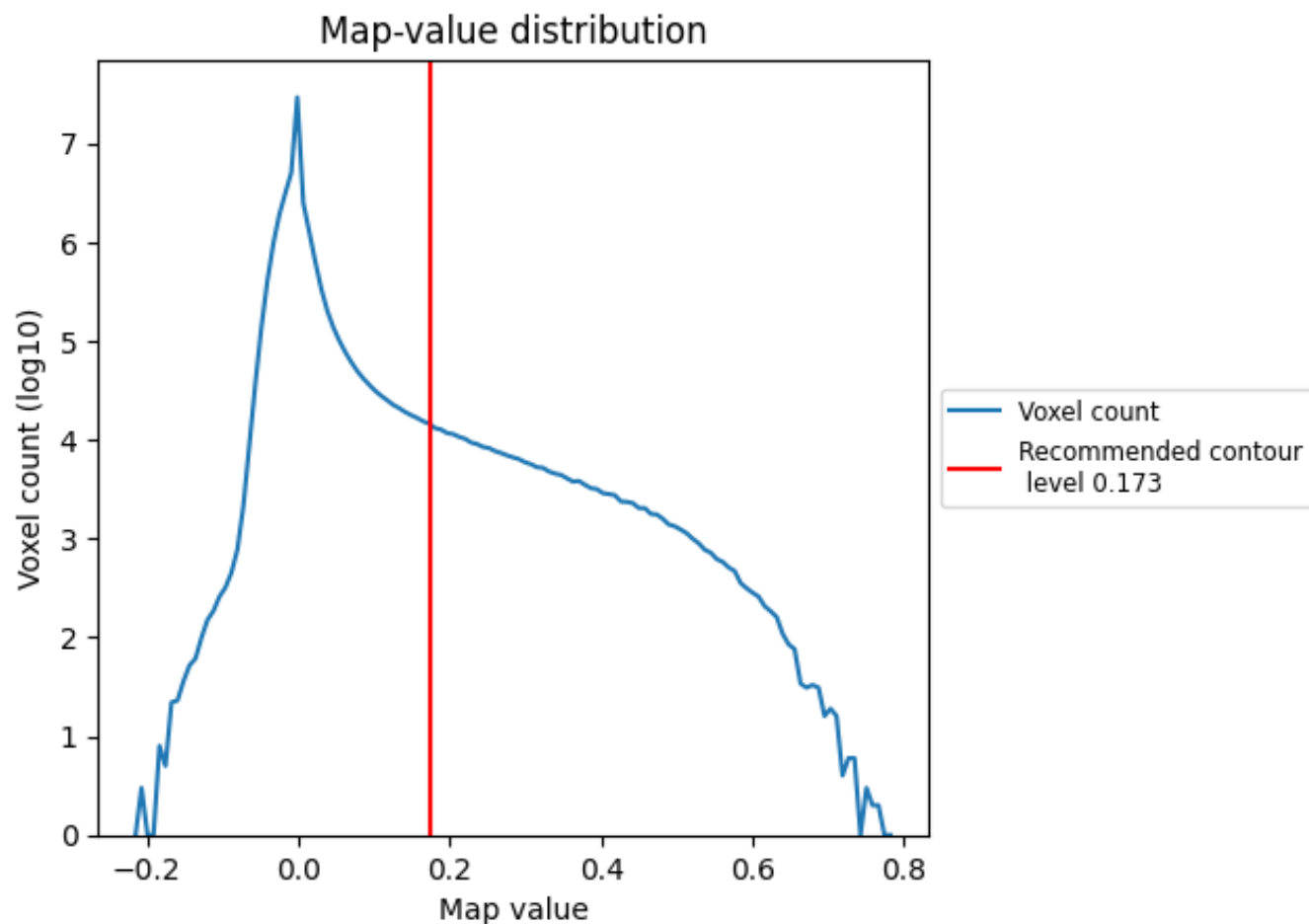
Z



## 7 Map analysis [i](#)

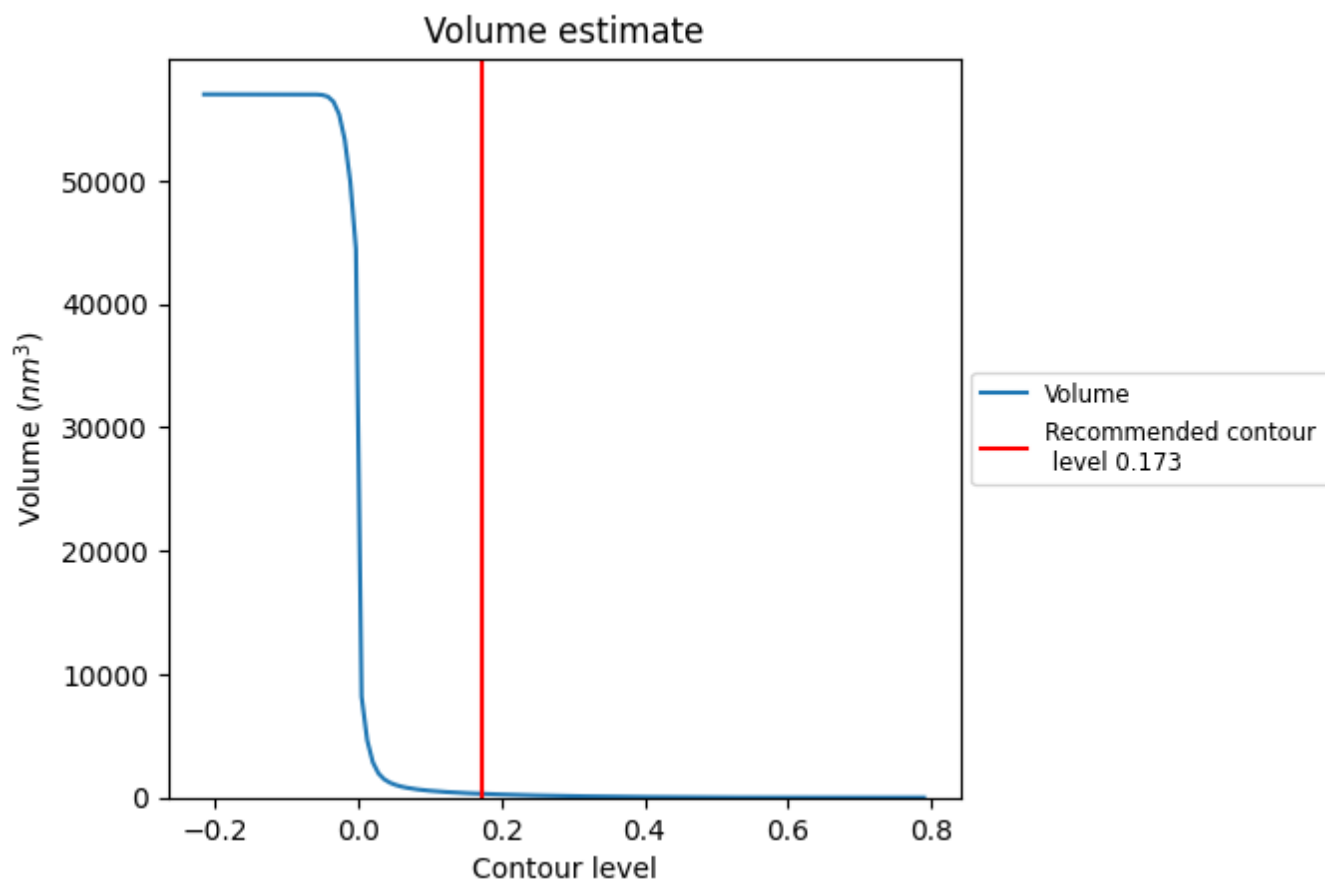
This section contains the results of statistical analysis of the map.

### 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.

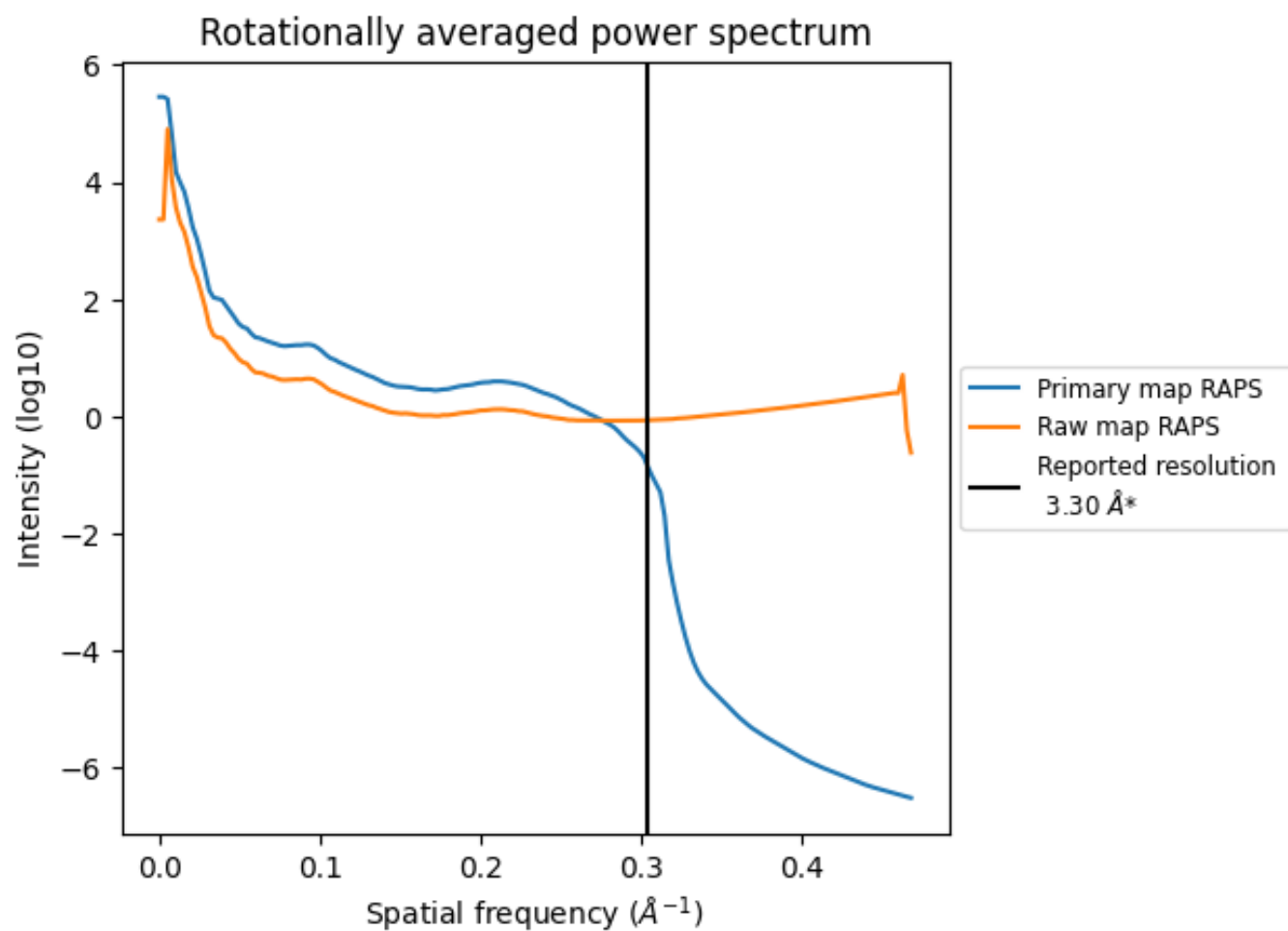
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 304  $\text{nm}^3$ ; 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 ⓘ

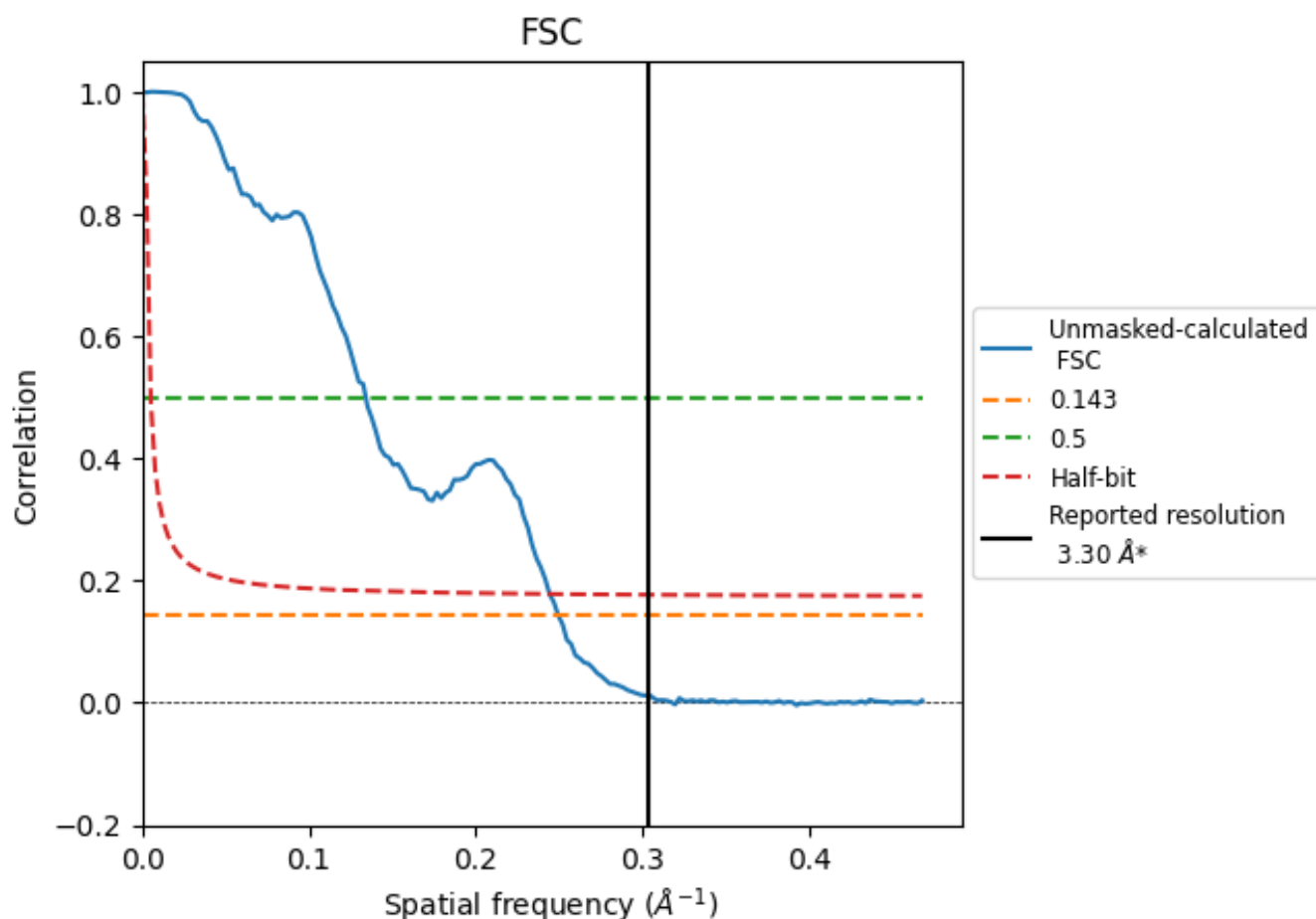


\*Reported resolution corresponds to spatial frequency of  $0.303 \text{ \AA}^{-1}$

## 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](#)

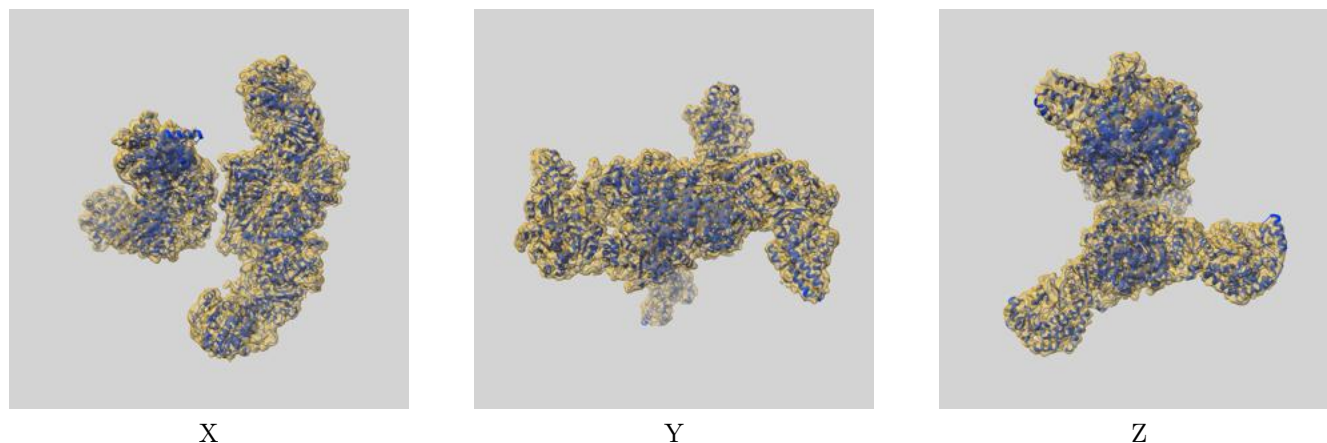
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.01	7.46	4.10

\*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](#)

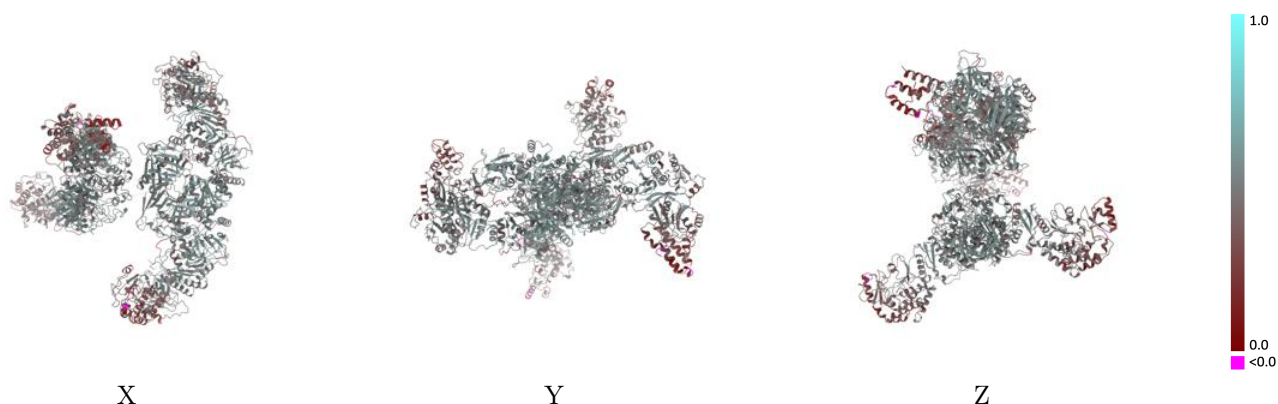
This section contains information regarding the fit between EMDB map EMD-43355 and PDB model 8VMC. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

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



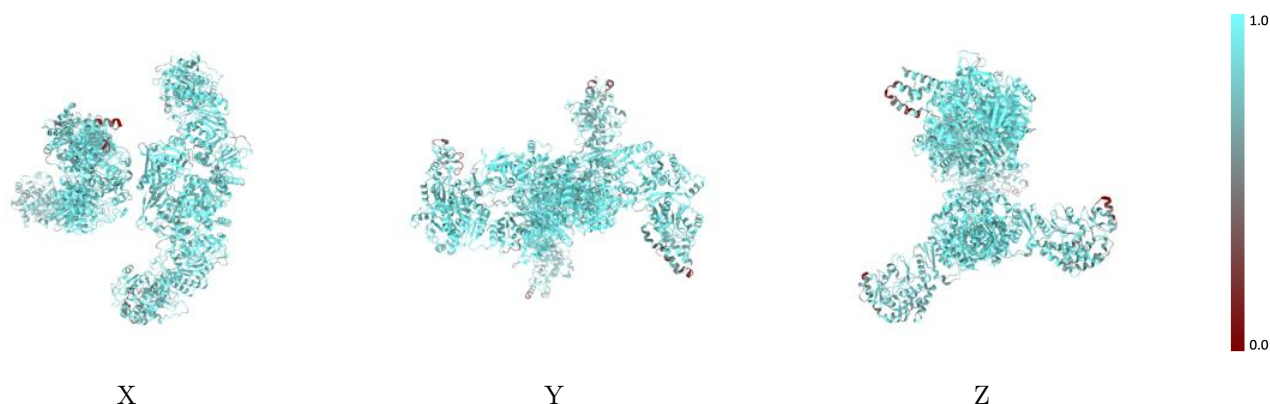
The images above show the 3D surface view of the map at the recommended contour level 0.173 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



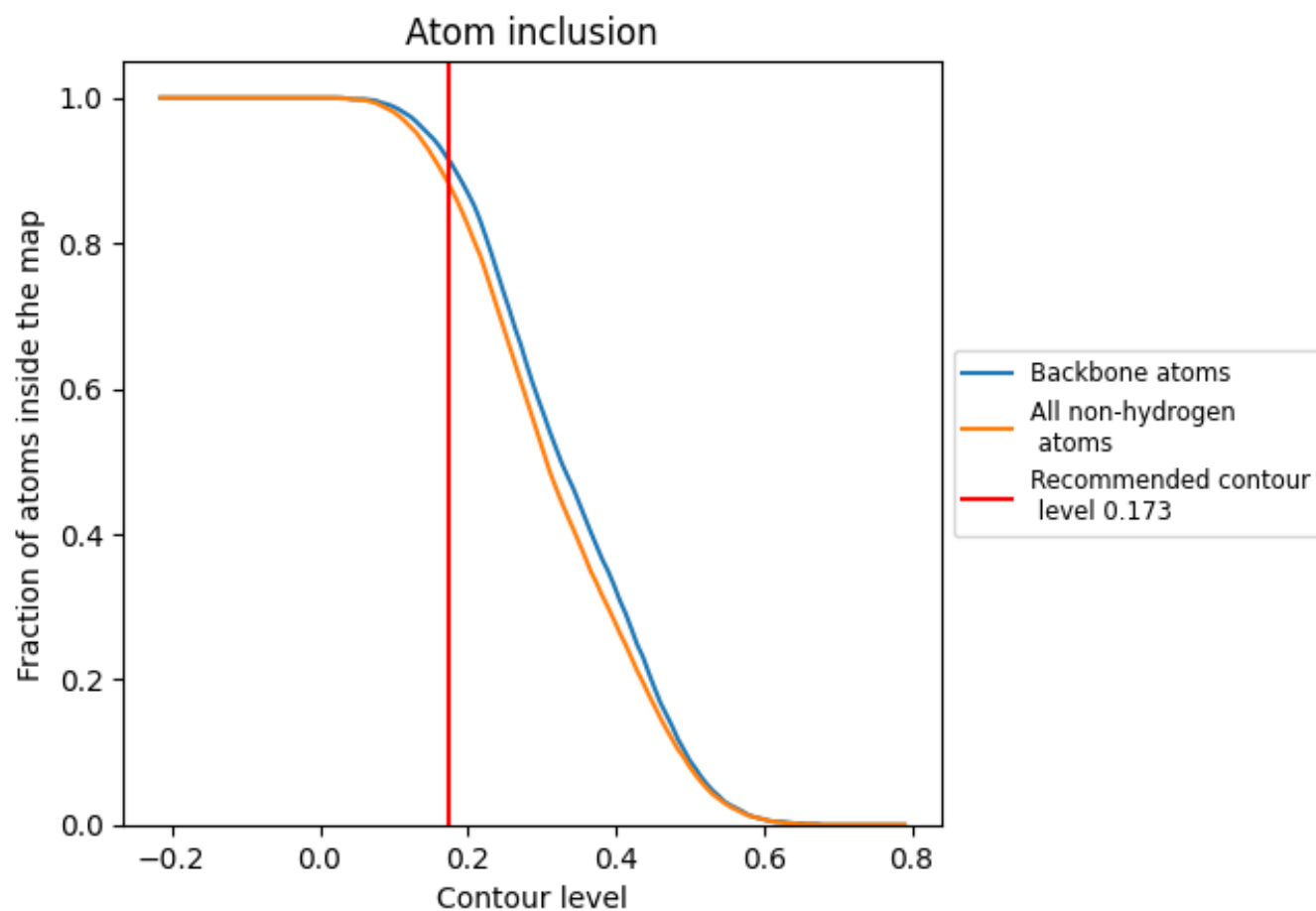
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	<div></div> 0.8840	<div></div> 0.4640
A	<div></div> 0.8830	<div></div> 0.4640
B	<div></div> 0.8860	<div></div> 0.4640

