



## Full wwPDB EM Validation Report ⓘ

Feb 22, 2025 – 02:31 PM EST

PDB ID : 8VM5  
EMDB ID : EMD-43352  
Title : Composite structure of human FASN with NADPH in State 5  
Authors : Schultz, K.; Marmorstein, R.  
Deposited on : 2024-01-12  
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.dev117  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
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) : 2.41.4

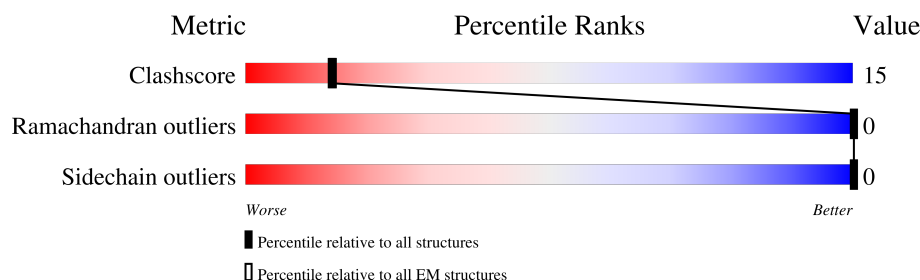
# 1 Overall quality at a glance

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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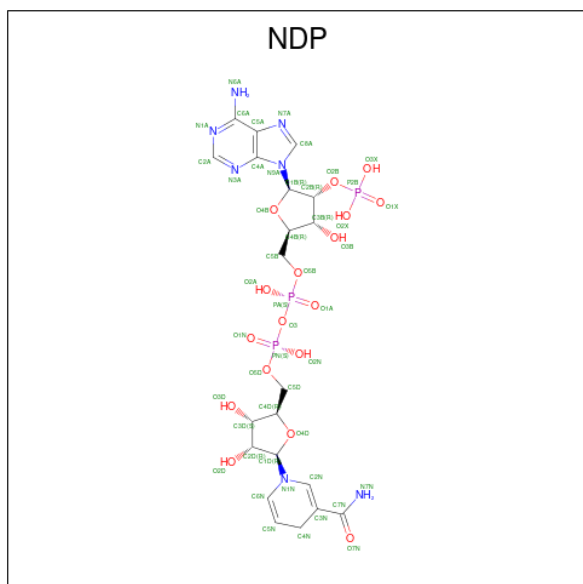
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	ALA	-	expression tag	UNP P49327
A	-4	MET	-	expression tag	UNP P49327
A	-3	GLY	-	expression tag	UNP P49327
A	-2	SER	-	expression tag	UNP P49327
A	-1	GLY	-	expression tag	UNP P49327
A	0	ILE	-	expression tag	UNP P49327
A	1	PRO	-	expression tag	UNP P49327
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 (three-letter code: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).

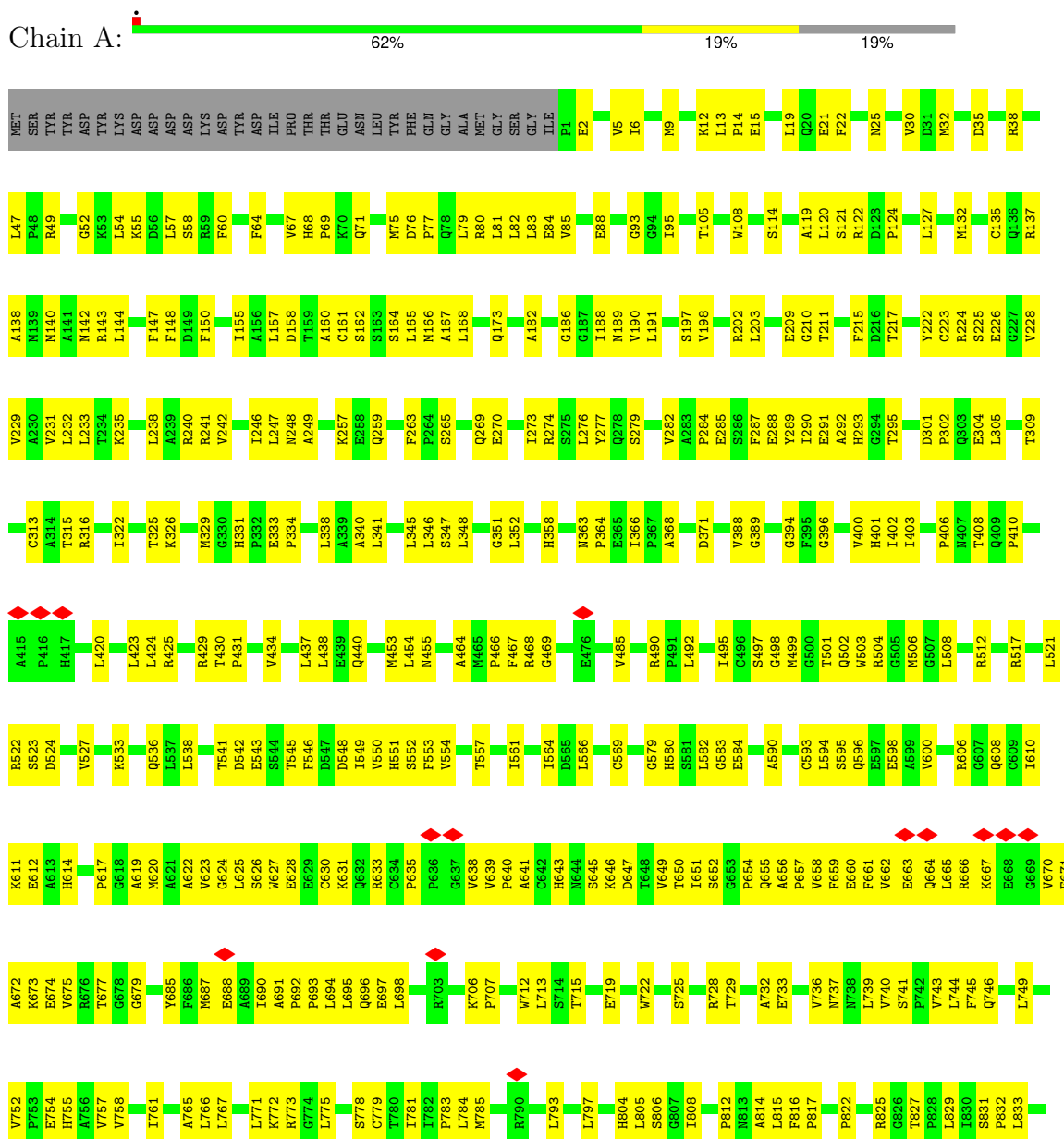


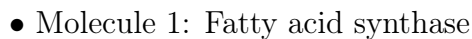
Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
2	A	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
2	B	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
2	B	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	

### 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





L120	G43
D123	G46
P124	L47
L127	R50
V128	S51
G129	G52
Y130	K53
M131	L54
M132	K55
V133	D56
G134	L57
C135	S58
A138	R59
M139	F60
N142	S63
R143	F64
L144	F65
F147	K70
F150	Q71
L157	A72
D158	H73
T159	T74
A160	M75
C161	D76
S162	P77
S163	Q78
S164	L79
L165	R80
M166	L81
A167	L82
L168	L83
A171	E84
I175	V85
Q179	T86
A182	I90
I184	V91
I188	D92
N189	G93
V190	G94
L191	I95
L192	D98
K193	S99
F194	L100
T196	R101
T197	G102
	T103
	H104
	T105
	W108
	S114
	S117



E2113	L1888	R1515	Y1270	C1141	L899	L767	L694	W627	V554	V472	A368	L276	V198	
LYS	I1889	H1516	T1271	V1145	V912	Q768	L695	E628	S555	L473	L369	Y277	Q199	
ALA	A1272	F1517	T1273	T1150	V913	A769	Q696	E629	S556	E476	L374	A283	P200	
ALA	T1274	E1521	D1274	THR	V935	V770	K699	C630	T557	R477	Q375	P284	R202	
ALA	R1275	E1521	R1275	THR	E945	K773	K700	Q632	A558	Q483	V376	E265		
TYR	E1286	T1535	E1286	VAL	E958	G774	V701	R633	I559	Q484	V377	E288	M205	
ARG	Q1289	T1535	Q1289	GLN	V958	K776	R703	C634	Q485	V485	D378	L206	L206	
ASP	Q1292	I1544	Q1292	GLY	E958	K776	R704	P635	I561		Q379	S207	S207	
ASP	Q1294	R1552	Q1294	GLY	E958	K776	R704	P635	I561		P380	P208	P208	
SER	Q1295	R1552	Q1295	LEU	E958	K776	R704	P635	I561		L381	E209	E209	
GLN	Q1296	R1552	Q1296	LEU	E958	K776	R704	P635	I561		A292	A292	G210	
ARG	Q1297	R1552	Q1297	LEU	E958	K776	R704	P635	I561		H293	H293	T211	
ASP	Q1298	R1552	Q1298	LEU	E958	K776	R704	P635	I561		V383	G294	C212	
LEU	R1301	R1552	Q1299	VAL	E958	K776	R704	P635	I561		N391	T295	F215	
VAL	R1302	R1552	Q1300	VAL	E958	K776	R704	P635	I561		F393	D301	G221	
GLU	R1303	R1552	Q1301	GLY	E958	K776	R704	P635	I561		P302	P302	G221	
ALA	R1304	R1552	Q1302	ASP	E958	K776	R704	P635	I561		Q303	Q303	Y222	
VAL	R1305	R1552	Q1303	ASP	E958	K776	R704	P635	I561		E304	E304	C223	
ALA	R1306	R1552	Q1304	ASP	E958	K776	R704	P635	I561		H401	H401	E226	
HIS	R1307	R1552	Q1305	ALA	E958	K776	R704	P635	I561		I402	I402	G227	
ILE	R1308	R1552	Q1306	ALA	E958	K776	R704	P635	I561		L404	L404	V228	
LEU	R1309	R1552	Q1307	ILE	E958	K776	R704	P635	I561		R405	R405	V231	
GLY	R1310	R1552	Q1308	PR0	E958	K776	R704	P635	I561		P406	P406		
ILE	R1311	R1552	Q1309	ARG	E958	K776	R704	P635	I561		H417	H417	T234	
ARG	R1312	R1552	Q1310	ASP	E958	K776	R704	P635	I561		L420	L420	K235	
ASP	R1313	R1552	Q1311	ASP	E958	K776	R704	P635	I561		P421	P421	K236	
ASP	R1314	R1552	Q1312	ASP	E958	K776	R704	P635	I561		R422	R422	S237	
ASP	R1315	R1552	Q1313	ASP	E958	K776	R704	P635	I561		L424	L424	R240	
ASP	R1316	R1552	Q1314	ASP	E958	K776	R704	P635	I561		R429	R429	R241	
ASP	R1317	R1552	Q1315	ASP	E958	K776	R704	P635	I561		T430	T430	V242	
ASP	R1318	R1552	Q1316	ASP	E958	K776	R704	P635	I561		P431	P431	T245	
ASP	R1319	R1552	Q1317	ASP	E958	K776	R704	P635	I561		E333	E333	I246	
ASP	R1320	R1552	Q1318	ASP	E958	K776	R704	P635	I561		P334	P334	L247	
ASP	R1321	R1552	Q1319	ASP	E958	K776	R704	P635	I561		A335	A335	N248	
ASP	R1322	R1552	Q1320	ASP	E958	K776	R704	P635	I561		L337	L337	A249	
ASP	R1323	R1552	Q1321	ASP	E958	K776	R704	P635	I561		E439	E439	G250	
ASP	R1324	R1552	Q1322	ASP	E958	K776	R704	P635	I561		Q440	Q440	T251	
ASP	R1325	R1552	Q1323	ASP	E958	K776	R704	P635	I561		R443	R443	W252	
ASP	R1326	R1552	Q1324	ASP	E958	K776	R704	P635	I561		L451	L451	T253	
ASP	R1327	R1552	Q1325	ASP	E958	K776	R704	P635	I561		S452	S452	D254	
ASP	R1328	R1552	Q1326	ASP	E958	K776	R704	P635	I561		M453	M453	G255	
ASP	R1329	R1552	Q1327	ASP	E958	K776	R704	P635	I561		L454	L454	F256	
ASP	R1330	R1552	Q1328	ASP	E958	K776	R704	P635	I561		V460	V460	P258	
ASP	R1331	R1552	Q1329	ASP	E958	K776	R704	P635	I561		P461	P461	Q259	
ASP	R1332	R1552	Q1330	ASP	E958	K776	R704	P635	I561		A354	A354	V261	
ASP	R1333	R1552	Q1331	ASP	E958	K776	R704	P635	I561		P355	P355	T262	
ASP	R1334	R1552	Q1332	ASP	E958	K776	R704	P635	I561		N356	N356	F263	
ASP	R1335	R1552	Q1333	ASP	E958	K776	R704	P635	I561		E365	E365	E270	
ASP	R1336	R1552	Q1334	ASP	E958	K776	R704	P635	I561		I366	I366	R274	
ASP	R1337	R1552	Q1335	ASP	E958	K776	R704	P635	I561		P367	P367	S275	
ASP	R1338	R1552	Q1336	ASP	E958	K776	R704	P635	I561					
ASP	R1339	R1552	Q1337	ASP	E958	K776	R704	P635	I561					
ASP	R1340	R1552	Q1338	ASP	E958	K776	R704	P635	I561					
ASP	R1341	R1552	Q1339	ASP	E958	K776	R704	P635	I561					
ASP	R1342	R1552	Q1340	ASP	E958	K776	R704	P635	I561					
ASP	R1343	R1552	Q1341	ASP	E958	K776	R704	P635	I561					
ASP	R1344	R1552	Q1342	ASP	E958	K776	R704	P635	I561					
ASP	R1345	R1552	Q1343	ASP	E958	K776	R704	P635	I561					
ASP	R1346	R1552	Q1344	ASP	E958	K776	R704	P635	I561					
ASP	R1347	R1552	Q1345	ASP	E958	K776	R704	P635	I561					
ASP	R1348	R1552	Q1346	ASP	E958	K776	R704	P635	I561					
ASP	R1349	R1552	Q1347	ASP	E958	K776	R704	P635	I561					
ASP	R1350	R1552	Q1348	ASP	E958	K776	R704	P635	I561					
ASP	R1351	R1552	Q1349	ASP	E958	K776	R704	P635	I561					
ASP	R1352	R1552	Q1350	ASP	E958	K776	R704	P635	I561					
ASP	R1353	R1552	Q1351	ASP	E958	K776	R704	P635	I561					
ASP	R1354	R1552	Q1352	ASP	E958	K776	R704	P635	I561					
ASP	R1355	R1552	Q1353	ASP	E958	K776	R704	P635	I561					
ASP	R1356	R1552	Q1354	ASP	E958	K776	R704	P635	I561					
ASP	R1357	R1552	Q1355	ASP	E958	K776	R704	P635	I561					
ASP	R1358	R1552	Q1356	ASP	E958	K776	R704	P635	I561					
ASP	R1359	R1552	Q1357	ASP	E958	K776	R704	P635	I561					
ASP	R1360	R1552	Q1358	ASP	E958	K776	R704	P635	I561					
ASP	R1361	R1552	Q1359	ASP	E958	K776	R704	P635	I561					
ASP	R1362	R1552	Q1360	ASP	E958	K776	R704	P635	I561					
ASP	R1363	R1552	Q1361	ASP	E958	K776	R704	P635	I561					
ASP	R1364	R1552	Q1362	ASP	E958	K776	R704	P635	I561					
ASP	R1365	R1552	Q1363	ASP	E958	K776	R704	P635	I561					
ASP	R1366	R1552	Q1364	ASP	E958	K776	R704	P635	I561					
ASP	R1367	R1552	Q1365	ASP	E958	K776	R704	P635	I561					
ASP	R1368	R1552	Q1366	ASP	E958	K776	R704	P635	I561					
ASP	R1369	R1552	Q1367	ASP	E958	K776	R704	P635	I561					
ASP	R1370	R1552	Q1368	ASP	E958	K776	R704	P635	I561					
ASP	R1371	R1552	Q1369	ASP	E958	K776	R704	P635	I561					
ASP	R1372	R1552	Q1370	ASP	E958	K776	R704	P635	I561					
ASP	R1373	R1552	Q1371	ASP	E958	K776	R704	P635	I561					
ASP	R1374	R1552	Q1372	ASP	E958	K776	R704	P635	I561					
ASP	R1375	R1552	Q1373	ASP	E958	K776	R704	P635	I561					
ASP	R1376	R1552	Q1374	ASP	E958	K776	R704	P635	I561					
ASP	R1377	R1552	Q1375	ASP	E958	K776	R704	P635	I561					
ASP	R1378	R1552	Q1376	ASP	E958	K776	R704	P635	I561					
ASP	R1379	R1552	Q1377	ASP	E958	K776	R704	P635	I561					
ASP	R1380	R1552	Q1378	ASP	E958	K776	R704	P635	I561					
ASP	R1381	R1552	Q1379	ASP	E958	K776	R704	P635	I561					
ASP	R1382	R1552	Q1380	ASP	E958	K776	R704	P635	I561					
ASP	R1383	R1552	Q1381	ASP	E958	K776	R704	P635	I561					
ASP	R1384	R1552	Q1382	ASP	E958	K776	R704	P635	I561					
ASP	R1385	R1552	Q1383	ASP	E958	K776	R704	P635	I561					
ASP	R1386	R1552	Q1384	ASP	E958	K776	R704	P635	I561					
ASP	R1387	R1552	Q1385	ASP	E958	K776	R704	P635	I561					
ASP	R1388	R1552	Q1386	ASP	E958	K776	R704	P635	I561					
ASP	R1389	R1552	Q1387	ASP	E958	K776	R704	P635	I561					
ASP	R1390	R1552	Q1388	ASP	E958	K776	R704	P635	I561					
ASP	R1391	R1552	Q1389	ASP	E958	K776	R704	P635	I561					
ASP	R1392	R1552	Q1390	ASP	E958	K776	R704	P635	I561					
ASP	R1393	R1552	Q1391	ASP	E958	K776	R704	P635	I561					
ASP	R1394	R1552	Q1392	ASP	E958	K776	R704	P635	I561					
ASP	R1395	R1552	Q1393	ASP	E958	K776	R704	P635	I561					
ASP	R1396	R1552	Q1394	ASP	E958	K776	R704	P635	I561					
ASP	R1397	R1552	Q1395	ASP	E958	K776	R704	P635	I561					
ASP	R1398	R1552	Q1396	ASP	E958	K776	R704	P635	I561					
ASP														



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	157272	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	0.741	Depositor
Minimum map value	-0.185	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.161	Depositor
Map size ( $\text{\AA}$ )	384.84, 384.84, 384.84	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.069, 1.069, 1.069	Depositor

## 5 Model quality

### 5.1 Standard geometry

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	0.28	0/16198	0.48	0/22023
1	B	0.28	0/16222	0.48	0/22055
All	All	0.28	0/32420	0.48	0/44078

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	468	0
1	B	15857	9380	15826	523	0
2	A	96	52	52	2	0
2	B	96	52	52	5	0
All	All	31882	18827	31739	970	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 15.

All (970) 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:292:ALA:HB2	1:B:322:ILE:HD11	1.36	1.08
1:A:164:SER:HB2	1:A:338:LEU:HD13	1.39	1.03
1:B:619:ALA:HB3	1:B:658:VAL:HG11	1.38	1.02
1:A:687:MET:HE2	1:A:739:LEU:HD11	1.38	1.02
1:A:725:SER:HA	1:A:728:ARG:HH12	1.24	1.02
1:A:640:PRO:HA	1:A:651:ILE:HG22	1.39	0.99
1:A:620:MET:HB3	1:A:677:THR:HG21	1.41	0.99
1:B:417:HIS:HA	1:B:420:LEU:HD13	1.44	0.98
1:A:2:GLU:HG2	1:A:235:LYS:HB2	1.48	0.95
1:B:716:SER:HB3	1:B:738:ASN:HA	1.50	0.94
1:B:1446:ILE:HG23	1:B:1474:LEU:HD12	1.50	0.92
1:A:5:VAL:HB	1:A:242:VAL:HG13	1.53	0.90
1:B:322:ILE:HG21	1:B:374:LEU:HD21	1.53	0.89
1:A:247:LEU:HD23	1:A:282:VAL:HG21	1.52	0.89
1:B:508:LEU:HD22	1:B:539:LEU:HD23	1.54	0.88
1:A:440:GLN:HG3	1:A:833:LEU:HD22	1.55	0.87
1:A:641:ALA:H	1:A:651:ILE:HA	1.39	0.86
1:B:13:LEU:HD22	1:B:329:MET:HE3	1.57	0.85
1:B:5:VAL:HB	1:B:242:VAL:HG13	1.55	0.85
1:A:54:LEU:HG	1:A:226:GLU:HG3	1.60	0.83
1:A:79:LEU:HD21	1:A:143:ARG:HG3	1.60	0.83
1:B:57:LEU:HD22	1:B:81:LEU:HD11	1.61	0.83
1:A:549:ILE:HD12	1:A:610:ILE:HB	1.60	0.83
1:B:499:MET:HE3	1:B:581:SER:HB3	1.60	0.82
1:B:193:LYS:HE2	1:B:195:ASN:HD22	1.45	0.82
1:B:468:ARG:HD2	1:B:485:VAL:HG21	1.61	0.81
1:B:622:ALA:N	1:B:673:LYS:O	2.14	0.81
1:B:274:ARG:HA	1:B:277:TYR:CE1	2.16	0.81
1:A:274:ARG:HA	1:A:277:TYR:CE1	2.16	0.81
1:B:78:GLN:HB3	1:B:188:ILE:HD12	1.61	0.80
1:A:9:MET:HE2	1:A:19:LEU:HD13	1.65	0.79
1:A:468:ARG:HD2	1:A:485:VAL:HG21	1.64	0.79
1:A:719:GLU:HA	1:A:722:TRP:CD1	2.18	0.79
1:B:39:ARG:HG2	1:B:53:LYS:HD2	1.63	0.78
1:B:549:ILE:HD11	1:B:611:LYS:HG3	1.65	0.78
1:B:33:VAL:HG12	1:B:50:ARG:HB3	1.66	0.78
1:B:491:PRO:HG2	1:B:756:ALA:HA	1.66	0.78
1:A:161:CYS:HB2	1:A:394:GLY:HA2	1.64	0.77
1:A:625:LEU:HD11	1:A:633:ARG:HD3	1.65	0.77
1:B:348:LEU:HD13	1:B:406:PRO:HB3	1.65	0.77
1:A:396:GLY:HA3	1:B:142:ASN:HD22	1.50	0.77
1:A:12:LYS:HD2	1:A:81:LEU:HD22	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:HIS:HB3	1:A:71:GLN:OE1	1.85	0.76
1:B:695:LEU:HD11	1:B:699:LYS:HE2	1.65	0.76
1:A:715:THR:O	1:A:744:LEU:N	2.17	0.76
1:A:1010:GLU:OE2	1:A:1019:ARG:NH2	2.18	0.76
1:B:719:GLU:HA	1:B:722:TRP:HE3	1.50	0.76
1:A:209:GLU:OE1	1:A:209:GLU:N	2.19	0.76
1:A:752:VAL:HB	1:A:775:LEU:HD11	1.67	0.76
1:A:124:PRO:HA	1:A:127:LEU:HD23	1.67	0.75
1:B:158:ASP:O	1:B:163:SER:HB3	1.85	0.75
1:B:1680:VAL:HG21	2:B:2601:NDP:H6N	1.68	0.75
1:B:1827:LYS:HZ1	1:B:1849:ILE:HG22	1.51	0.75
1:B:639:VAL:HG13	1:B:640:PRO:HD2	1.68	0.75
1:A:692:PRO:O	1:A:695:LEU:HG	1.86	0.75
1:A:657:PRO:HA	1:A:660:GLU:HG2	1.68	0.75
1:A:639:VAL:HG13	1:A:640:PRO:HD2	1.69	0.74
1:B:635:PRO:HD3	1:B:661:PHE:CD1	2.22	0.74
1:B:654:PRO:HB2	1:B:657:PRO:HD2	1.67	0.74
1:B:460:VAL:HG22	1:B:461:PRO:HD2	1.70	0.74
1:A:168:LEU:HD22	1:A:402:ILE:HD11	1.69	0.74
1:B:276:LEU:HD12	1:B:401:HIS:HB3	1.69	0.74
1:B:333:GLU:HB2	1:B:334:PRO:HD3	1.70	0.74
1:B:674:GLU:N	1:B:674:GLU:OE1	2.21	0.74
1:B:451:LEU:HD21	1:B:473:LEU:HD12	1.71	0.73
1:A:550:VAL:O	1:A:554:VAL:HG23	1.88	0.73
1:A:38:ARG:NH1	1:A:54:LEU:O	2.22	0.73
1:B:293:HIS:N	1:B:304:GLU:OE2	2.19	0.73
1:B:1031:ASP:OD2	1:B:1035:GLN:NE2	2.21	0.73
1:A:499:MET:HE1	1:A:552:SER:HB2	1.70	0.72
1:A:620:MET:HB3	1:A:677:THR:CG2	2.18	0.72
1:B:716:SER:CB	1:B:738:ASN:HA	2.19	0.72
1:A:277:TYR:CE2	1:A:284:PRO:HG3	2.25	0.72
1:A:363:ASN:HB3	1:A:366:ILE:HD13	1.71	0.72
1:A:84:GLU:O	1:A:88:GLU:HG3	1.89	0.71
1:A:127:LEU:O	1:B:202:ARG:NH1	2.23	0.71
1:B:79:LEU:HD21	1:B:143:ARG:HG3	1.70	0.71
1:B:597:GLU:OE1	1:B:597:GLU:N	2.22	0.71
1:A:429:ARG:NH1	1:A:464:ALA:O	2.23	0.71
1:A:549:ILE:HD11	1:A:611:LYS:HG2	1.72	0.71
1:B:1457:VAL:HG21	1:B:1471:CYS:HB3	1.71	0.71
1:B:662:VAL:O	1:B:666:ARG:HG2	1.91	0.71
1:A:6:ILE:HG12	1:A:233:LEU:HD21	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:SER:O	1:A:598:GLU:N	2.24	0.70
1:B:1244:GLU:O	1:B:1273:THR:OG1	2.08	0.70
1:A:784:LEU:O	1:A:785:MET:HG3	1.90	0.70
1:B:606:ARG:NH2	1:B:739:LEU:HD13	2.06	0.70
1:A:733:GLU:OE1	1:A:733:GLU:N	2.22	0.70
1:B:54:LEU:HD12	1:B:57:LEU:HD21	1.73	0.70
1:B:165:LEU:HD22	1:B:402:ILE:HD13	1.74	0.70
1:B:628:GLU:OE1	1:B:631:LYS:HD2	1.92	0.70
1:B:1588:ILE:HD13	1:B:1598:LEU:HD23	1.71	0.70
1:A:665:LEU:HB3	1:A:670:VAL:CG2	2.21	0.70
1:A:1410:ASP:OD1	1:A:1411:SER:N	2.24	0.70
1:B:708:ARG:NH2	1:B:714:SER:HB2	2.06	0.70
1:A:79:LEU:HD13	1:A:140:MET:HA	1.74	0.70
1:A:469:GLY:HA2	1:A:805:LEU:HD21	1.73	0.70
1:A:564:ILE:HD13	1:A:590:ALA:HB2	1.73	0.70
1:A:656:ALA:HB3	1:A:657:PRO:HD3	1.73	0.70
1:A:737:ASN:HA	1:A:740:VAL:CG2	2.21	0.70
1:B:623:VAL:HG12	1:B:625:LEU:HG	1.73	0.70
1:B:100:LEU:O	1:B:103:THR:OG1	2.10	0.70
1:A:492:LEU:HD12	1:A:757:VAL:O	1.91	0.69
1:B:769:ALA:O	1:B:773:ARG:HG2	1.92	0.69
1:A:423:LEU:HD12	1:A:424:LEU:H	1.57	0.69
1:A:584:GLU:HG3	1:A:712:TRP:HZ2	1.55	0.69
1:A:1278:GLN:OE1	1:A:1278:GLN:N	2.26	0.69
1:B:697:GLU:O	1:B:701:VAL:HG23	1.93	0.69
1:A:666:ARG:NH2	1:A:672:ALA:O	2.26	0.69
1:A:425:ARG:HB2	1:A:804:HIS:CD2	2.27	0.69
1:A:623:VAL:HG13	1:A:665:LEU:HD13	1.74	0.69
1:A:257:LYS:HE3	1:A:263:PHE:O	1.92	0.69
1:B:618:GLY:N	1:B:679:GLY:O	2.24	0.69
1:A:654:PRO:HB2	1:A:657:PRO:HD2	1.75	0.68
1:A:165:LEU:HD11	1:A:402:ILE:HD12	1.76	0.68
1:B:765:ALA:HB1	1:B:768:GLN:HG2	1.76	0.68
1:B:623:VAL:HG21	1:B:661:PHE:HE2	1.59	0.68
1:B:1837:GLU:N	1:B:1837:GLU:OE1	2.27	0.68
1:B:124:PRO:HA	1:B:127:LEU:HD23	1.76	0.68
1:B:724:SER:O	1:B:728:ARG:HG2	1.94	0.68
1:A:737:ASN:HA	1:A:740:VAL:HG22	1.76	0.68
1:B:277:TYR:CE2	1:B:284:PRO:HG3	2.29	0.68
1:A:503:TRP:CH2	1:A:506:MET:HA	2.29	0.67
1:A:831:SER:OG	1:A:832:PRO:HD3	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:LEU:HD22	1:B:366:ILE:HD13	1.77	0.67
1:B:708:ARG:HD3	1:B:727:ALA:O	1.92	0.67
1:B:440:GLN:HG3	1:B:833:LEU:HD22	1.76	0.67
1:B:654:PRO:HB2	1:B:657:PRO:CD	2.25	0.67
1:A:333:GLU:HB2	1:A:334:PRO:HD3	1.77	0.67
1:B:365:GLU:O	1:B:367:PRO:HD3	1.93	0.67
1:A:138:ALA:O	1:A:142:ASN:ND2	2.27	0.67
1:B:47:LEU:HD22	1:B:197:SER:HB3	1.77	0.67
1:B:540:SER:OG	1:B:545:THR:HG21	1.96	0.66
1:B:619:ALA:HB3	1:B:658:VAL:CG1	2.20	0.66
1:A:622:ALA:O	1:A:672:ALA:HA	1.96	0.66
1:A:725:SER:HA	1:A:728:ARG:NH1	2.05	0.66
1:A:504:ARG:HD2	1:A:541:THR:O	1.96	0.66
1:A:499:MET:HG3	1:A:553:PHE:CE1	2.31	0.66
1:A:522:ARG:NH1	1:A:596:GLN:OE1	2.29	0.66
1:B:506:MET:HG3	1:B:559:ILE:CD1	2.25	0.66
1:A:25:ASN:HB2	1:A:32:MET:HE1	1.77	0.66
1:B:620:MET:O	1:B:674:GLU:HB2	1.95	0.66
1:B:1195:GLN:O	1:B:1199:ALA:N	2.26	0.66
1:A:431:PRO:HG3	1:A:467:PHE:CE2	2.31	0.66
1:A:6:ILE:HA	1:A:233:LEU:HD23	1.78	0.65
1:B:1145:VAL:HG21	1:B:1356:ILE:HG12	1.77	0.65
1:A:15:GLU:OE2	1:A:38:ARG:NH2	2.29	0.65
1:B:259:GLN:OE1	1:B:259:GLN:N	2.29	0.65
1:A:706:LYS:O	1:A:729:THR:OG1	2.11	0.65
1:A:35:ASP:OD1	1:A:49:ARG:HB3	1.97	0.65
1:B:625:LEU:HD21	1:B:670:VAL:HG21	1.78	0.65
1:A:276:LEU:CD1	1:A:401:HIS:HB3	2.27	0.65
1:B:343:LYS:HZ3	1:B:354:ALA:HB3	1.62	0.65
1:B:485:VAL:HG22	1:B:805:LEU:O	1.96	0.65
1:B:51:SER:HA	1:B:223:CYS:SG	2.35	0.65
1:B:831:SER:OG	1:B:832:PRO:HD3	1.96	0.65
1:A:2:GLU:CG	1:A:235:LYS:HB2	2.25	0.65
1:A:625:LEU:CD1	1:A:633:ARG:HD3	2.27	0.65
1:B:661:PHE:CZ	1:B:665:LEU:HD21	2.32	0.65
1:A:168:LEU:HD22	1:A:402:ILE:CD1	2.26	0.65
1:A:606:ARG:HE	1:A:739:LEU:HD13	1.62	0.64
1:A:1145:VAL:HG21	1:A:1356:ILE:HG12	1.79	0.64
1:B:460:VAL:CG2	1:B:461:PRO:HD2	2.28	0.64
1:A:341:LEU:O	1:A:345:LEU:HG	1.98	0.64
1:B:602:ALA:O	1:B:606:ARG:HG3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:LEU:HD12	1:A:401:HIS:HB3	1.80	0.64
1:A:315:THR:HG22	1:A:315:THR:O	1.98	0.64
1:B:663:GLU:O	1:B:667:LYS:HG3	1.96	0.64
1:A:9:MET:HE2	1:A:19:LEU:CD1	2.27	0.64
1:B:165:LEU:HD22	1:B:402:ILE:CD1	2.28	0.64
1:A:138:ALA:CB	1:B:160:ALA:HB2	2.28	0.64
1:A:692:PRO:HA	1:A:695:LEU:CD2	2.28	0.63
1:B:380:PRO:O	1:B:381:LEU:HD23	1.98	0.63
1:A:1893:LEU:HD12	1:A:1916:SER:CB	2.29	0.63
1:B:290:ILE:O	1:B:322:ILE:HD12	1.98	0.63
1:B:431:PRO:HG3	1:B:467:PHE:CE1	2.34	0.63
1:B:706:LYS:N	1:B:729:THR:OG1	2.30	0.63
1:A:617:PRO:HA	1:A:679:GLY:O	1.97	0.63
1:A:437:LEU:HD22	1:A:454:LEU:HD21	1.81	0.63
1:B:542:ASP:OD2	1:B:544:SER:OG	2.17	0.63
1:A:732:ALA:O	1:A:736:VAL:HG23	1.99	0.63
1:B:182:ALA:CB	1:B:234:THR:HG22	2.29	0.63
1:B:719:GLU:HA	1:B:722:TRP:CE3	2.33	0.63
1:A:566:LEU:HD22	1:A:815:LEU:CD2	2.29	0.62
1:B:438:LEU:HD22	1:B:471:ALA:CB	2.29	0.62
1:A:293:HIS:N	1:A:304:GLU:OE2	2.23	0.62
1:A:620:MET:HA	1:A:652:SER:HA	1.80	0.62
1:B:276:LEU:CD1	1:B:401:HIS:HB3	2.28	0.62
1:A:203:LEU:HD12	1:B:132:MET:HE3	1.81	0.62
1:A:285:GLU:N	1:A:285:GLU:OE1	2.32	0.62
1:A:627:TRP:CZ3	1:A:640:PRO:HB2	2.34	0.62
1:A:754:GLU:HG3	1:A:778:SER:OG	1.99	0.62
1:B:33:VAL:CG1	1:B:50:ARG:HB3	2.29	0.62
1:A:557:THR:O	1:A:561:ILE:HG13	2.00	0.62
1:A:737:ASN:OD1	1:A:741:SER:HB3	2.00	0.62
1:B:291:GLU:HG2	1:B:340:ALA:HB1	1.81	0.62
1:B:326:LYS:HE3	1:B:331:HIS:CD2	2.35	0.62
1:B:333:GLU:CB	1:B:334:PRO:HD3	2.28	0.62
1:B:429:ARG:NH1	1:B:464:ALA:O	2.27	0.62
1:A:645:SER:HA	1:A:746:GLN:HB2	1.82	0.62
1:B:188:ILE:HG22	1:B:228:VAL:HG13	1.82	0.62
1:B:316:ARG:NH1	1:B:320:LEU:HD13	2.13	0.62
1:B:166:MET:HE1	1:B:251:THR:HG21	1.82	0.62
1:B:706:LYS:HB3	1:B:707:PRO:HD2	1.82	0.62
1:B:719:GLU:HG2	1:B:722:TRP:CZ3	2.35	0.62
1:A:6:ILE:HG12	1:A:233:LEU:CD2	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:LEU:HB2	1:A:630:CYS:HB2	1.82	0.61
1:A:772:LYS:HD3	1:A:781:ILE:HD13	1.81	0.61
1:A:1336:LEU:O	1:A:1405:ARG:NH1	2.32	0.61
1:B:325:THR:HB	1:B:343:LYS:HD3	1.81	0.61
1:B:659:PHE:O	1:B:663:GLU:HG3	1.99	0.61
1:B:1272:ALA:O	1:B:1294:GLN:NE2	2.33	0.61
1:A:189:ASN:ND2	1:A:334:PRO:HD2	2.15	0.61
1:A:549:ILE:HD11	1:A:611:LYS:CG	2.30	0.61
1:A:736:VAL:O	1:A:740:VAL:HG22	2.00	0.61
1:A:1411:SER:OG	1:A:1439:ARG:NH2	2.34	0.61
1:B:476:GLU:OE2	1:B:477:ARG:NH1	2.33	0.61
1:B:290:ILE:HG23	1:B:322:ILE:CD1	2.31	0.61
1:A:434:VAL:O	1:A:438:LEU:HG	2.01	0.61
1:B:293:HIS:O	1:B:326:LYS:HD2	2.00	0.61
1:B:544:SER:HA	1:B:547:ASP:CG	2.21	0.61
1:A:270:GLU:OE2	1:A:274:ARG:NH2	2.26	0.61
1:B:438:LEU:HD22	1:B:471:ALA:HB3	1.83	0.61
1:B:597:GLU:O	1:B:601:LEU:HG	2.00	0.61
1:A:1909:VAL:HG12	1:A:1911:LYS:H	1.65	0.61
1:A:25:ASN:HA	1:A:30:VAL:HG12	1.83	0.60
1:A:508:LEU:HD11	1:A:538:LEU:O	2.01	0.60
1:B:615:LEU:HD21	1:B:680:MET:CE	2.31	0.60
1:A:606:ARG:O	1:A:610:ILE:HG13	2.01	0.60
1:A:694:LEU:CD2	1:A:736:VAL:HG22	2.31	0.60
1:B:494:PHE:O	1:B:495:ILE:HD13	2.01	0.60
1:A:396:GLY:HA3	1:B:142:ASN:ND2	2.15	0.60
1:B:322:ILE:HG21	1:B:374:LEU:CD2	2.30	0.60
1:A:550:VAL:HG21	1:A:611:LYS:HE2	1.84	0.60
1:A:124:PRO:HA	1:A:127:LEU:CD2	2.32	0.60
1:A:215:PHE:CE1	1:A:305:LEU:HD11	2.36	0.60
1:B:544:SER:HA	1:B:547:ASP:OD2	2.01	0.60
1:B:719:GLU:HG2	1:B:722:TRP:CE3	2.37	0.60
1:A:633:ARG:HH22	1:A:664:GLN:HE21	1.47	0.60
1:B:166:MET:HE1	1:B:251:THR:CG2	2.31	0.60
1:B:765:ALA:HB1	1:B:768:GLN:CG	2.32	0.60
1:B:498:GLY:HA3	1:B:580:HIS:HD2	1.66	0.59
1:B:606:ARG:O	1:B:610:ILE:HG13	2.02	0.59
1:B:1021:LEU:HD11	1:B:1073:ALA:HB1	1.83	0.59
1:A:1617:VAL:HG12	1:A:1628:LEU:HD13	1.84	0.59
1:B:499:MET:CE	1:B:581:SER:HB3	2.32	0.59
1:A:423:LEU:HD12	1:A:424:LEU:N	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:689:ALA:O	1:B:692:PRO:HD2	2.03	0.59
1:A:713:LEU:HD22	1:A:722:TRP:CH2	2.38	0.59
1:B:495:ILE:HD12	1:B:578:VAL:HB	1.82	0.59
1:A:259:GLN:N	1:A:259:GLN:OE1	2.29	0.59
1:B:182:ALA:HB1	1:B:234:THR:HG22	1.82	0.59
1:B:290:ILE:HG23	1:B:322:ILE:HD12	1.85	0.59
1:B:580:HIS:CE1	1:B:743:VAL:HG11	2.37	0.59
1:B:737:ASN:HA	1:B:740:VAL:HG22	1.85	0.59
1:B:329:MET:HE1	1:B:332:PRO:HG3	1.85	0.59
1:B:588:GLY:HA3	1:B:594:LEU:HD12	1.85	0.59
1:B:695:LEU:O	1:B:699:LYS:HG2	2.03	0.59
1:B:703:ARG:HB2	1:B:704:GLU:OE1	2.03	0.59
1:A:2057:ALA:HB3	1:A:2105:VAL:HG22	1.85	0.59
1:B:692:PRO:HB2	1:B:693:PRO:CD	2.33	0.59
1:A:620:MET:HB2	1:A:652:SER:OG	2.02	0.58
1:A:1176:GLN:N	1:A:1176:GLN:OE1	2.36	0.58
1:B:635:PRO:HD2	1:B:638:VAL:HG21	1.85	0.58
1:B:1130:GLU:N	1:B:1130:GLU:OE1	2.34	0.58
1:A:155:ILE:HG22	1:A:157:LEU:HD12	1.86	0.58
1:A:517:ARG:O	1:A:521:LEU:HG	2.03	0.58
1:A:25:ASN:HB2	1:A:32:MET:CE	2.33	0.58
1:A:584:GLU:OE2	1:A:712:TRP:NE1	2.35	0.58
1:B:423:LEU:HD23	1:B:812:PRO:HB3	1.85	0.58
1:A:566:LEU:HD22	1:A:815:LEU:HD22	1.85	0.58
1:B:241:ARG:HH21	1:B:453:MET:HE2	1.69	0.58
1:B:288:GLU:O	1:B:288:GLU:HG2	2.03	0.58
1:B:615:LEU:HD21	1:B:680:MET:HE3	1.85	0.58
1:B:754:GLU:OE1	1:B:776:LYS:HD2	2.04	0.58
1:A:105:THR:HG23	1:A:182:ALA:C	2.24	0.58
1:A:440:GLN:HG3	1:A:833:LEU:CD2	2.30	0.58
1:A:524:ASP:OD1	1:A:533:LYS:HA	2.04	0.58
1:B:57:LEU:HD22	1:B:81:LEU:CD1	2.32	0.58
1:B:13:LEU:HD22	1:B:329:MET:CE	2.31	0.57
1:A:38:ARG:NH1	1:A:55:LYS:HA	2.19	0.57
1:A:1837:GLU:OE2	1:A:1841:ARG:NH2	2.37	0.57
1:A:1974:VAL:HG12	1:A:1994:PRO:HG3	1.86	0.57
1:B:645:SER:HB3	1:B:770:VAL:HG13	1.84	0.57
1:A:437:LEU:HD22	1:A:454:LEU:CD2	2.34	0.57
1:A:498:GLY:HA2	1:A:582:LEU:O	2.05	0.57
1:A:499:MET:CE	1:A:552:SER:HB2	2.32	0.57
1:A:1562:GLN:NE2	1:A:1607:ASP:OD1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2042:GLU:OE2	1:A:2059:GLN:NE2	2.37	0.57
1:B:610:ILE:HG23	1:B:680:MET:HE2	1.86	0.57
1:B:695:LEU:CD1	1:B:699:LYS:HE2	2.33	0.57
1:B:736:VAL:O	1:B:740:VAL:HG22	2.04	0.57
1:B:1198:LEU:O	1:B:1202:LEU:N	2.34	0.57
1:A:772:LYS:CE	1:A:781:ILE:HD13	2.35	0.57
1:B:1021:LEU:HD12	1:B:1074:GLN:O	2.03	0.57
1:A:21:GLU:O	1:A:25:ASN:ND2	2.37	0.57
1:A:247:LEU:CD2	1:A:282:VAL:HG21	2.29	0.57
1:B:718:PRO:HD2	1:B:721:GLN:NE2	2.19	0.57
1:A:645:SER:HA	1:A:746:GLN:CG	2.34	0.57
1:A:1786:LEU:HD21	1:B:1774:LEU:HB2	1.85	0.57
1:B:509:SER:O	1:B:512:ARG:HG3	2.04	0.57
1:A:235:LYS:CG	1:A:238:LEU:HD13	2.35	0.57
1:A:713:LEU:HD22	1:A:722:TRP:CZ3	2.40	0.57
1:B:580:HIS:ND1	1:B:743:VAL:HG11	2.20	0.57
1:B:645:SER:CB	1:B:648:THR:HG1	2.17	0.57
1:B:36:ASP:OD1	1:B:37:ASP:N	2.35	0.57
1:B:504:ARG:HA	1:B:546:PHE:CE2	2.40	0.57
1:B:1080:VAL:HG22	1:B:1087:THR:HG23	1.87	0.57
1:B:537:LEU:O	1:B:540:SER:OG	2.23	0.56
1:B:1680:VAL:HG21	2:B:2601:NDP:C6N	2.34	0.56
1:A:222:TYR:HD2	1:A:331:HIS:HB3	1.69	0.56
1:A:620:MET:HG3	1:A:651:ILE:O	2.05	0.56
1:B:322:ILE:HG22	1:B:375:GLN:O	2.04	0.56
1:B:550:VAL:O	1:B:554:VAL:HG23	2.04	0.56
1:B:726:LEU:HD12	1:B:727:ALA:N	2.19	0.56
1:B:787:LYS:HD3	1:B:788:ASP:CG	2.25	0.56
1:B:1486:VAL:HG13	1:B:1486:VAL:O	2.04	0.56
1:B:92:ASP:HA	1:B:830:ILE:HB	1.87	0.56
1:B:254:ASP:HB2	1:B:257:LYS:NZ	2.20	0.56
1:A:612:GLU:O	1:A:614:HIS:ND1	2.38	0.56
1:B:692:PRO:HB2	1:B:693:PRO:HD3	1.86	0.56
1:A:351:GLY:C	1:A:352:LEU:HD12	2.26	0.56
1:A:79:LEU:CD1	1:A:140:MET:HA	2.35	0.56
1:A:661:PHE:O	1:A:665:LEU:HG	2.05	0.56
1:B:74:THR:HG21	1:B:130:TYR:HE1	1.71	0.56
1:B:468:ARG:HD2	1:B:485:VAL:CG2	2.33	0.56
1:A:161:CYS:CB	1:A:394:GLY:HA2	2.35	0.56
1:A:499:MET:HG2	1:A:582:LEU:HD23	1.87	0.56
1:B:664:GLN:OE1	1:B:667:LYS:HD2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:ALA:HB2	1:A:322:ILE:HD11	1.86	0.56
1:A:495:ILE:HD12	1:A:771:LEU:HD21	1.86	0.56
1:B:542:ASP:OD1	1:B:543:GLU:N	2.39	0.56
1:B:1451:SER:OG	1:B:1453:VAL:HG13	2.06	0.56
1:A:189:ASN:HD22	1:A:334:PRO:HD2	1.69	0.56
1:A:737:ASN:O	1:A:741:SER:N	2.35	0.56
1:A:752:VAL:CB	1:A:775:LEU:HD11	2.35	0.56
1:B:105:THR:HB	1:B:150:PHE:CD1	2.41	0.56
1:A:635:PRO:HD3	1:A:661:PHE:CZ	2.41	0.55
1:B:79:LEU:O	1:B:83:LEU:HD13	2.06	0.55
1:B:72:ALA:O	1:B:80:ARG:NH1	2.39	0.55
1:B:1417:VAL:HG12	1:B:1417:VAL:O	2.06	0.55
1:B:1827:LYS:NZ	1:B:1849:ILE:HG22	2.21	0.55
1:A:1488:PRO:HA	1:A:1493:LEU:HD23	1.88	0.55
1:B:626:SER:HB2	1:B:629:GLU:HG3	1.89	0.55
1:B:654:PRO:HG3	1:B:686:PHE:CZ	2.42	0.55
1:B:706:LYS:O	1:B:729:THR:HA	2.07	0.55
1:A:93:GLY:O	1:A:240:ARG:HB2	2.06	0.55
1:B:63:SER:OG	1:B:429:ARG:NH2	2.38	0.55
1:B:128:VAL:HG21	1:B:130:TYR:CE1	2.41	0.55
1:B:656:ALA:HB3	1:B:657:PRO:HD3	1.88	0.55
1:A:79:LEU:HD21	1:A:143:ARG:CG	2.34	0.55
1:A:287:PHE:HZ	1:A:403:ILE:HD13	1.72	0.55
1:B:261:VAL:HG13	1:B:262:THR:HG23	1.88	0.55
1:B:1205:GLU:OE1	1:B:1209:LEU:HD12	2.06	0.55
1:A:68:HIS:CG	1:A:69:PRO:HD2	2.41	0.55
1:B:13:LEU:HB3	1:B:14:PRO:HD2	1.88	0.55
1:B:343:LYS:NZ	1:B:354:ALA:HB3	2.21	0.55
1:B:627:TRP:HE1	1:B:631:LYS:HE2	1.71	0.55
1:B:628:GLU:O	1:B:631:LYS:HB2	2.07	0.55
1:B:1233:GLU:OE1	1:B:1515:ARG:NH2	2.36	0.55
1:B:1889:ILE:HD11	1:B:1912:LEU:HD11	1.89	0.55
1:A:542:ASP:HB3	1:A:545:THR:HB	1.87	0.55
1:B:655:GLN:O	1:B:658:VAL:HG12	2.06	0.55
1:A:633:ARG:NH2	1:A:664:GLN:HG3	2.21	0.55
1:B:251:THR:HG23	1:B:399:ASN:O	2.07	0.55
1:B:721:GLN:OE1	1:B:721:GLN:N	2.35	0.55
1:A:1602:GLU:HB3	1:A:1650:VAL:HG23	1.89	0.55
1:B:1205:GLU:O	1:B:1209:LEU:N	2.39	0.55
1:B:71:GLN:HG3	1:B:75:MET:HE3	1.87	0.54
1:B:717:ILE:HD13	1:B:727:ALA:HB1	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:ASP:OD1	1:B:399:ASN:ND2	2.40	0.54
1:A:620:MET:CB	1:A:677:THR:HG21	2.27	0.54
1:B:786:LYS:HE3	1:B:789:HIS:HD2	1.72	0.54
1:A:211:THR:HG21	1:A:358:HIS:CE1	2.42	0.54
1:B:549:ILE:HD11	1:B:611:LYS:CG	2.35	0.54
1:B:642:CYS:CB	1:B:743:VAL:HB	2.38	0.54
1:B:1521:GLU:OE1	1:B:1521:GLU:N	2.38	0.54
1:B:322:ILE:CG2	1:B:374:LEU:HD21	2.32	0.54
1:B:687:MET:CE	1:B:690:ILE:HG13	2.38	0.54
1:A:64:PHE:HE1	1:A:464:ALA:HB1	1.73	0.54
1:A:105:THR:O	1:A:150:PHE:HB3	2.07	0.54
1:A:626:SER:O	1:A:630:CYS:N	2.33	0.54
1:B:417:HIS:O	1:B:422:ARG:NH2	2.40	0.54
1:B:715:THR:O	1:B:744:LEU:HG	2.08	0.54
1:B:732:ALA:O	1:B:736:VAL:HG23	2.08	0.54
1:B:1997:SER:O	1:B:2001:ASN:ND2	2.41	0.54
1:A:293:HIS:CE1	1:A:326:LYS:HE2	2.42	0.54
1:A:346:LEU:CD2	1:A:829:LEU:HD11	2.37	0.54
1:A:793:LEU:O	1:A:797:LEU:HG	2.08	0.54
1:B:23:TRP:CH2	1:B:347:SER:HA	2.41	0.54
1:B:124:PRO:HA	1:B:127:LEU:CD2	2.38	0.54
1:B:639:VAL:CG1	1:B:640:PRO:HD2	2.38	0.54
1:B:661:PHE:CE2	1:B:665:LEU:HD11	2.43	0.54
1:B:717:ILE:CD1	1:B:727:ALA:HB1	2.37	0.54
1:A:13:LEU:HD22	1:A:329:MET:HE1	1.89	0.54
1:B:497:SER:HB3	1:B:760:GLU:OE2	2.07	0.54
1:A:646:LYS:HG3	1:A:647:ASP:OD1	2.08	0.53
1:A:1200:GLN:HG2	1:A:1205:GLU:OE2	2.08	0.53
1:A:25:ASN:HA	1:A:30:VAL:CG1	2.38	0.53
1:A:1287:LEU:O	1:A:1292:VAL:HG22	2.08	0.53
1:B:133:VAL:HG12	1:B:133:VAL:O	2.08	0.53
1:B:664:GLN:O	1:B:667:LYS:HB2	2.09	0.53
1:B:1224:LEU:O	1:B:1228:LEU:HD13	2.08	0.53
1:A:121:SER:HB3	1:B:199:GLN:NE2	2.24	0.53
1:A:593:CYS:O	1:A:594:LEU:HD23	2.08	0.53
1:B:164:SER:HB3	1:B:338:LEU:HG	1.90	0.53
1:B:508:LEU:HD22	1:B:539:LEU:CD2	2.33	0.53
1:B:743:VAL:O	1:B:744:LEU:HD23	2.08	0.53
1:A:248:ASN:ND2	1:A:279:SER:OG	2.42	0.53
1:A:54:LEU:HD21	1:A:226:GLU:O	2.09	0.53
1:A:158:ASP:O	1:B:138:ALA:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:LYS:HB2	1:A:536:GLN:HB3	1.90	0.53
1:B:105:THR:HG23	1:B:182:ALA:C	2.28	0.53
1:B:508:LEU:HD21	1:B:538:LEU:C	2.28	0.53
1:B:721:GLN:O	1:B:724:SER:OG	2.16	0.53
1:B:898:THR:OG1	1:B:935:VAL:HG11	2.08	0.53
1:A:593:CYS:SG	1:A:594:LEU:HG	2.49	0.53
1:A:1267:GLN:OE1	1:A:1267:GLN:N	2.42	0.53
1:A:1286:GLU:OE1	1:A:1286:GLU:N	2.37	0.53
1:A:1486:VAL:O	1:A:1493:LEU:HD22	2.09	0.53
1:B:440:GLN:HG3	1:B:833:LEU:CD2	2.38	0.53
1:B:610:ILE:CG2	1:B:680:MET:HE2	2.39	0.53
1:A:138:ALA:HB3	1:B:160:ALA:HB2	1.91	0.53
1:A:368:ALA:HA	1:A:371:ASP:OD2	2.09	0.53
1:A:635:PRO:HG3	1:A:661:PHE:CG	2.44	0.53
1:B:301:ASP:HB2	1:B:302:PRO:HD3	1.91	0.53
1:A:550:VAL:HG22	1:A:608:GLN:HA	1.91	0.53
1:A:620:MET:HB2	1:A:652:SER:CB	2.39	0.53
1:B:191:LEU:O	1:B:192:LEU:HD12	2.09	0.53
1:B:257:LYS:HD2	1:B:263:PHE:O	2.09	0.53
1:A:161:CYS:HA	1:A:333:GLU:O	2.09	0.52
1:A:635:PRO:HD3	1:A:661:PHE:CE1	2.43	0.52
1:A:326:LYS:HE3	1:A:331:HIS:ND1	2.24	0.52
1:A:2034:TYR:O	1:A:2038:ASN:ND2	2.42	0.52
1:B:503:TRP:CD2	1:B:787:LYS:HG2	2.44	0.52
1:A:425:ARG:HE	1:A:812:PRO:HD2	1.74	0.52
1:A:550:VAL:CG2	1:A:608:GLN:HA	2.39	0.52
1:A:1535:THR:HG23	1:A:1535:THR:O	2.09	0.52
1:A:1555:GLN:N	1:A:1555:GLN:OE1	2.43	0.52
1:B:610:ILE:HD13	1:B:682:PHE:CE1	2.44	0.52
1:B:615:LEU:HD12	1:B:615:LEU:O	2.09	0.52
1:B:737:ASN:HA	1:B:740:VAL:CG2	2.39	0.52
1:A:249:ALA:CB	1:A:402:ILE:HG12	2.39	0.52
1:A:138:ALA:HB1	1:B:160:ALA:HB2	1.90	0.52
1:A:596:GLN:O	1:A:600:VAL:HG23	2.10	0.52
1:B:198:VAL:O	1:B:202:ARG:HG2	2.10	0.52
1:A:346:LEU:HD21	1:A:829:LEU:HD11	1.91	0.52
1:A:660:GLU:O	1:A:663:GLU:HG2	2.09	0.52
1:A:692:PRO:HA	1:A:695:LEU:HD21	1.91	0.52
1:A:693:PRO:O	1:A:697:GLU:HG2	2.09	0.52
1:A:1786:LEU:HG	1:B:1774:LEU:HB3	1.92	0.52
1:B:13:LEU:HB3	1:B:14:PRO:CD	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:LEU:HD13	1:B:402:ILE:HD13	1.92	0.52
1:B:468:ARG:NH1	1:B:807:GLY:HA2	2.25	0.52
1:A:249:ALA:HB2	1:A:402:ILE:HG12	1.92	0.52
1:A:1246:LEU:HD23	1:A:1320:ALA:HB1	1.92	0.52
1:B:305:LEU:HD22	1:B:366:ILE:CD1	2.40	0.52
1:B:504:ARG:NH2	1:B:541:THR:O	2.34	0.52
1:A:619:ALA:O	1:A:658:VAL:HG11	2.10	0.52
1:A:1784:ILE:HG13	1:A:1789:VAL:HG21	1.92	0.52
1:B:83:LEU:HD12	1:B:144:LEU:CD2	2.39	0.52
1:B:86:THR:HG23	1:B:184:ILE:HG21	1.93	0.52
1:B:542:ASP:OD1	1:B:544:SER:N	2.34	0.52
1:B:557:THR:O	1:B:561:ILE:HG13	2.10	0.52
1:B:782:ILE:HG22	1:B:782:ILE:O	2.09	0.52
1:A:333:GLU:HB2	1:A:334:PRO:CD	2.39	0.51
1:A:639:VAL:CG1	1:A:640:PRO:HD2	2.40	0.51
1:B:1014:GLU:N	1:B:1014:GLU:OE1	2.43	0.51
1:B:633:ARG:NH2	1:B:668:GLU:OE2	2.34	0.51
1:B:706:LYS:H	1:B:729:THR:HG1	1.57	0.51
1:A:1616:LEU:HD13	1:A:1650:VAL:HG22	1.92	0.51
1:A:1677:SER:HA	1:A:1708:LEU:HD11	1.93	0.51
1:A:348:LEU:HD22	1:A:406:PRO:HB3	1.92	0.51
1:A:765:ALA:HB2	1:A:783:PRO:HB3	1.92	0.51
1:A:1893:LEU:HD12	1:A:1916:SER:HB3	1.90	0.51
1:B:326:LYS:NZ	1:B:336:SER:HB2	2.26	0.51
1:B:714:SER:OG	1:B:717:ILE:HG12	2.10	0.51
1:B:1206:ARG:CZ	1:B:1209:LEU:HD13	2.40	0.51
1:A:166:MET:HE1	1:A:400:VAL:HG22	1.91	0.51
1:A:222:TYR:CD2	1:A:331:HIS:HB3	2.44	0.51
1:B:76:ASP:OD1	1:B:77:PRO:HD2	2.10	0.51
1:B:207:SER:HB3	1:B:221:GLY:C	2.31	0.51
1:B:560:GLN:O	1:B:564:ILE:HG13	2.11	0.51
1:A:242:VAL:HG23	1:A:822:PRO:HB3	1.92	0.51
1:A:934:GLU:OE1	1:A:936:ARG:NH2	2.44	0.51
1:B:527:VAL:HG12	1:B:527:VAL:O	2.10	0.51
1:B:1373:SER:O	1:B:1376:ALA:N	2.44	0.51
1:A:57:LEU:HD22	1:A:81:LEU:HD11	1.93	0.51
1:B:615:LEU:HD11	1:B:680:MET:HE3	1.93	0.51
1:B:25:ASN:CB	1:B:32:MET:HE3	2.40	0.51
1:A:81:LEU:O	1:A:85:VAL:HG23	2.10	0.51
1:A:424:LEU:HD12	1:A:455:ASN:OD1	2.11	0.51
1:A:579:GLY:HA3	1:A:584:GLU:OE1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:SER:HB3	1:B:199:GLN:HE21	1.76	0.50
1:A:657:PRO:HA	1:A:660:GLU:CG	2.38	0.50
1:A:694:LEU:HD22	1:A:736:VAL:HG22	1.92	0.50
1:A:1974:VAL:O	1:A:1974:VAL:HG13	2.10	0.50
1:B:524:ASP:OD1	1:B:534:VAL:HB	2.10	0.50
1:A:191:LEU:HD21	1:A:224:ARG:CB	2.42	0.50
1:A:347:SER:HB3	1:A:352:LEU:O	2.11	0.50
1:B:424:LEU:HD22	1:B:473:LEU:HD11	1.92	0.50
1:B:1647:SER:OG	1:B:1828:CYS:SG	2.70	0.50
1:B:493:TRP:CD2	1:B:576:GLY:HA3	2.45	0.50
1:B:501:THR:HG23	1:B:501:THR:O	2.12	0.50
1:A:165:LEU:HD23	1:A:400:VAL:HB	1.92	0.50
1:B:656:ALA:O	1:B:660:GLU:HG3	2.11	0.50
1:B:1879:THR:O	1:B:1907:ARG:NH1	2.42	0.50
1:B:1889:ILE:CD1	1:B:1912:LEU:HD11	2.41	0.50
1:A:52:GLY:O	1:A:225:SER:HA	2.12	0.50
1:B:47:LEU:HD21	1:B:197:SER:C	2.32	0.50
1:A:108:TRP:HB3	1:A:167:ALA:HB1	1.92	0.50
1:A:623:VAL:CG1	1:A:665:LEU:HD13	2.40	0.50
1:B:369:LEU:CD2	1:B:376:VAL:HG23	2.42	0.50
1:B:483:GLN:HG2	1:B:484:GLN:N	2.27	0.50
1:B:503:TRP:CE2	1:B:506:MET:HB3	2.47	0.50
1:B:2042:GLU:OE2	1:B:2059:GLN:NE2	2.45	0.50
1:A:165:LEU:CD1	1:A:402:ILE:HD12	2.42	0.50
1:B:589:TYR:HE2	1:B:596:GLN:HB2	1.76	0.50
1:B:1552:ARG:O	1:B:1555:GLN:NE2	2.45	0.50
1:B:534:VAL:O	1:B:538:LEU:HD13	2.11	0.49
1:A:203:LEU:HD12	1:B:132:MET:CE	2.40	0.49
1:B:743:VAL:C	1:B:744:LEU:HD23	2.33	0.49
1:B:991:TYR:OH	1:B:1007:GLY:N	2.44	0.49
1:B:1178:LEU:HD12	1:B:1214:LEU:HD11	1.94	0.49
1:A:235:LYS:HG2	1:A:238:LEU:HD13	1.94	0.49
1:B:209:GLU:N	1:B:209:GLU:OE1	2.45	0.49
1:B:1071:ASP:OD1	1:B:1072:LYS:N	2.39	0.49
1:B:1111:VAL:O	1:B:1111:VAL:HG13	2.12	0.49
1:A:625:LEU:CB	1:A:630:CYS:HB2	2.42	0.49
1:A:673:LYS:HD2	1:A:674:GLU:N	2.27	0.49
1:B:98:ASP:HA	1:B:101:ARG:HG3	1.93	0.49
1:B:758:VAL:HG11	1:B:771:LEU:HD23	1.93	0.49
1:A:549:ILE:HD12	1:A:610:ILE:CB	2.36	0.49
1:B:661:PHE:O	1:B:665:LEU:HG	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:691:ALA:HA	1:B:694:LEU:HB3	1.95	0.49
1:A:645:SER:HA	1:A:746:GLN:CB	2.43	0.49
1:A:1570:SER:OG	1:A:1646:ALA:O	2.29	0.49
1:B:305:LEU:HB2	1:B:366:ILE:HD13	1.94	0.49
1:B:618:GLY:H	1:B:679:GLY:C	2.15	0.49
1:B:766:LEU:HD23	1:B:766:LEU:O	2.12	0.49
1:A:120:LEU:HD12	1:A:135:CYS:SG	2.52	0.49
1:A:582:LEU:HD12	1:A:583:GLY:H	1.77	0.49
1:A:695:LEU:HD12	1:A:696:GLN:N	2.28	0.49
1:B:165:LEU:HD13	1:B:402:ILE:CD1	2.43	0.49
1:B:190:VAL:HA	1:B:226:GLU:HG2	1.93	0.49
1:B:1125:GLU:N	1:B:1125:GLU:OE1	2.46	0.49
1:A:946:VAL:O	1:A:953:VAL:HG12	2.12	0.49
1:B:222:TYR:HB3	1:B:295:THR:HG23	1.95	0.49
1:B:719:GLU:HA	1:B:722:TRP:HB2	1.95	0.49
1:B:754:GLU:O	1:B:755:HIS:HB2	2.13	0.49
1:B:1274:ASP:OD1	1:B:1275:ARG:N	2.46	0.49
1:A:1336:LEU:HD11	1:A:1340:GLY:HA3	1.95	0.49
1:B:325:THR:HG21	1:B:340:ALA:HA	1.93	0.49
1:B:510:LEU:CD2	1:B:793:LEU:HD13	2.42	0.49
1:A:627:TRP:CE3	1:A:643:HIS:HB2	2.48	0.48
1:A:628:GLU:O	1:A:631:LYS:HB3	2.13	0.48
1:A:1904:LEU:HB3	1:A:1909:VAL:HG21	1.94	0.48
1:A:114:SER:OG	1:A:137:ARG:NH1	2.46	0.48
1:B:621:ALA:O	1:B:651:ILE:HG12	2.13	0.48
1:A:82:LEU:HG	1:A:144:LEU:HD11	1.95	0.48
1:A:241:ARG:NH2	1:A:827:THR:O	2.46	0.48
1:A:619:ALA:O	1:A:658:VAL:HG21	2.13	0.48
1:B:114:SER:O	1:B:117:SER:OG	2.27	0.48
1:B:171:ALA:O	1:B:175:ILE:HG13	2.14	0.48
1:B:768:GLN:NE2	1:B:783:PRO:HB3	2.28	0.48
1:A:13:LEU:HD13	1:A:22:PHE:CZ	2.49	0.48
1:A:60:PHE:HB3	1:A:842:TRP:CD1	2.48	0.48
1:A:772:LYS:CD	1:A:781:ILE:HD13	2.43	0.48
1:B:168:LEU:HD21	1:B:246:ILE:CD1	2.43	0.48
1:B:283:ALA:HB1	1:B:285:GLU:OE1	2.14	0.48
1:B:617:PRO:HB2	1:B:655:GLN:OE1	2.12	0.48
1:A:606:ARG:NH2	1:A:739:LEU:HA	2.29	0.48
1:A:620:MET:CG	1:A:652:SER:HB2	2.44	0.48
1:A:1189:GLN:O	1:A:1193:ASN:ND2	2.45	0.48
1:B:601:LEU:HB3	1:B:701:VAL:HG13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:658:VAL:O	1:B:662:VAL:HG23	2.13	0.48
1:B:499:MET:HE2	1:B:582:LEU:N	2.29	0.48
1:A:30:VAL:O	1:A:30:VAL:HG13	2.13	0.48
1:A:229:VAL:HG12	1:A:338:LEU:HD23	1.94	0.48
1:B:8:GLY:O	1:B:231:VAL:HG13	2.13	0.48
1:B:86:THR:CG2	1:B:184:ILE:HG21	2.43	0.48
1:B:417:HIS:CA	1:B:420:LEU:HD13	2.32	0.48
1:B:621:ALA:HA	1:B:674:GLU:CB	2.44	0.48
1:B:717:ILE:HG13	1:B:717:ILE:O	2.13	0.48
1:B:437:LEU:HD22	1:B:454:LEU:HD22	1.96	0.48
1:A:692:PRO:HD2	1:A:693:PRO:HD2	1.95	0.48
1:A:1396:TYR:CE1	1:A:1398:SER:HB2	2.48	0.48
1:A:1970:ASN:C	1:A:1971:LEU:HD12	2.34	0.48
1:B:544:SER:O	1:B:547:ASP:HB2	2.13	0.48
1:A:190:VAL:C	1:A:191:LEU:HD12	2.34	0.48
1:A:663:GLU:O	1:A:667:LYS:HG2	2.13	0.48
1:A:761:ILE:HD13	1:A:784:LEU:HD12	1.95	0.48
1:A:766:LEU:HD12	1:A:766:LEU:O	2.14	0.48
1:A:1771:LYS:CE	1:A:1795:LEU:HD22	2.44	0.48
1:B:25:ASN:HB2	1:B:32:MET:CE	2.44	0.47
1:B:93:GLY:O	1:B:95:ILE:HD12	2.14	0.47
1:B:532:LEU:HD13	1:B:537:LEU:HD11	1.96	0.47
1:B:654:PRO:HG3	1:B:686:PHE:CE1	2.48	0.47
1:A:265:SER:O	1:A:269:GLN:HG3	2.14	0.47
1:A:624:GLY:N	1:A:671:PHE:O	2.47	0.47
1:B:71:GLN:HG3	1:B:75:MET:CE	2.44	0.47
1:B:247:LEU:HD21	1:B:405:ARG:HE	1.79	0.47
1:B:695:LEU:HD12	1:B:732:ALA:HB1	1.96	0.47
1:B:1928:GLN:OE1	1:B:1931:ARG:NH2	2.45	0.47
1:A:497:SER:OG	1:A:501:THR:HG21	2.14	0.47
1:A:593:CYS:HG	1:A:712:TRP:HZ3	1.60	0.47
1:A:1275:ARG:NH2	1:A:1321:ALA:O	2.47	0.47
1:B:247:LEU:HD11	1:B:405:ARG:HB2	1.96	0.47
1:B:627:TRP:NE1	1:B:631:LYS:HE2	2.28	0.47
1:A:6:ILE:HG23	1:A:231:VAL:CG1	2.44	0.47
1:A:13:LEU:HB3	1:A:14:PRO:HD2	1.96	0.47
1:A:420:LEU:HD22	1:A:512:ARG:HE	1.79	0.47
1:A:542:ASP:O	1:A:545:THR:HG22	2.15	0.47
1:B:7:ALA:O	1:B:241:ARG:HG3	2.13	0.47
1:B:621:ALA:HA	1:B:674:GLU:HB3	1.95	0.47
1:B:642:CYS:SG	1:B:743:VAL:HB	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1893:LEU:HD12	1:A:1916:SER:OG	2.14	0.47
1:A:661:PHE:CE2	1:A:665:LEU:HD11	2.50	0.47
1:B:159:THR:HG22	1:B:159:THR:O	2.14	0.47
1:B:215:PHE:HZ	1:B:292:ALA:HB3	1.80	0.47
1:B:740:VAL:HG23	1:B:741:SER:N	2.29	0.47
1:A:76:ASP:OD1	1:A:77:PRO:HD2	2.14	0.47
1:A:138:ALA:HB2	1:B:158:ASP:CG	2.35	0.47
1:A:186:GLY:HA2	1:A:229:VAL:O	2.14	0.47
1:A:623:VAL:HG12	1:A:625:LEU:H	1.79	0.47
1:A:1020:LEU:HD22	1:A:1032:THR:CG2	2.45	0.47
1:A:1128:LEU:HD21	1:A:1217:GLY:C	2.35	0.47
1:B:108:TRP:HB3	1:B:167:ALA:HB1	1.95	0.47
1:B:247:LEU:HD12	1:B:403:ILE:HG22	1.95	0.47
1:B:253:THR:HG22	1:B:255:GLY:H	1.80	0.47
1:B:322:ILE:HG23	1:B:376:VAL:HG22	1.96	0.47
1:B:340:ALA:O	1:B:344:VAL:HG23	2.15	0.47
1:B:694:LEU:O	1:B:698:LEU:HG	2.15	0.47
1:B:706:LYS:O	1:B:729:THR:OG1	2.26	0.47
1:A:363:ASN:HB3	1:A:366:ILE:CD1	2.40	0.47
1:A:466:PRO:HG2	1:A:467:PHE:HD1	1.79	0.47
1:A:635:PRO:HD3	1:A:661:PHE:CE2	2.49	0.47
1:A:658:VAL:O	1:A:662:VAL:HG23	2.15	0.47
1:B:862:TYR:CD1	1:B:894:ILE:HG23	2.50	0.47
1:A:247:LEU:HD23	1:A:282:VAL:CG2	2.36	0.47
1:A:290:ILE:HG23	1:A:290:ILE:O	2.15	0.47
1:A:431:PRO:HG3	1:A:467:PHE:CD2	2.50	0.47
1:A:690:ILE:O	1:A:690:ILE:HG22	2.14	0.47
1:A:825:ARG:HG2	1:A:825:ARG:HH11	1.78	0.47
1:A:891:TYR:OH	1:A:923:THR:HG22	2.14	0.47
1:A:1418:ASP:OD2	1:A:1446:ILE:N	2.45	0.47
1:A:58:SER:O	1:A:841:ALA:HA	2.14	0.47
1:A:550:VAL:HG22	1:A:608:GLN:CA	2.45	0.47
1:A:1134:LEU:HD13	1:A:1214:LEU:HD23	1.97	0.47
1:B:23:TRP:CZ3	1:B:347:SER:HA	2.50	0.47
1:B:165:LEU:CD2	1:B:402:ILE:HD13	2.45	0.47
1:B:348:LEU:HD11	1:B:406:PRO:HG3	1.96	0.47
1:B:801:GLY:O	1:B:804:HIS:HB3	2.15	0.47
1:A:119:ALA:O	1:A:122:ARG:NH1	2.44	0.46
1:B:43:GLY:O	1:B:46:GLY:N	2.37	0.46
1:A:47:LEU:HD13	1:A:197:SER:CB	2.46	0.46
1:A:215:PHE:HZ	1:A:292:ALA:HB3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:655:GLN:OE1	1:A:655:GLN:N	2.34	0.46
1:B:1846:GLY:HA3	2:B:2601:NDP:H61A	1.80	0.46
1:A:309:THR:HA	1:A:313:CYS:HB2	1.97	0.46
1:A:657:PRO:CA	1:A:660:GLU:HG2	2.41	0.46
1:A:1391:LEU:HD23	1:A:1391:LEU:O	2.16	0.46
1:B:120:LEU:HD12	1:B:135:CYS:SG	2.54	0.46
1:B:584:GLU:HG3	1:B:738:ASN:OD1	2.15	0.46
1:B:760:GLU:OE1	1:B:760:GLU:HA	2.15	0.46
1:B:1141:CYS:O	1:B:1145:VAL:HG23	2.16	0.46
1:B:123:ASP:OD1	1:B:123:ASP:N	2.49	0.46
1:B:254:ASP:HB2	1:B:257:LYS:HZ2	1.81	0.46
1:B:1270:TYR:HB3	1:B:1292:VAL:HG12	1.97	0.46
1:B:1909:VAL:HG11	1:B:1912:LEU:HD13	1.98	0.46
1:A:495:ILE:HD12	1:A:758:VAL:HG11	1.97	0.46
1:A:1414:PHE:CE2	1:A:1493:LEU:HD21	2.51	0.46
1:B:634:CYS:HB2	1:B:638:VAL:CG1	2.45	0.46
1:B:655:GLN:HA	1:B:658:VAL:HG12	1.97	0.46
1:B:1110:GLN:NE2	1:B:2085:PRO:O	2.48	0.46
1:A:545:THR:HG23	1:A:546:PHE:CD1	2.51	0.46
1:A:767:LEU:HB3	1:A:771:LEU:CD1	2.46	0.46
1:B:132:MET:HB3	1:B:132:MET:HE2	1.81	0.46
1:B:549:ILE:HG13	1:B:550:VAL:N	2.30	0.46
1:A:645:SER:HA	1:A:746:GLN:NE2	2.31	0.46
1:A:719:GLU:HA	1:A:722:TRP:NE1	2.31	0.46
1:A:1325:PRO:O	1:A:1329:LEU:HD13	2.16	0.46
1:A:1973:VAL:HG12	2:A:2602:NDP:H52A	1.98	0.46
1:B:25:ASN:HB2	1:B:32:MET:HE3	1.98	0.46
1:A:147:PHE:HD2	1:A:148:PHE:CE2	2.34	0.46
1:B:93:GLY:O	1:B:240:ARG:HB2	2.16	0.46
1:A:287:PHE:O	1:A:316:ARG:NH2	2.49	0.46
1:B:83:LEU:HD12	1:B:144:LEU:HD21	1.96	0.46
1:B:168:LEU:HD21	1:B:246:ILE:HD13	1.97	0.46
1:B:504:ARG:HD2	1:B:543:GLU:OE1	2.14	0.46
1:A:114:SER:OG	1:A:137:ARG:HB2	2.15	0.46
1:A:198:VAL:O	1:A:202:ARG:HG2	2.16	0.46
1:B:212:CYS:SG	1:B:222:TYR:HA	2.55	0.46
1:A:13:LEU:HB3	1:A:14:PRO:CD	2.45	0.45
1:A:468:ARG:CD	1:A:485:VAL:HG21	2.42	0.45
1:A:1130:GLU:OE1	1:A:1130:GLU:N	2.45	0.45
1:A:1725:ASP:OD1	1:A:1726:THR:N	2.47	0.45
1:B:494:PHE:CE1	1:B:759:LEU:HD12	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:642:CYS:HB3	1:B:743:VAL:HB	1.97	0.45
1:B:720:ALA:HB3	1:B:721:GLN:OE1	2.16	0.45
1:A:541:THR:O	1:A:541:THR:HG22	2.15	0.45
1:A:655:GLN:O	1:A:659:PHE:HD2	1.98	0.45
1:A:923:THR:HG23	1:A:923:THR:O	2.16	0.45
1:A:1788:ASN:O	1:A:1789:VAL:HG23	2.15	0.45
1:B:157:LEU:O	1:B:157:LEU:HD12	2.16	0.45
1:B:235:LYS:HE3	1:B:237:SER:OG	2.16	0.45
1:B:431:PRO:HG3	1:B:467:PHE:CD1	2.51	0.45
1:B:532:LEU:HD22	1:B:551:HIS:CD2	2.52	0.45
1:B:665:LEU:O	1:B:669:GLY:N	2.49	0.45
1:B:1486:VAL:HG23	1:B:1493:LEU:HB2	1.98	0.45
1:A:137:ARG:O	1:A:140:MET:HG2	2.15	0.45
1:A:173:GLN:NE2	1:B:179:GLN:OE1	2.50	0.45
1:A:292:ALA:CB	1:A:322:ILE:HD11	2.46	0.45
1:A:523:SER:O	1:A:527:VAL:HG22	2.16	0.45
1:A:569:CYS:SG	1:A:814:ALA:HB1	2.57	0.45
1:A:775:LEU:HG	1:A:779:CYS:SG	2.56	0.45
1:B:81:LEU:O	1:B:85:VAL:HG23	2.16	0.45
1:B:490:ARG:HH22	1:B:780:THR:HG23	1.80	0.45
1:B:623:VAL:HG21	1:B:661:PHE:CE2	2.46	0.45
1:B:1371:ILE:O	1:B:1372:LEU:HD12	2.16	0.45
1:B:56:ASP:OD1	1:B:57:LEU:N	2.49	0.45
1:B:378:ASP:OD1	1:B:379:GLN:N	2.49	0.45
1:B:879:THR:C	1:B:880:LEU:HD12	2.37	0.45
1:A:60:PHE:HB3	1:A:842:TRP:NE1	2.31	0.45
1:A:162:SER:OG	1:A:394:GLY:N	2.49	0.45
1:A:388:VAL:HG12	1:A:389:GLY:N	2.32	0.45
1:B:523:SER:O	1:B:527:VAL:HG23	2.17	0.45
1:B:687:MET:HA	1:B:690:ILE:HG12	1.99	0.45
1:A:52:GLY:HA3	1:A:225:SER:OG	2.16	0.45
1:A:95:ILE:HD12	1:A:232:LEU:HD21	1.97	0.45
1:A:538:LEU:HD23	1:A:546:PHE:HZ	1.82	0.45
1:B:566:LEU:HD22	1:B:815:LEU:HD22	1.99	0.45
1:A:52:GLY:HA3	1:A:225:SER:CB	2.46	0.45
1:A:1527:PRO:HB2	1:A:1872:LEU:HD12	1.99	0.45
1:A:1561:ALA:HB1	1:A:1627:LEU:HD11	1.98	0.45
1:B:25:ASN:HB3	1:B:32:MET:HE3	1.98	0.45
1:B:492:LEU:HD12	1:B:757:VAL:O	2.16	0.45
1:B:661:PHE:CD2	1:B:665:LEU:HD11	2.52	0.45
1:B:717:ILE:HD13	1:B:727:ALA:CB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:LEU:HD21	1:A:224:ARG:HB3	1.99	0.45
1:A:217:THR:HG22	1:A:364:PRO:HD3	1.99	0.45
1:A:273:ILE:O	1:A:277:TYR:CD1	2.70	0.45
1:A:506:MET:HG2	1:A:546:PHE:HE2	1.82	0.45
1:A:633:ARG:HH22	1:A:664:GLN:NE2	2.15	0.45
1:B:166:MET:CE	1:B:251:THR:HG21	2.45	0.45
1:A:548:ASP:HB3	1:A:551:HIS:ND1	2.32	0.45
1:A:635:PRO:HD3	1:A:661:PHE:CD1	2.52	0.45
1:A:694:LEU:HD13	1:A:739:LEU:HD23	1.98	0.45
1:A:765:ALA:CB	1:A:783:PRO:HB3	2.47	0.45
1:B:157:LEU:HD13	1:B:159:THR:OG1	2.16	0.45
1:B:368:ALA:HB1	1:B:374:LEU:HB3	1.98	0.45
1:B:1389:VAL:CG2	1:B:1501:LEU:HD11	2.47	0.45
1:A:289:TYR:HE1	1:A:291:GLU:HB2	1.83	0.45
1:A:937:LEU:C	1:A:938:LEU:HD12	2.37	0.45
1:B:752:VAL:O	1:B:776:LYS:NZ	2.29	0.45
1:A:816:PHE:HB3	1:A:817:PRO:CD	2.47	0.44
1:B:246:ILE:HG12	1:B:404:LEU:HD21	1.97	0.44
1:B:327:SER:HB3	1:B:356:ASN:OD1	2.17	0.44
1:B:1078:VAL:HG23	1:B:1089:ALA:HB2	1.98	0.44
1:B:369:LEU:HD21	1:B:376:VAL:HG23	1.98	0.44
1:A:12:LYS:CD	1:A:81:LEU:HD22	2.44	0.44
1:A:67:VAL:HG11	1:A:75:MET:CE	2.47	0.44
1:A:293:HIS:HB3	1:A:304:GLU:OE1	2.17	0.44
1:A:542:ASP:OD1	1:A:543:GLU:N	2.50	0.44
1:A:627:TRP:N	1:A:649:VAL:HG21	2.32	0.44
1:A:1942:SER:O	1:A:1943:THR:OG1	2.16	0.44
1:A:1125:GLU:N	1:A:1125:GLU:OE1	2.50	0.44
1:A:1275:ARG:O	1:A:1296:GLN:NE2	2.47	0.44
1:B:160:ALA:O	1:B:161:CYS:HB3	2.18	0.44
1:B:682:PHE:HB3	1:B:683:HIS:ND1	2.33	0.44
1:A:168:LEU:HD21	1:A:246:ILE:HD13	1.98	0.44
1:B:767:LEU:O	1:B:771:LEU:HD13	2.17	0.44
1:B:1535:THR:HG22	1:B:1544:ILE:HD13	1.99	0.44
1:A:165:LEU:HG	1:A:400:VAL:CG1	2.47	0.44
1:A:1020:LEU:HD22	1:A:1032:THR:HG22	1.98	0.44
1:B:332:PRO:O	1:B:336:SER:HB3	2.17	0.44
1:B:1286:GLU:OE2	1:B:1289:GLN:NE2	2.50	0.44
1:A:210:GLY:O	1:A:223:CYS:HB3	2.18	0.44
1:A:580:HIS:CD2	1:A:743:VAL:HG11	2.52	0.44
1:B:579:GLY:O	1:B:715:THR:HG21	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:641:ALA:N	1:A:650:THR:O	2.51	0.44
2:A:2601:NDP:P2B	2:A:2601:NDP:HO3A	2.41	0.44
1:B:193:LYS:CE	1:B:195:ASN:HD22	2.24	0.44
1:A:188:ILE:HG22	1:A:228:VAL:HG13	2.00	0.44
1:B:14:PRO:CD	1:B:329:MET:HE3	2.48	0.44
1:B:622:ALA:O	1:B:672:ALA:HA	2.18	0.44
1:B:740:VAL:HG23	1:B:741:SER:H	1.82	0.44
1:B:2033:ASN:OD1	1:B:2034:TYR:N	2.51	0.44
1:A:105:THR:HA	1:A:182:ALA:O	2.17	0.43
1:A:737:ASN:CA	1:A:740:VAL:HG22	2.45	0.43
1:A:740:VAL:HG23	1:A:741:SER:N	2.33	0.43
1:A:1973:VAL:HG23	1:A:2034:TYR:HE1	1.83	0.43
1:B:293:HIS:HB3	1:B:304:GLU:OE1	2.18	0.43
1:B:615:LEU:HD11	1:B:680:MET:CE	2.48	0.43
1:B:719:GLU:HG2	1:B:722:TRP:HZ3	1.83	0.43
1:B:1902:GLN:OE1	1:B:1932:TRP:NE1	2.47	0.43
1:A:76:ASP:O	1:A:80:ARG:HG3	2.17	0.43
1:A:160:ALA:O	1:A:161:CYS:HB2	2.18	0.43
1:A:692:PRO:CD	1:A:693:PRO:HD2	2.48	0.43
1:A:466:PRO:HG2	1:A:467:PHE:CD1	2.54	0.43
1:A:499:MET:HG3	1:A:553:PHE:HE1	1.82	0.43
1:A:612:GLU:HA	1:A:614:HIS:CE1	2.52	0.43
1:A:685:TYR:O	1:A:688:GLU:HB3	2.18	0.43
1:A:706:LYS:HB3	1:A:707:PRO:HD2	2.00	0.43
1:A:1651:VAL:HG23	1:A:1652:TYR:N	2.33	0.43
1:B:680:MET:HB3	1:B:682:PHE:CE1	2.53	0.43
1:B:1029:PHE:O	1:B:1032:THR:OG1	2.30	0.43
1:B:164:SER:OG	1:B:335:ALA:HA	2.18	0.43
1:B:165:LEU:HB3	1:B:400:VAL:HG11	2.00	0.43
1:B:685:TYR:O	1:B:688:GLU:HG3	2.18	0.43
1:A:908:GLU:OE1	1:A:908:GLU:N	2.52	0.43
1:A:687:MET:HE2	1:A:739:LEU:CD1	2.28	0.43
1:B:1242:VAL:HG13	1:B:1270:TYR:HA	2.00	0.43
1:A:229:VAL:HG11	1:A:338:LEU:HB3	1.99	0.43
1:A:430:THR:OG1	1:A:431:PRO:HD2	2.18	0.43
1:A:990:VAL:HG13	1:A:1039:LEU:CD1	2.48	0.43
1:B:248:ASN:OD1	1:B:249:ALA:N	2.48	0.43
1:B:499:MET:HA	1:B:556:LEU:CD2	2.48	0.43
1:B:1319:VAL:HG12	1:B:1319:VAL:O	2.18	0.43
1:B:1571:LEU:CD2	1:B:1622:LEU:HD11	2.48	0.43
1:A:325:THR:HG21	1:A:340:ALA:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:PRO:HG3	1:A:661:PHE:HB2	2.00	0.43
1:B:1568:TYR:HB3	1:B:1853:VAL:HG11	2.00	0.43
1:A:138:ALA:HB2	1:B:158:ASP:OD1	2.18	0.43
1:A:1786:LEU:HD11	1:B:1775:SER:HA	2.01	0.43
1:A:2020:SER:OG	1:A:2021:SER:N	2.51	0.43
1:B:205:MET:O	1:B:221:GLY:HA3	2.19	0.43
1:B:771:LEU:HB3	1:B:781:ILE:HD11	2.00	0.43
1:B:1366:GLN:O	1:B:1369:GLN:N	2.52	0.43
1:A:68:HIS:CD2	1:A:69:PRO:HD2	2.54	0.43
1:A:1785:PHE:HB2	1:B:1774:LEU:HD22	2.00	0.43
1:B:11:GLY:HA2	1:B:85:VAL:HG13	2.00	0.43
1:B:59:ARG:HD2	1:B:838:HIS:HB3	2.00	0.43
1:B:60:PHE:CD1	1:B:80:ARG:HB3	2.54	0.43
1:A:1753:LEU:HD13	1:A:1773:ASP:OD2	2.18	0.42
1:B:10:SER:OG	1:B:831:SER:HB2	2.19	0.42
1:B:90:ILE:HG12	1:B:184:ILE:HD11	2.00	0.42
1:B:549:ILE:CD1	1:B:611:LYS:HG3	2.42	0.42
1:A:698:LEU:HB3	1:A:732:ALA:HB1	2.01	0.42
1:A:1826:LEU:HD12	1:A:1826:LEU:N	2.34	0.42
1:B:506:MET:HG3	1:B:559:ILE:HD11	2.00	0.42
1:A:315:THR:O	1:A:315:THR:CG2	2.65	0.42
1:B:723:HIS:HB2	1:B:728:ARG:NH2	2.34	0.42
1:B:2020:SER:OG	1:B:2021:SER:N	2.53	0.42
1:B:2097:LEU:C	1:B:2097:LEU:HD23	2.40	0.42
1:A:64:PHE:CE1	1:A:464:ALA:HB1	2.53	0.42
1:A:288:GLU:HG2	1:A:288:GLU:O	2.18	0.42
1:A:506:MET:O	1:A:538:LEU:HD22	2.19	0.42
1:A:772:LYS:NZ	1:A:781:ILE:HD13	2.34	0.42
1:A:1446:ILE:HG21	1:A:1486:VAL:HG21	2.02	0.42
1:B:635:PRO:HD2	1:B:638:VAL:CG2	2.49	0.42
1:A:155:ILE:HG23	1:B:157:LEU:HB2	2.02	0.42
1:A:492:LEU:HB2	1:A:808:ILE:HD13	2.01	0.42
1:A:745:PHE:CE2	1:A:749:LEU:HD21	2.54	0.42
1:A:1287:LEU:O	1:A:1290:HIS:O	2.38	0.42
1:B:70:LYS:HE3	1:B:130:TYR:OH	2.20	0.42
1:B:325:THR:HG21	1:B:340:ALA:CA	2.49	0.42
1:B:1883:ALA:O	1:B:1911:LYS:NZ	2.53	0.42
1:A:1134:LEU:CD1	1:A:1214:LEU:HD23	2.50	0.42
1:B:78:GLN:CB	1:B:188:ILE:HD12	2.41	0.42
1:B:90:ILE:CG1	1:B:184:ILE:HD11	2.50	0.42
1:B:329:MET:SD	1:B:339:ALA:HB1	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:646:LYS:HD2	1:B:646:LYS:HA	1.83	0.42
1:B:765:ALA:HB2	1:B:783:PRO:HB3	2.00	0.42
1:B:1019:ARG:HH12	1:B:1069:LEU:HD13	1.85	0.42
1:B:1120:THR:HG21	1:B:1517:PHE:CE2	2.55	0.42
1:A:691:ALA:O	1:A:695:LEU:N	2.33	0.42
1:A:754:GLU:O	1:A:755:HIS:HB2	2.18	0.42
1:B:65:PHE:HA	1:B:147:PHE:CE1	2.54	0.42
1:B:391:ASN:HB2	1:B:393:PHE:CZ	2.55	0.42
1:B:1593:THR:HG21	1:B:1906:GLN:HG2	2.02	0.42
1:A:550:VAL:HG22	1:A:608:GLN:N	2.35	0.42
1:A:728:ARG:HB2	1:A:728:ARG:CZ	2.50	0.42
1:A:752:VAL:CG1	1:A:775:LEU:HD11	2.50	0.42
1:A:816:PHE:HB3	1:A:817:PRO:HD2	2.02	0.42
1:A:993:GLU:O	1:A:997:ARG:HG2	2.19	0.42
1:B:391:ASN:HB3	1:B:401:HIS:HD2	1.85	0.42
1:B:443:ARG:CZ	1:B:443:ARG:HB3	2.50	0.42
1:B:510:LEU:HD23	1:B:510:LEU:HA	1.86	0.42
1:B:1846:GLY:HA3	2:B:2601:NDP:N6A	2.35	0.42
1:B:270:GLU:HG2	1:B:274:ARG:HH12	1.84	0.42
1:B:579:GLY:HA3	1:B:587:CYS:SG	2.59	0.42
1:B:786:LYS:HG2	1:B:787:LYS:N	2.35	0.42
1:B:889:THR:HG21	1:B:1030:MET:HB3	2.01	0.42
1:B:991:TYR:CZ	1:B:1006:GLN:HA	2.55	0.42
1:B:1389:VAL:HG22	1:B:1501:LEU:HD11	2.02	0.42
1:A:38:ARG:HH12	1:A:55:LYS:HA	1.84	0.42
1:A:1237:SER:OG	1:A:1238:LEU:N	2.53	0.42
1:A:1922:THR:HG22	1:A:1923:GLY:N	2.35	0.42
1:B:56:ASP:O	1:B:57:LEU:HD23	2.20	0.42
1:B:623:VAL:CG2	1:B:651:ILE:HD13	2.49	0.42
1:B:745:PHE:HE1	1:B:749:LEU:HD11	1.85	0.42
1:B:1313:LEU:HD22	1:B:1342:LEU:CD1	2.49	0.42
1:B:1366:GLN:HG3	1:B:1369:GLN:H	1.84	0.42
1:A:1250:GLY:O	1:A:1316:ASN:ND2	2.53	0.41
1:B:50:ARG:NH2	1:B:211:THR:OG1	2.53	0.41
1:B:497:SER:OG	1:B:501:THR:HG21	2.19	0.41
1:B:498:GLY:HA2	1:B:580:HIS:O	2.20	0.41
1:B:2063:ILE:HG12	2:B:2602:NDP:C7N	2.50	0.41
1:A:132:MET:HE2	1:B:200:PHE:CZ	2.54	0.41
1:A:293:HIS:CD2	1:A:295:THR:HG23	2.54	0.41
1:A:490:ARG:NH1	1:A:806:SER:HB3	2.35	0.41
1:A:502:GLN:OE1	1:A:502:GLN:N	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:627:TRP:O	1:A:631:LYS:HB2	2.19	0.41
1:B:391:ASN:HB2	1:B:393:PHE:CE1	2.54	0.41
1:B:515:ARG:HB2	1:B:566:LEU:HD23	2.01	0.41
1:B:745:PHE:CE1	1:B:749:LEU:HD11	2.55	0.41
1:A:325:THR:HG21	1:A:340:ALA:CA	2.50	0.41
1:A:408:THR:O	1:A:410:PRO:HD3	2.21	0.41
1:A:533:LYS:HB2	1:A:536:GLN:CB	2.51	0.41
1:A:638:VAL:HG12	1:A:639:VAL:N	2.35	0.41
1:A:938:LEU:HD23	1:B:945:GLU:HB2	2.01	0.41
1:B:6:ILE:HG23	1:B:231:VAL:CG1	2.51	0.41
1:A:675:VAL:O	1:A:677:THR:HG23	2.20	0.41
1:A:1771:LYS:HE3	1:A:1795:LEU:HD22	2.03	0.41
1:B:10:SER:HB2	1:B:831:SER:HB3	2.02	0.41
1:B:274:ARG:HA	1:B:277:TYR:CD1	2.54	0.41
1:B:351:GLY:O	1:B:383:VAL:HG23	2.21	0.41
1:B:1223:ALA:HB1	1:B:1392:LYS:CD	2.50	0.41
1:B:1714:GLN:OE1	1:B:1714:GLN:N	2.52	0.41
1:A:773:ARG:HA	1:A:773:ARG:HD3	1.91	0.41
1:B:1432:LEU:HD12	1:B:1980:LEU:HD23	2.02	0.41
1:A:665:LEU:O	1:A:670:VAL:HG22	2.21	0.41
1:A:692:PRO:N	1:A:693:PRO:HD2	2.35	0.41
1:A:1232:VAL:HG22	1:A:1240:MET:SD	2.61	0.41
1:B:4:VAL:O	1:B:245:THR:HG23	2.21	0.41
1:B:322:ILE:HG23	1:B:322:ILE:O	2.21	0.41
1:B:935:VAL:HG13	1:B:935:VAL:O	2.21	0.41
1:B:18:ASN:ND2	1:B:832:PRO:HB3	2.36	0.41
1:B:205:MET:HB3	1:B:222:TYR:CE1	2.55	0.41
1:B:625:LEU:HB2	1:B:630:CYS:SG	2.60	0.41
1:B:654:PRO:HG3	1:B:686:PHE:HZ	1.86	0.41
1:B:683:HIS:HA	1:B:739:LEU:O	2.21	0.41
1:B:2062:ALA:HB3	1:B:2085:PRO:HA	2.02	0.41
1:A:453:MET:HE2	1:A:453:MET:HB3	1.82	0.41
1:A:635:PRO:HG3	1:A:661:PHE:CB	2.50	0.41
1:A:692:PRO:HB2	1:A:693:PRO:HD3	2.02	0.41
1:B:139:MET:O	1:B:143:ARG:HG2	2.21	0.41
1:B:589:TYR:CE2	1:B:596:GLN:HB2	2.55	0.41
1:B:1485:GLU:OE1	1:B:1485:GLU:N	2.39	0.41
1:A:301:ASP:HB2	1:A:302:PRO:HD3	2.02	0.41
1:A:620:MET:O	1:A:675:VAL:HG12	2.21	0.41
1:A:673:LYS:HD2	1:A:674:GLU:H	1.85	0.41
1:A:991:TYR:CZ	1:A:1006:GLN:HA	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1795:LEU:HD12	1:B:1786:LEU:O	2.21	0.41
1:B:608:GLN:O	1:B:612:GLU:HG3	2.21	0.41
1:B:912:VAL:HG22	1:B:913:VAL:N	2.35	0.41
1:B:1888:ILE:HG21	1:B:1955:LEU:HD21	2.02	0.41
1:A:168:LEU:HD23	1:A:168:LEU:O	2.20	0.41
1:A:1261:SER:N	1:A:1262:PRO:CD	2.84	0.41
1:A:2018:VAL:HG11	1:A:2041:MET:HB3	2.03	0.41
1:B:276:LEU:HD23	1:B:276:LEU:HA	1.88	0.41
1:B:438:LEU:HD22	1:B:471:ALA:HB2	1.99	0.41
1:B:707:PRO:HA	1:B:728:ARG:O	2.21	0.41
1:B:752:VAL:HB	1:B:775:LEU:CD2	2.51	0.41
1:B:981:GLU:N	1:B:982:PRO:HD3	2.35	0.41
1:A:1300:ALA:O	1:A:1331:ASN:ND2	2.54	0.40
1:B:47:LEU:CD2	1:B:197:SER:HB3	2.46	0.40
1:B:567:LEU:HA	1:B:570:MET:HE2	2.03	0.40
1:B:692:PRO:CB	1:B:693:PRO:CD	2.99	0.40
1:A:83:LEU:HD23	1:A:144:LEU:CD2	2.51	0.40
1:A:189:ASN:HB2	1:A:334:PRO:HG2	2.04	0.40
1:A:469:GLY:CA	1:A:805:LEU:HD21	2.45	0.40
1:A:660:GLU:HA	1:A:663:GLU:HG2	2.03	0.40
1:B:493:TRP:CE2	1:B:576:GLY:HA3	2.57	0.40
1:B:899:LEU:HD22	1:B:958:VAL:HG22	2.04	0.40
1:B:1616:LEU:CD1	1:B:1650:VAL:HG22	2.51	0.40
1:A:698:LEU:HD23	1:A:698:LEU:HA	1.92	0.40
1:B:706:LYS:N	1:B:729:THR:HG1	2.14	0.40
1:B:1190:LEU:O	1:B:1195:GLN:NE2	2.54	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%)	1994 (97%)	66 (3%)	0	100	100
1	B	2063/2553 (81%)	2002 (97%)	61 (3%)	0	100	100
All	All	4123/5106 (81%)	3996 (97%)	127 (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%)	1708 (100%)	0	100	100
All	All	3413/4234 (81%)	3413 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	664	GLN
1	B	78	GLN
1	B	195	ASN
1	B	580	HIS
1	B	1345	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [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	2602	-	47,52,52	0.67	0	61,80,80	0.80	2 (3%)
2	NDP	A	2601	-	47,52,52	0.65	0	61,80,80	0.85	3 (4%)
2	NDP	B	2601	-	47,52,52	0.66	0	61,80,80	0.93	2 (3%)
2	NDP	A	2602	-	47,52,52	0.65	0	61,80,80	0.81	3 (4%)

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	2602	-	-	11/30/77/77	0/5/5/5
2	NDP	A	2601	-	-	14/30/77/77	0/5/5/5
2	NDP	B	2601	-	-	8/30/77/77	0/5/5/5
2	NDP	A	2602	-	-	11/30/77/77	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	-5.30	109.26	123.43
2	B	2602	NDP	P2B-O2B-C2B	-3.55	113.94	123.43
2	A	2602	NDP	P2B-O2B-C2B	-3.35	114.49	123.43
2	A	2601	NDP	C4B-O4B-C1B	-2.60	107.54	109.92

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2601	NDP	C5A-C6A-N6A	2.29	123.79	120.31
2	A	2602	NDP	C5A-C6A-N6A	2.25	123.75	120.31
2	A	2601	NDP	O3B-C3B-C2B	2.23	117.44	111.19
2	A	2601	NDP	C5A-C6A-N6A	2.23	123.70	120.31
2	A	2602	NDP	C3N-C2N-N1N	-2.13	120.07	123.20
2	B	2602	NDP	C5A-C6A-N6A	2.07	123.46	120.31

There are no chirality outliers.

All (44) 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	C2N-C3N-C7N-O7N
2	A	2602	NDP	C5B-O5B-PA-O2A
2	A	2602	NDP	C5B-O5B-PA-O3
2	A	2602	NDP	PN-O3-PA-O5B
2	A	2602	NDP	O4D-C4D-C5D-O5D
2	A	2602	NDP	O4D-C1D-N1N-C6N
2	A	2602	NDP	C2N-C3N-C7N-O7N
2	A	2602	NDP	C2N-C3N-C7N-N7N
2	B	2601	NDP	C5D-O5D-PN-O1N
2	B	2602	NDP	C5D-O5D-PN-O1N
2	B	2602	NDP	C2N-C3N-C7N-N7N
2	A	2602	NDP	C3D-C4D-C5D-O5D
2	A	2601	NDP	C3B-C2B-O2B-P2B
2	B	2601	NDP	O4D-C1D-N1N-C2N
2	A	2601	NDP	C1B-C2B-O2B-P2B
2	A	2602	NDP	C3B-C4B-C5B-O5B
2	B	2602	NDP	O4B-C4B-C5B-O5B
2	A	2602	NDP	O4B-C4B-C5B-O5B
2	B	2601	NDP	O4D-C4D-C5D-O5D
2	A	2601	NDP	O4D-C4D-C5D-O5D
2	B	2601	NDP	O4B-C4B-C5B-O5B
2	B	2602	NDP	O4D-C4D-C5D-O5D
2	B	2601	NDP	C3D-C4D-C5D-O5D
2	A	2601	NDP	C3D-C4D-C5D-O5D
2	A	2601	NDP	C2N-C3N-C7N-N7N
2	B	2602	NDP	C3B-C4B-C5B-O5B
2	A	2602	NDP	PA-O3-PN-O1N
2	A	2601	NDP	O4D-C1D-N1N-C2N
2	A	2601	NDP	C5D-O5D-PN-O2N

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Mol	Chain	Res	Type	Atoms
2	B	2601	NDP	C5D-O5D-PN-O3
2	B	2602	NDP	C5B-O5B-PA-O1A
2	B	2601	NDP	C2B-O2B-P2B-O2X
2	B	2602	NDP	C3B-C2B-O2B-P2B
2	B	2602	NDP	O4D-C1D-N1N-C6N
2	A	2601	NDP	C2B-O2B-P2B-O1X
2	A	2601	NDP	O4B-C4B-C5B-O5B
2	B	2602	NDP	C2D-C1D-N1N-C6N
2	A	2601	NDP	C2B-O2B-P2B-O2X
2	B	2602	NDP	C2B-O2B-P2B-O3X
2	A	2601	NDP	C3B-C4B-C5B-O5B
2	B	2601	NDP	C2B-O2B-P2B-O1X
2	B	2602	NDP	C1B-C2B-O2B-P2B

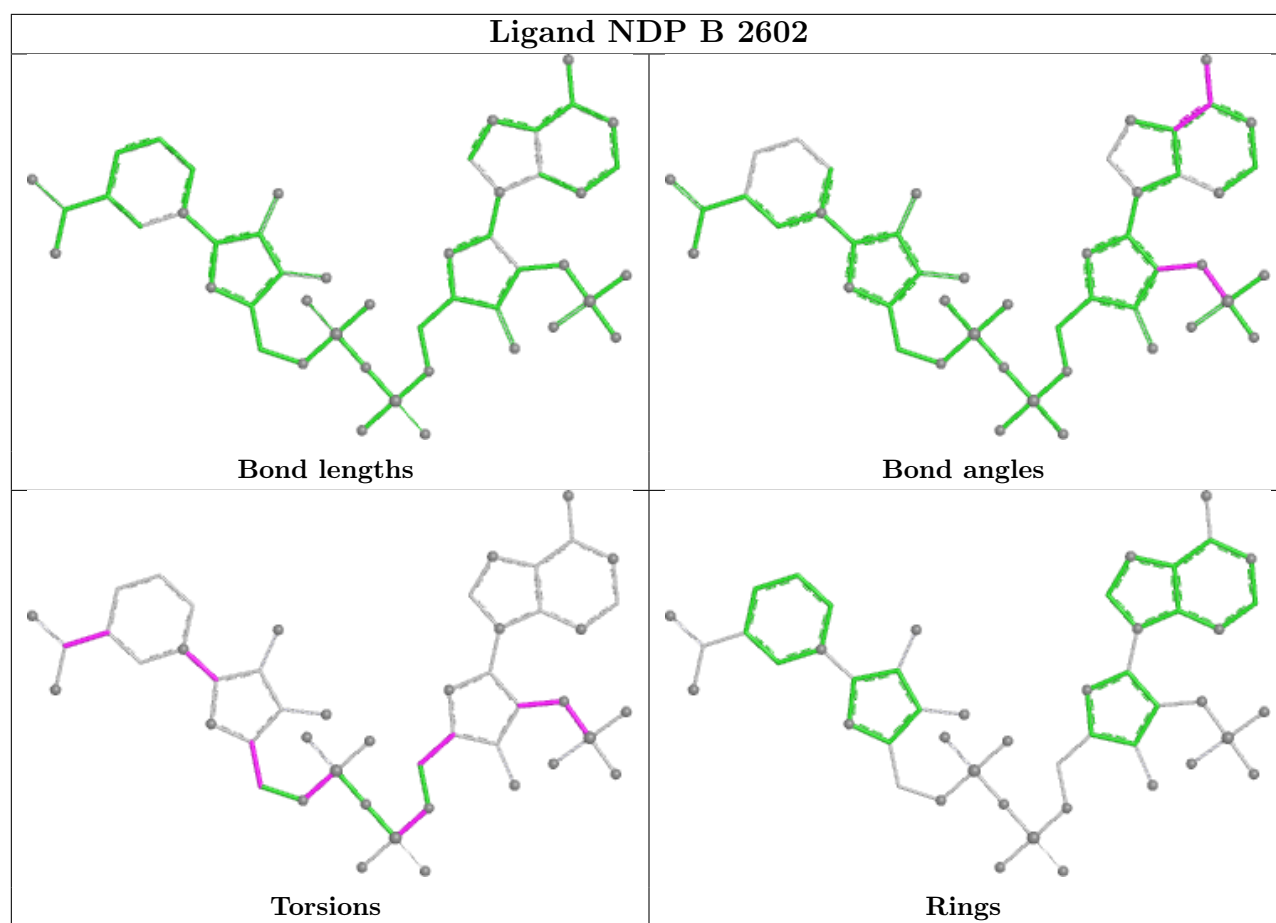
There are no ring outliers.

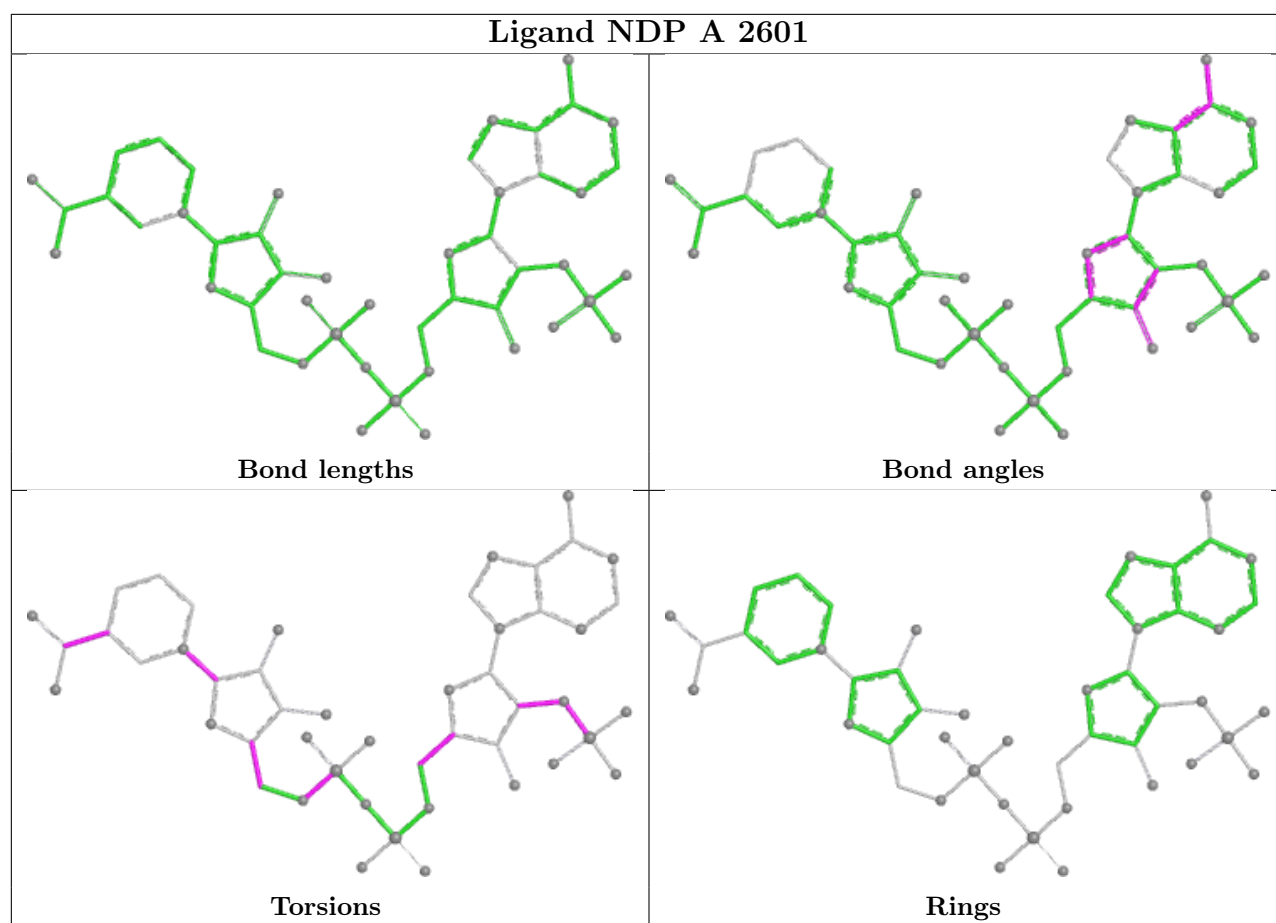
4 monomers are involved in 7 short contacts:

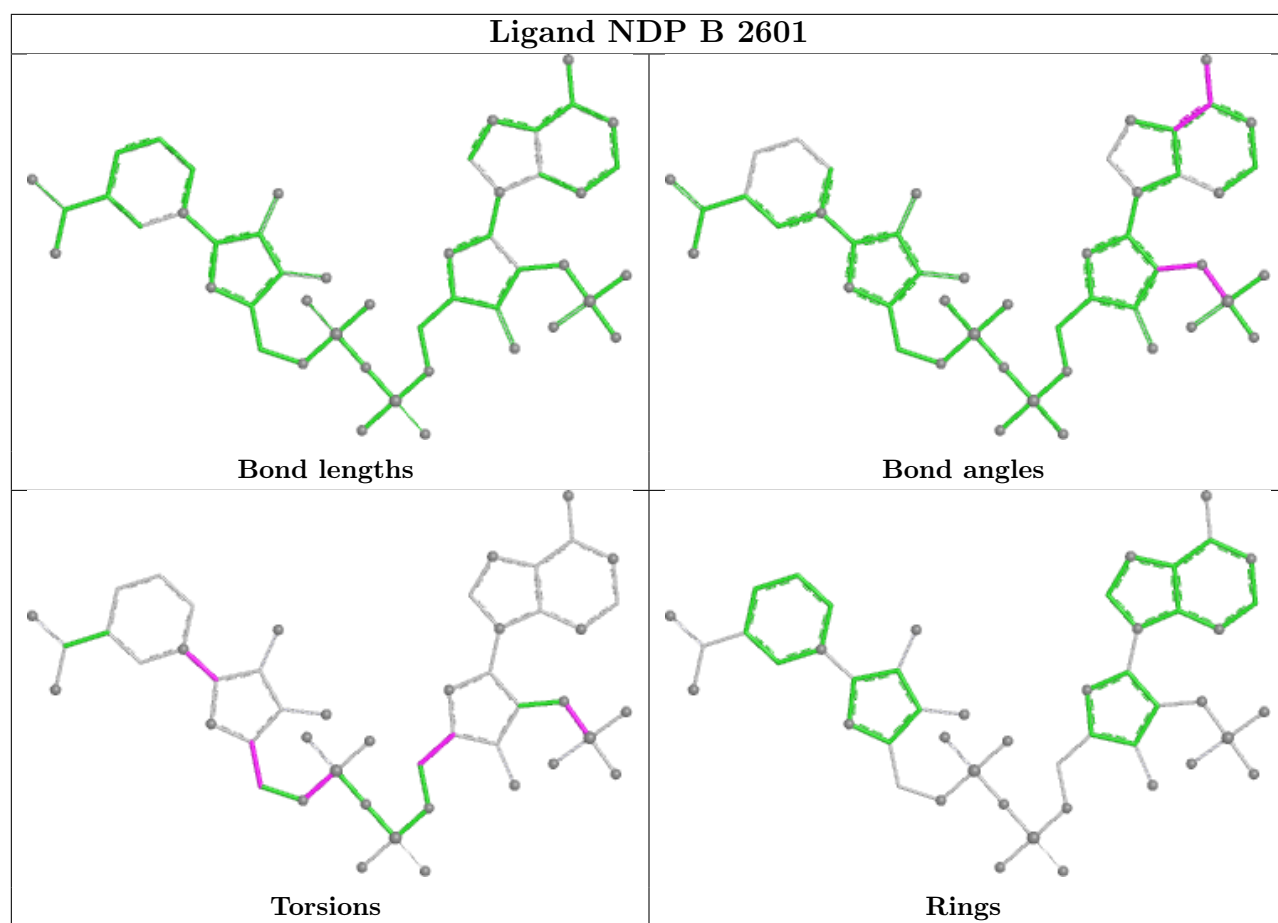
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2602	NDP	1	0
2	A	2601	NDP	1	0
2	B	2601	NDP	4	0
2	A	2602	NDP	1	0

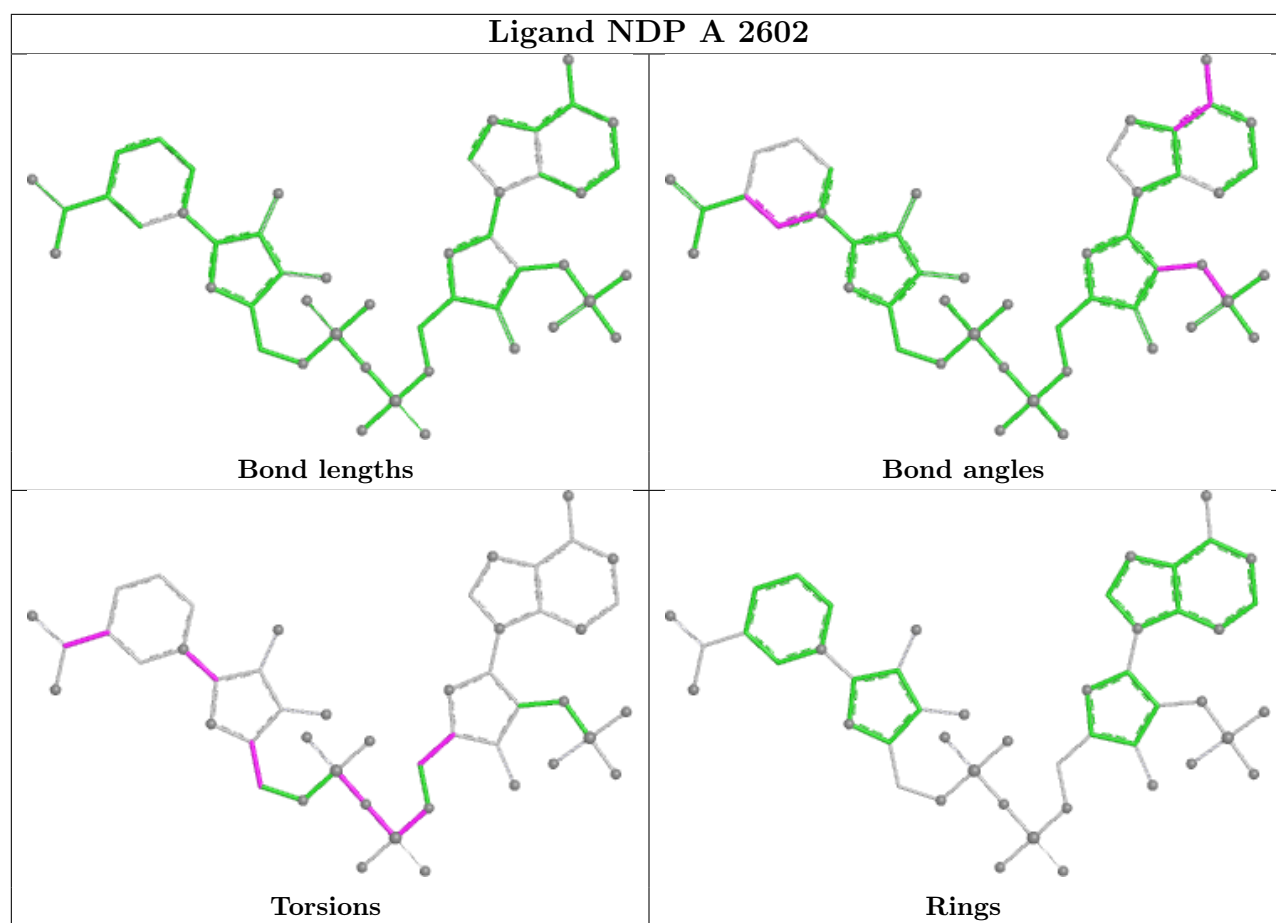
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

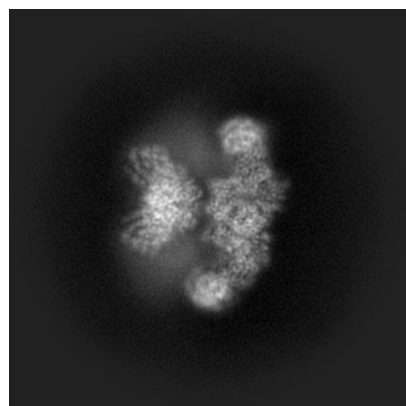
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43352. These allow visual inspection of the internal detail of the map and identification of artifacts.

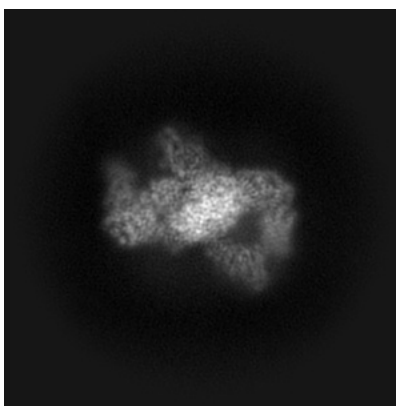
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

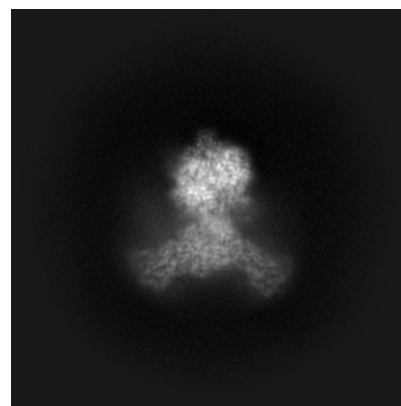
#### 6.1.1 Primary map



X

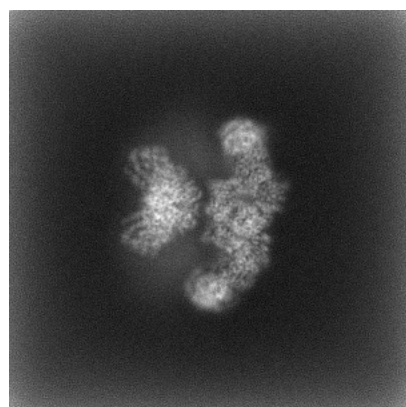


Y

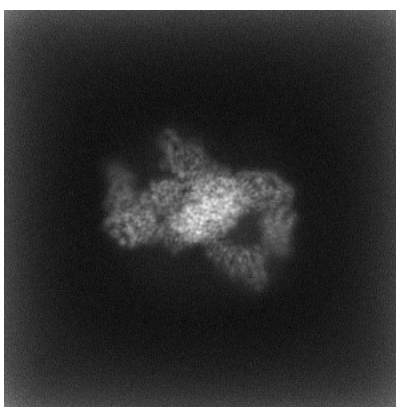


Z

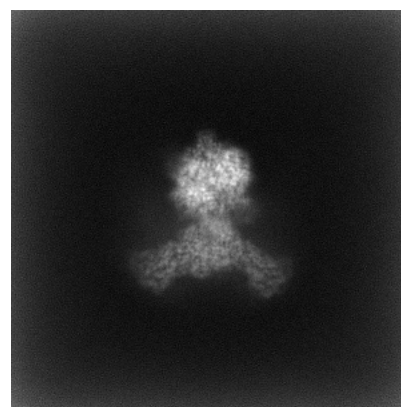
#### 6.1.2 Raw map



X



Y

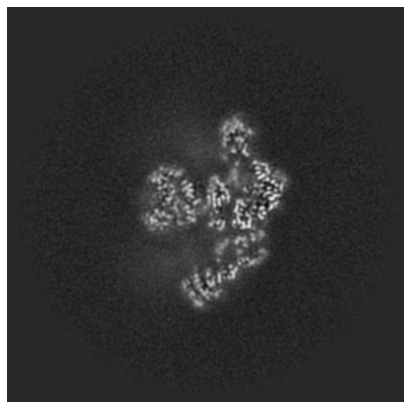


Z

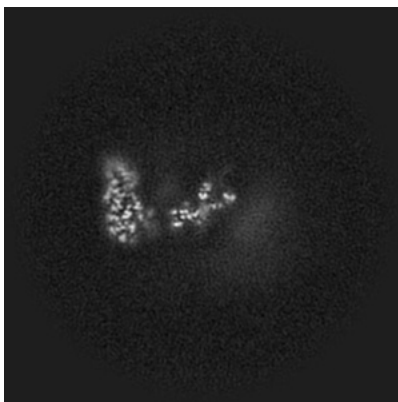
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

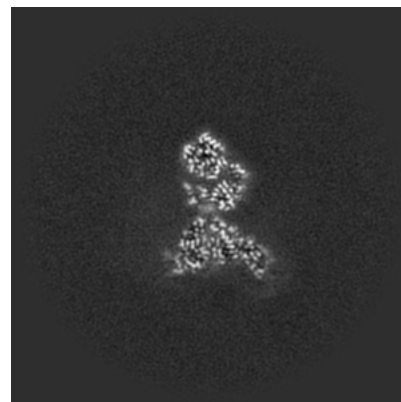
### 6.2.1 Primary map



X Index: 180

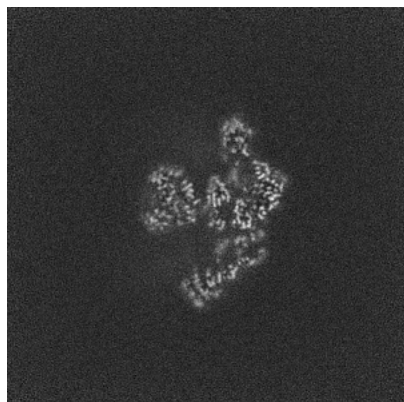


Y Index: 180



Z Index: 180

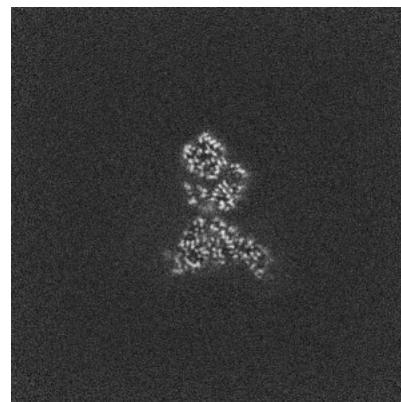
### 6.2.2 Raw map



X Index: 180



Y Index: 180

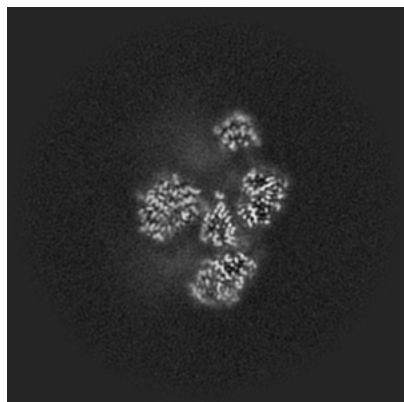


Z Index: 180

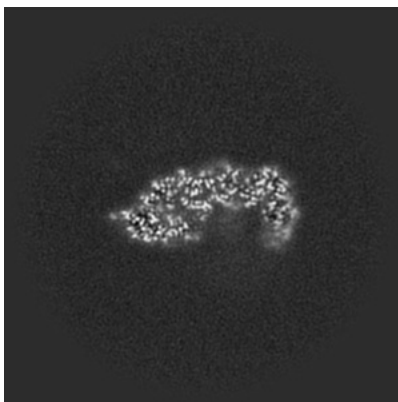
The images above show central slices of the map in three orthogonal directions.

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

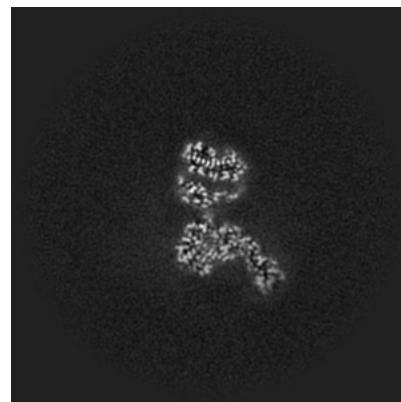
### 6.3.1 Primary map



X Index: 173

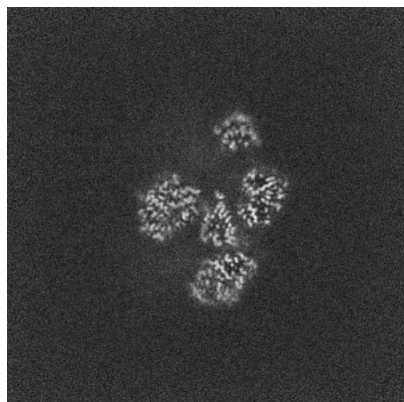


Y Index: 207

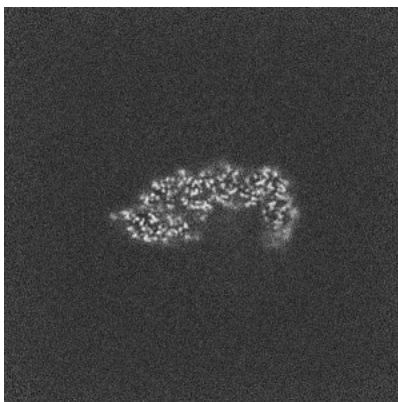


Z Index: 173

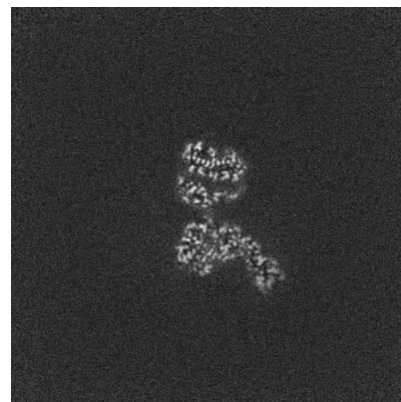
### 6.3.2 Raw map



X Index: 173



Y Index: 207



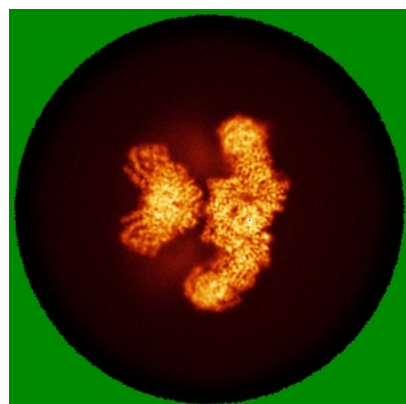
Z Index: 173

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

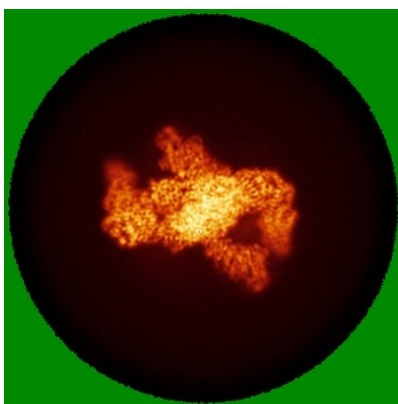


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

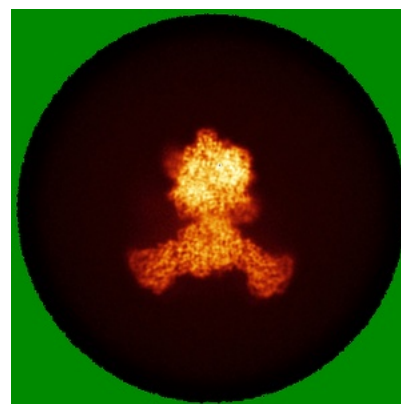
### 6.4.1 Primary map



X

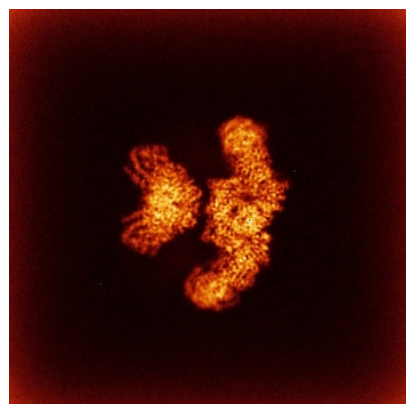


Y

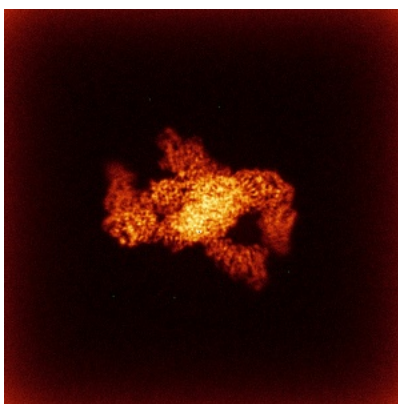


Z

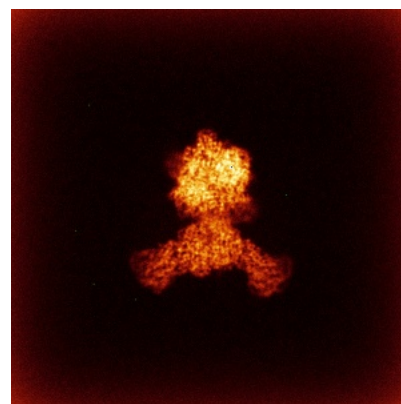
### 6.4.2 Raw map



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.

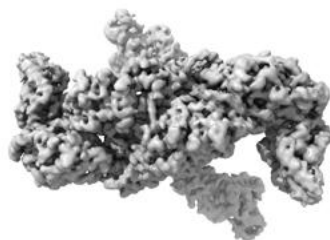


## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.161. 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



X



Y



Z

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.

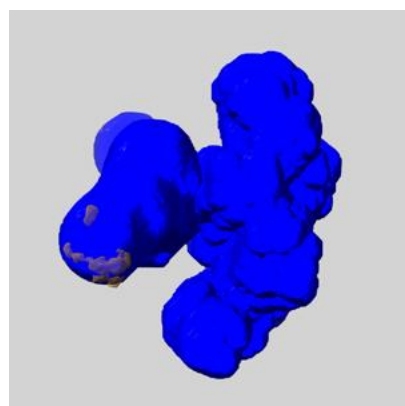
## 6.6 Mask visualisation [i](#)

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

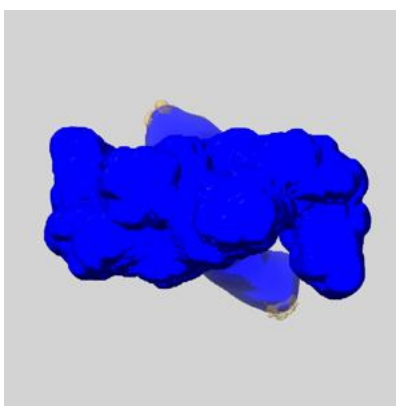
A mask typically either:

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

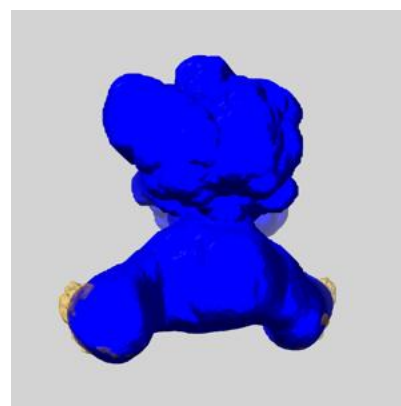
### 6.6.1 emd\_43352\_msk\_1.map [i](#)



X



Y

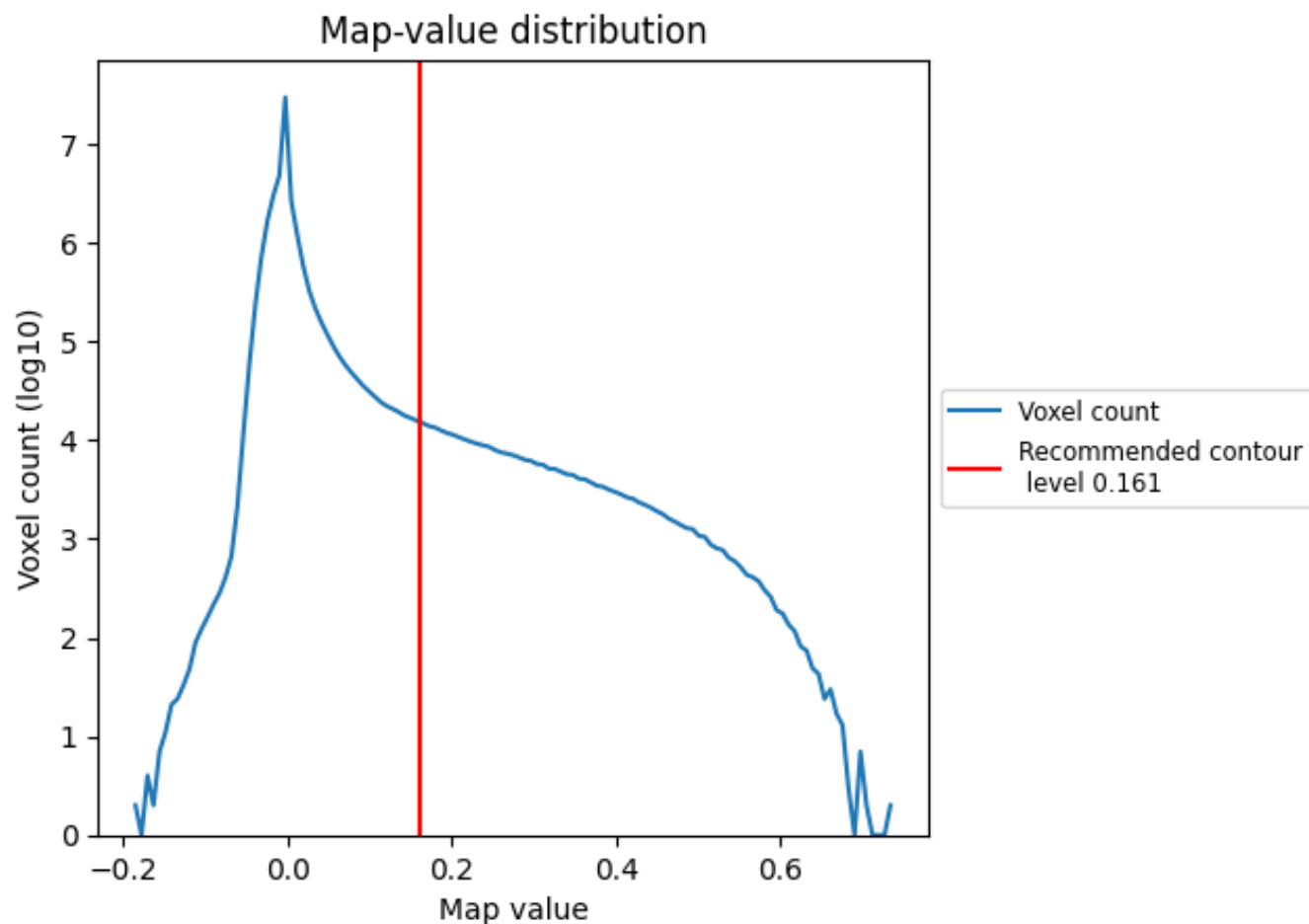


Z

## 7 Map analysis [i](#)

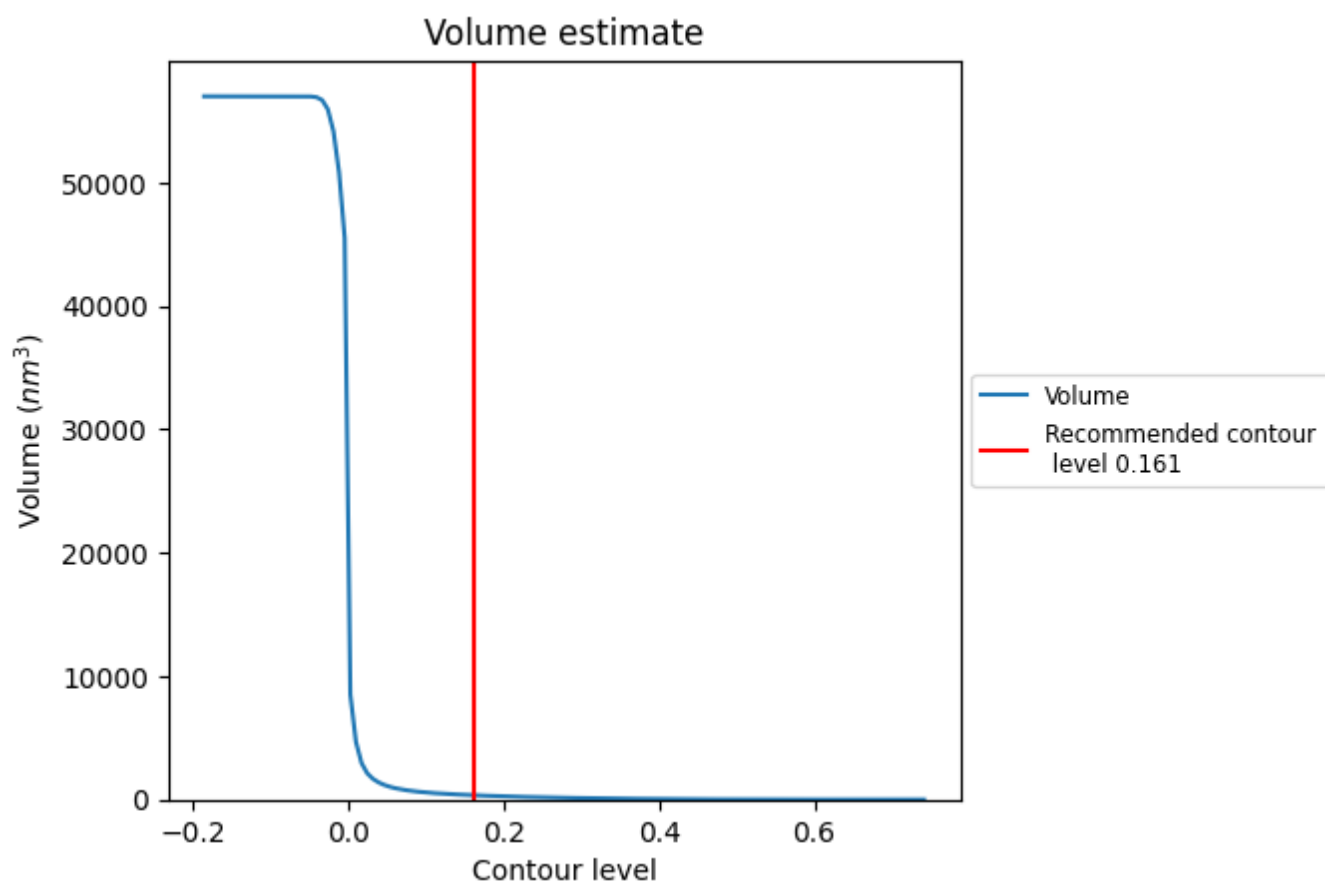
This section contains the results of statistical analysis of the map.

### 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.

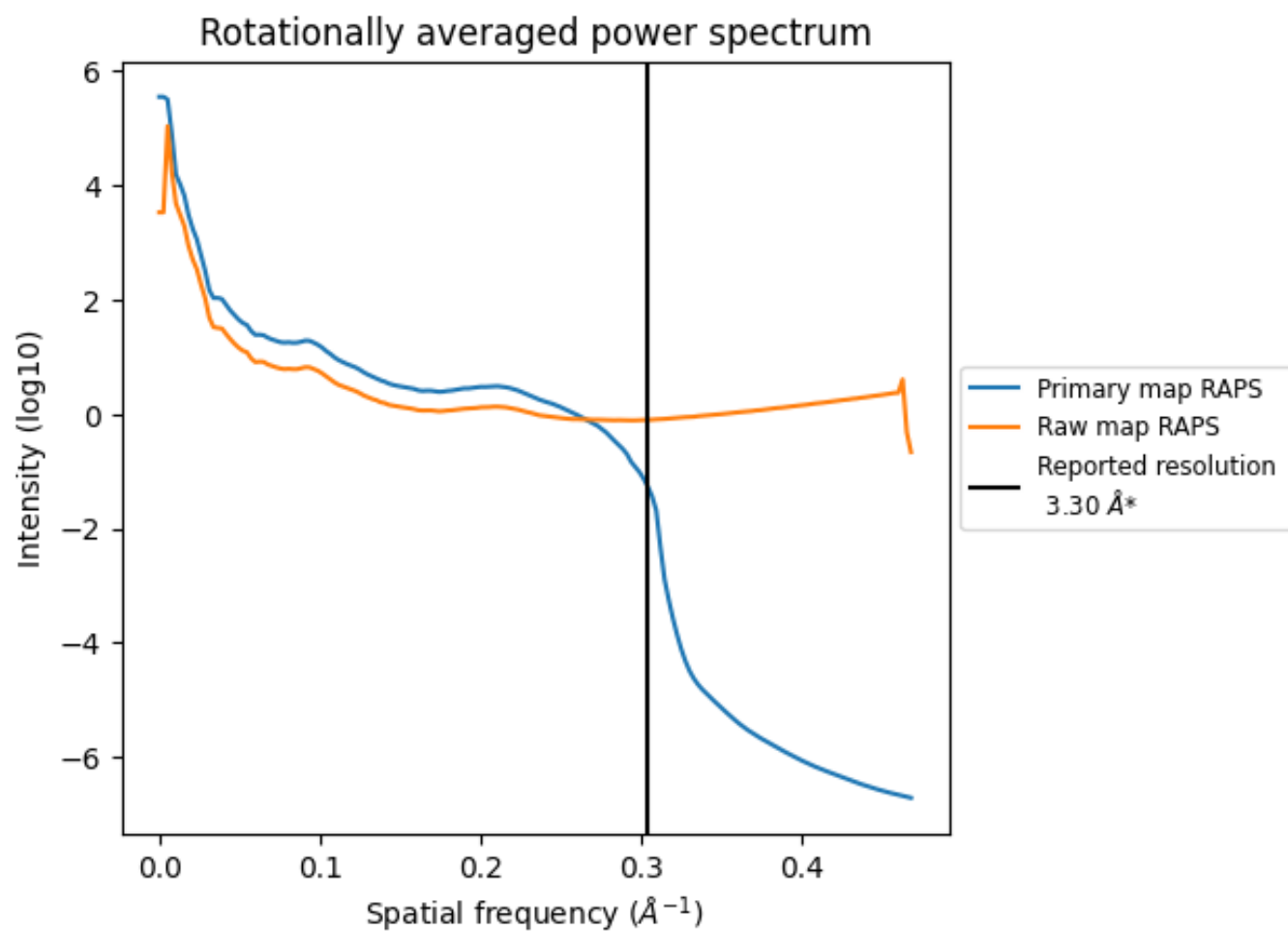
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 352  $\text{nm}^3$ ; this corresponds to an approximate mass of 318 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 ⓘ

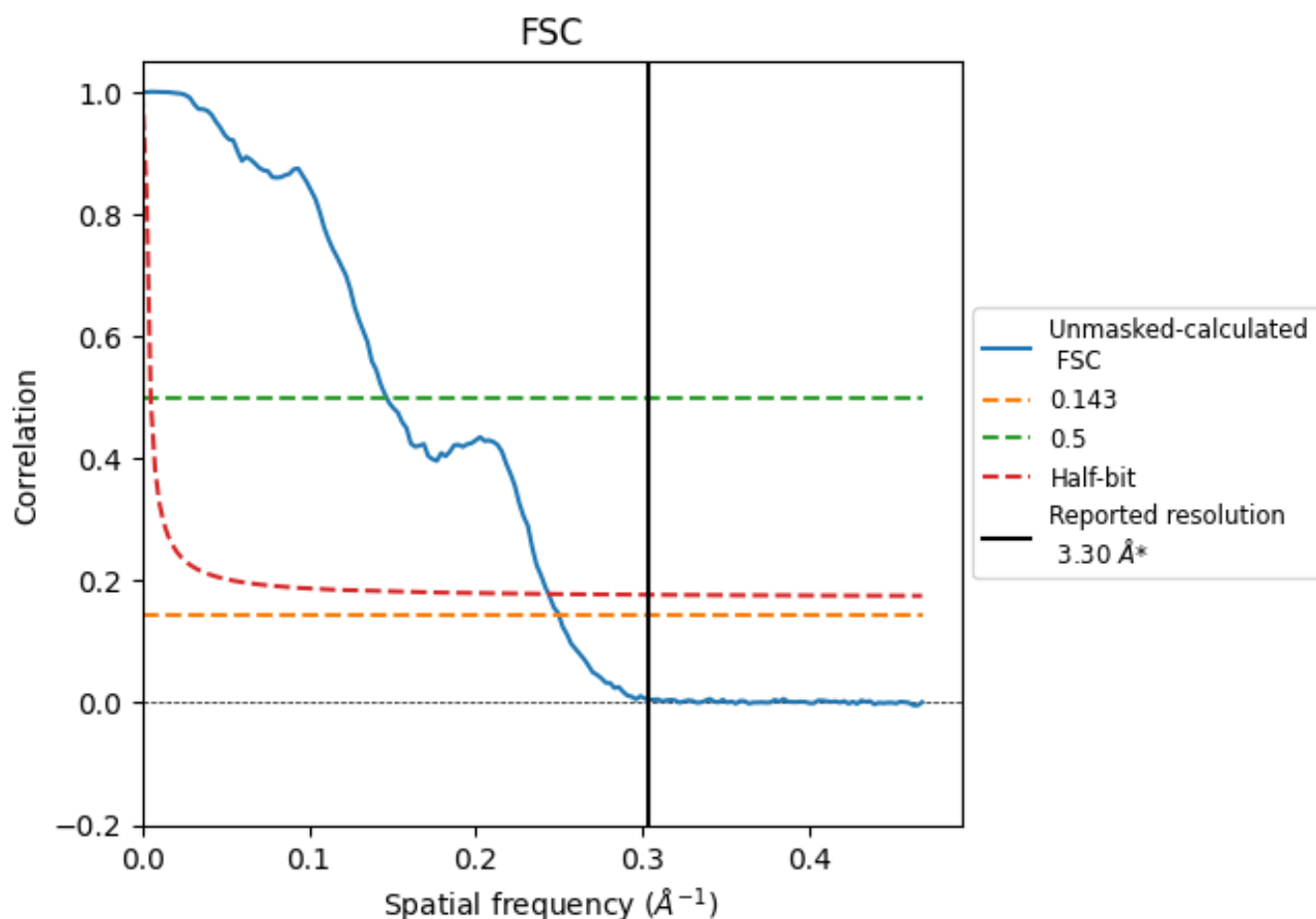


\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

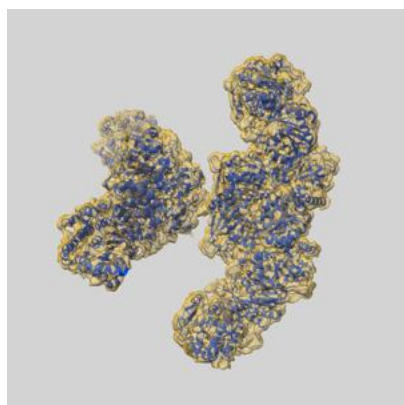
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.00	6.83	4.11

\*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 4.00 differs from the reported value 3.3 by more than 10 %

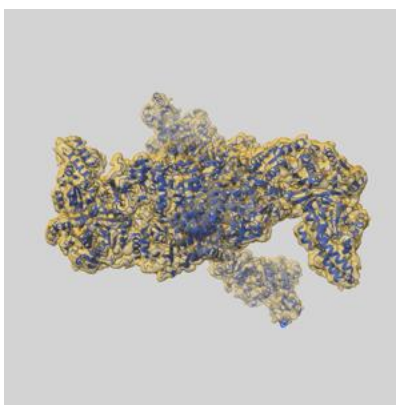
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-43352 and PDB model 8VM5. Per-residue inclusion information can be found in section 3 on page 7.

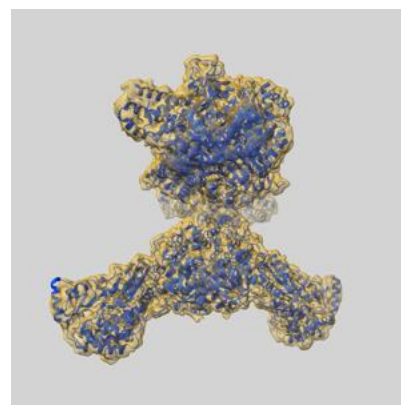
### 9.1 Map-model overlay [i](#)



X



Y

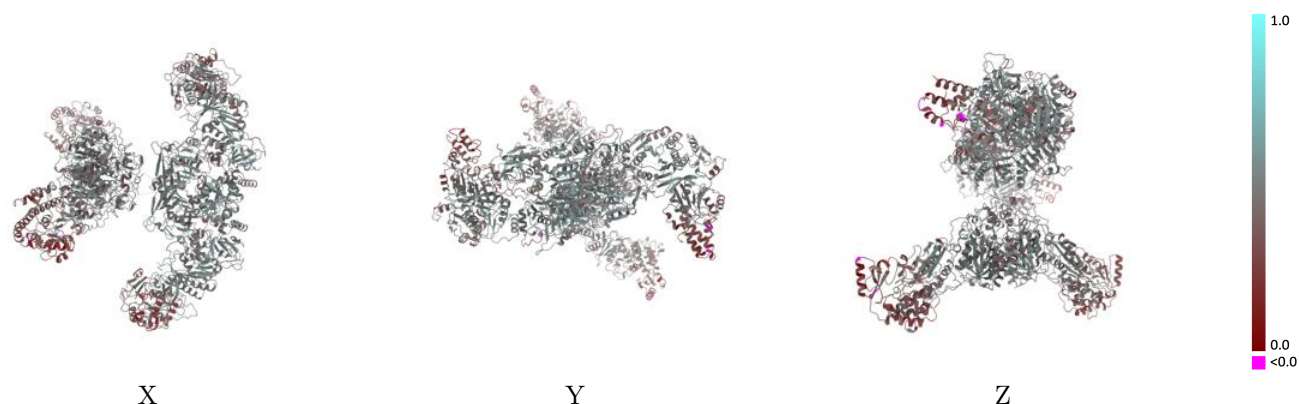


Z

The images above show the 3D surface view of the map at the recommended contour level 0.161 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.

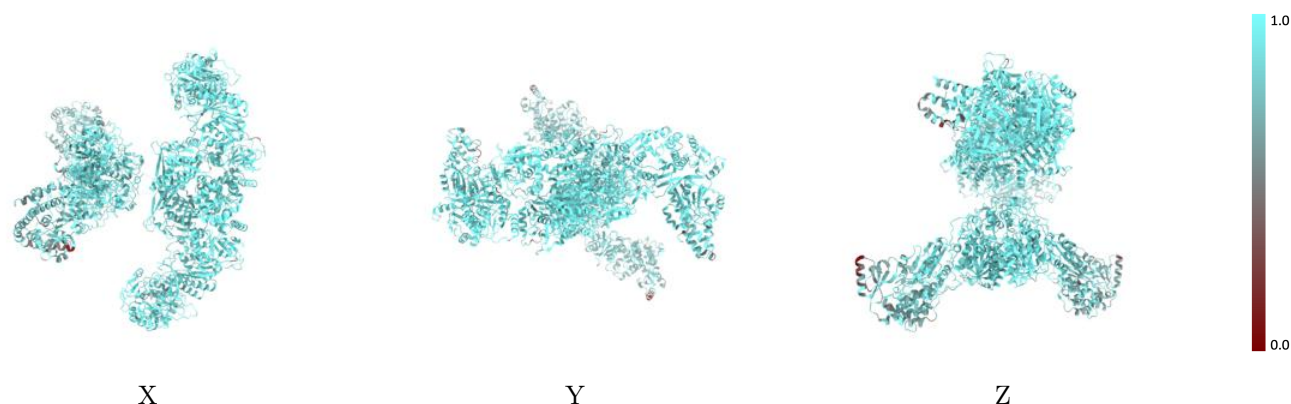


## 9.2 Q-score mapped to coordinate model [i](#)



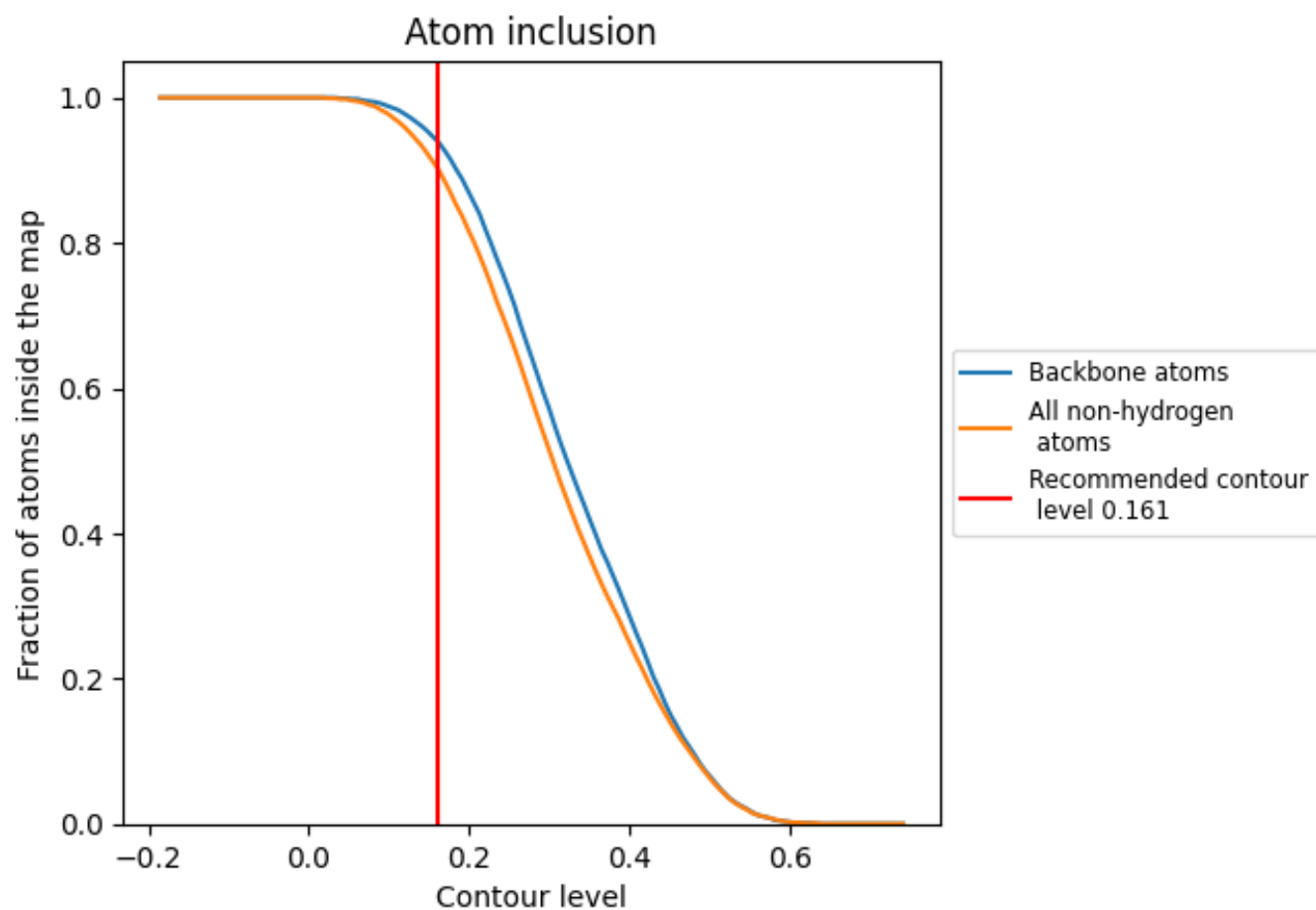
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.161).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 90% 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 (0.161) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9020	<div></div> 0.4520
A	<div></div> 0.9050	<div></div> 0.4530
B	<div></div> 0.9040	<div></div> 0.4510

