



## Full wwPDB EM Validation Report ⓘ

Feb 22, 2025 – 02:53 PM EST

PDB ID : 8VLO  
EMDB ID : EMD-43340  
Title : Composite structure of human FASN with NADPH in State 2  
Authors : Schultz, K.; Marmorstein, R.  
Deposited on : 2024-01-11  
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

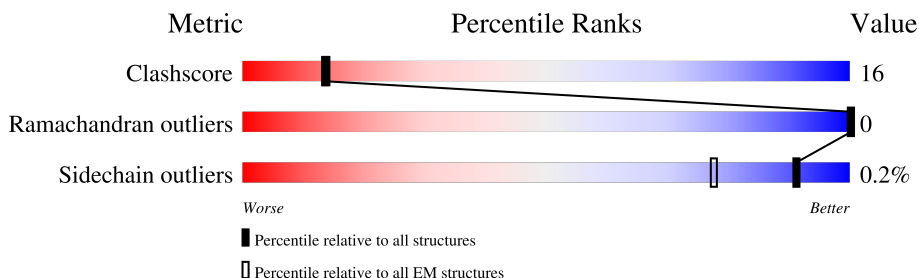
# 1 Overall quality at a glance

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 [i](#)

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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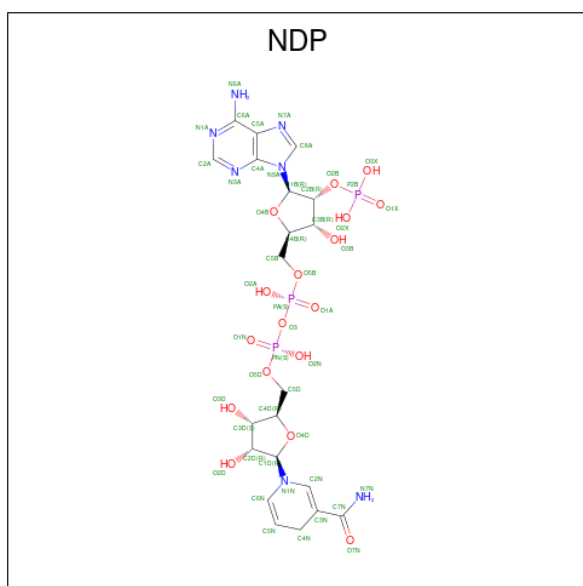
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	ALA	-	expression tag	UNP P49327
A	-4	MET	-	expression tag	UNP P49327
A	-3	GLY	-	expression tag	UNP P49327
A	-2	SER	-	expression tag	UNP P49327
A	-1	GLY	-	expression tag	UNP P49327
A	0	ILE	-	expression tag	UNP P49327
A	1	PRO	-	expression tag	UNP P49327
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).

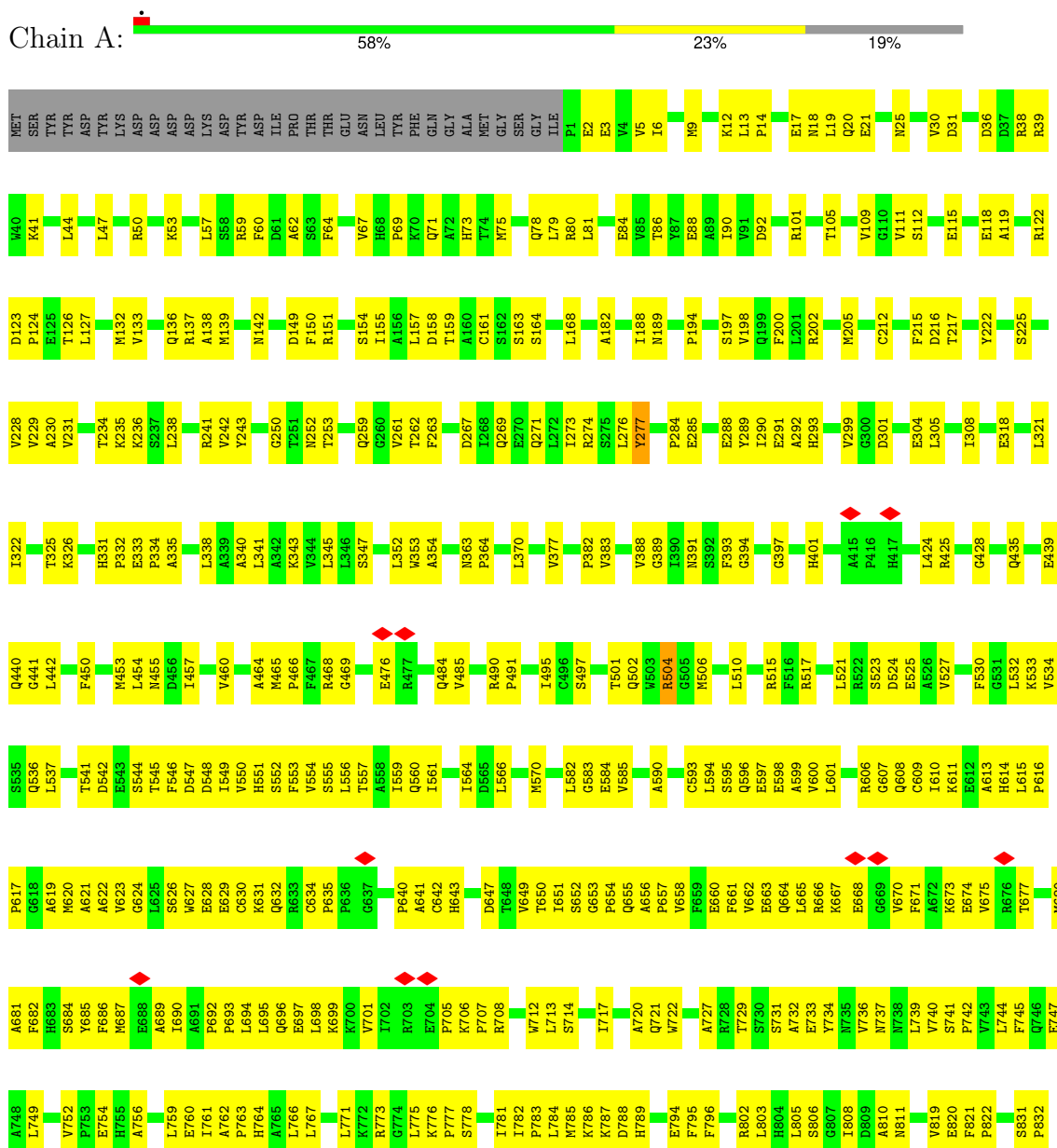


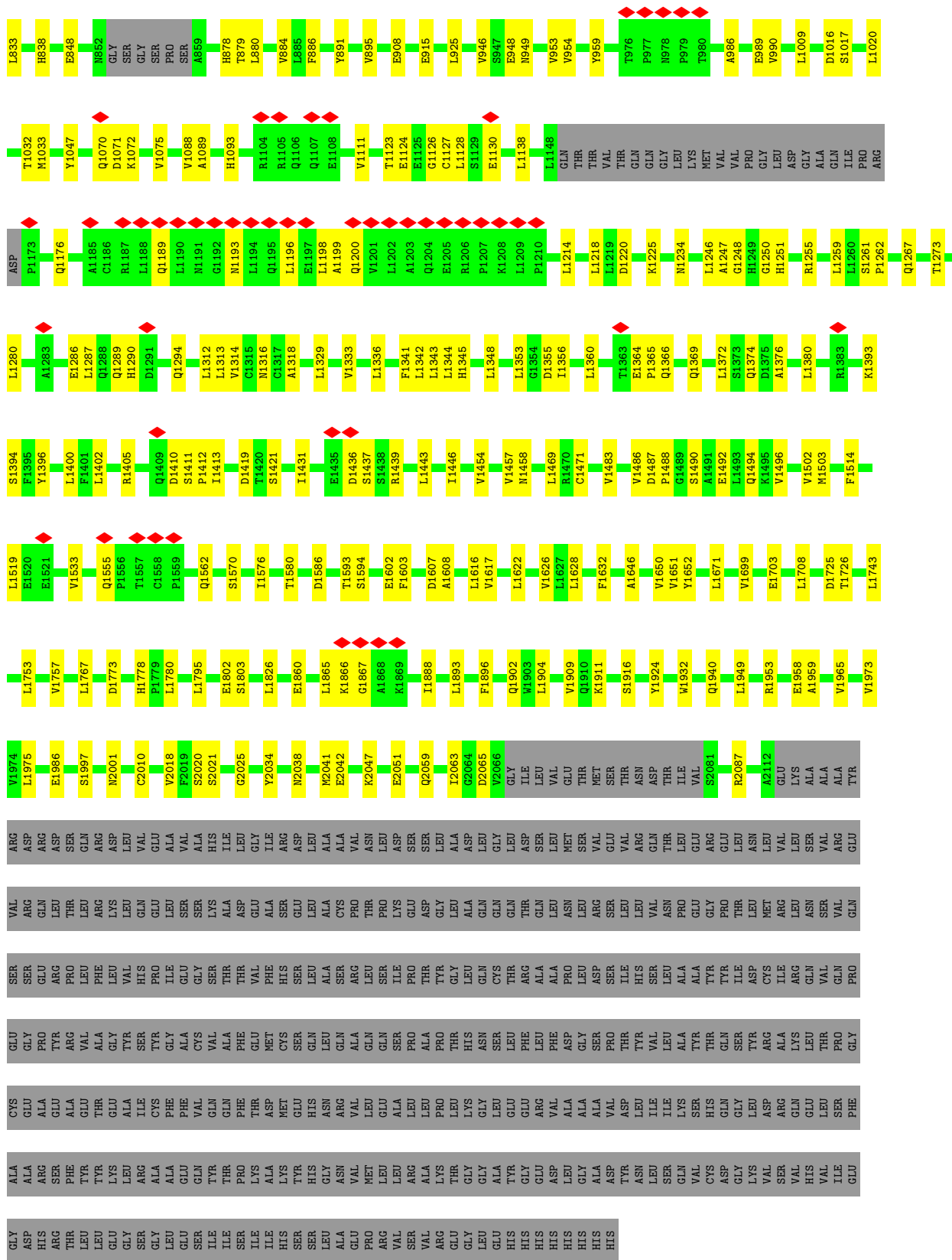
Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
2	A	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
2	B	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
2	B	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	

### 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





- Molecule 1: Fatty acid synthase



Chain B:



RET	SER	TYR	ASP	TYR	LYS	ASP	ASP	ASP	LYS	ASP	TYR	ASP	ILE	PRO	THR	THR	GLU	ASN	LEU	TYR	PHE	GLN	GLY	ALA	MET	GLY	SER	GLY	ILE	P1	V5	I6	A7	L13	P14	E17	W23	I27	V33	T34	D35	L44	R49	R50	S51	G52	R53	L54	K55					
D56	L57	F60	D61	A62	S63	F64	G65	V67	Q71	Q78	L79	R80	L81	L82	L83	E84	W85	T86	V87	E88	D92	I95	L100	W108	V109	G110	V111	T116	L120	E125	T126	L127	Y130	S131	M132	V133	Q136	R137	M139	L143	L144	F147	F148											
R151	T155	A156	L157	D158	C161	S162	S163	S164	L165	H166	A167	L168	A183	I184	I188	N189	V190	L191	L192	K193	P194	N195	T196	S197	Q198	F200	L201	R202	L203	G204	N205	E209	G210	F215	D216	T217	Y222	C223	R224	S225	E226	A230	V231	L232	L233	L238	R241							
V242	Y243	N248	A249	R252	T253	D254	K257	E258	V261	T262	F263	L268	R274	S275	L276	Y277	A280	A283	P284	E285	S286	L290	E291	A292	G294	T295	G296	T297	D301	P302	A303	K304	L305	L308	A314	T315	E318	P319	L320	L321	L322	T325	H331											
P332	E333	P334	A335	L338	A339	A340	A342	K343	A344	L345	L346	L348	L352	G353	A354	E365	I366	P367	D371	G372	R373	L374	Q375	V376	R384	F393	G394	F395	G396	R401	L402	L403	L404	R405	P406	P412	A415	L420	L424	R429	T430	P431	E432	Q435										
K436	L437	L438	E439	Q440	R443	M453	L454	N455	D456	L457	F467	R468	C469	R477	V485	P491	S497	G498	M499	Q502	W503	R504	M506	R512	L513	T520	D524	V527	K528	P529	L532	K533	V534	L537	L538	L539	S540	T541	D542	E543	S544	T545	I549											
V550	H551	S552	F553	V554	S555	L556	T559	Q560	L563	L567	M570	L577	H580	E584	V585	G588	C593	L594	S595	Q596	E597	E598	A599	V600	L601	Y604	W605	T610	R611	E612	A613	A619	A622	V623	G624	S626	W627	E628	P629	C630	K631	Q632	R633	C634	P635									
P636	G637	P640	A641	G642	H643	R644	T648	T650	I651	S652	G653	P654	Q655	G656	P657	V658	F659	E660	F661	V662	G663	Q664	L665	R666	W667	E668	Q669	E670	E674	G675	T677	M680	P681	F682	Y685	F686	M687	E688	A689	I690	A691	P692	P693	L694	L695	Q696	E697	L698	K699	K700	V701			
I702	R703	E704	P705	L706	F707	R708	W712	L713	S714	L717	F718	E719	A720	Q721	W722	L726	A727	R728	T729	S730	S731	A732	E733	W736	W737	W738	L739	W740	V743	L744	F745	Q746	E747	L749	V752	P753	E754	H755	A756	V757	V758	L759	E760	I761	A762	P763	H764	L767	Q768	A769	V770			
L771	K772	R773	G774	L775	K776	P777	L781	W782	K787	R790	L793	Q797	L797	L805	T808	D809	A810	F816	P824	L829	I830	L833	H838	W842	R852	GLY	SER	GLY	SER	PRO	SER	A859	A860	I861	H873	W876	D877	L884	G904	K927	T928													
E934	V935	E939	L943	V946	V953	V954	P972	T976	P977	N978	P979	T980	E981	R995	Y999	R1019	N1025	S1028	D1031	Q1035	L1066	Y1067	A1076	V1079	Q1109	Q1110	V1111	P1112	I1113	H1122	E1130	R1131	L1138	G1141	V1145	Q1146	A1147	L1148																
Q1149	T1150	THR	VAL	THR	GLN	GLN	GLY	LEU	LYS	VAL	VAL	PRO	GLY	LEU	ASP	GLY	ALA	GLN	ILE	PRO	ARG	ASP	P1173	S1174	Q1175	Q1176	E1177	L1182	C1186	R1187	L1188	Q1189	L1190	N1191	L1192	N1193	L1194	Q1195	L1196	E1197	L1198	A1199	Q1200	L1202	A1203	Q1204	E1205	R1206	P1207	K1208	L1209	P1210	L1218	L1219
L1224	C1227	L1228	L1229	T1230	E1233	L1238	K1241	E1244	H1249	L1252	I1256	S1261	P1262	L1265	D1274	R1275	Q1278	A1279	L1280	E1281	E1286	Q1289	Q1294	S1305	D1311	L1312	L1313	V1314	C1315	N1316	C1317	A1318	S1327	A1328	L1329	S1330	N1331	W1332	V1333															
L1336	F1341	L1342	L1343	L1344	H1345	T1346	L1347	R1348	R1349	G1350	H1351	I1356	L1360	E1364	P1365	Q1366	Y1367	Q1368	Q1369	I1370	I1371	L1372	S1373	Q1374	V1384	S1385	L1386	S1394	T1399	L1400	F1401	Q1409	D1410	S1411	V1417	W1424	L1428	L1432	E1435	D1436	R1439	P1440	V1441	V1453										

[illegible]

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	132786	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	0.744	Depositor
Minimum map value	-0.189	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.213	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

### 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	0.27	0/16198	0.48	0/22023
1	B	0.27	0/16222	0.48	0/22055
All	All	0.27	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	542	0
1	B	15857	9380	15826	468	0
2	A	96	52	52	5	0
2	B	96	52	52	4	0
All	All	31882	18827	31739	996	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 16.

All (996) 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:A:533:LYS:HE3	1:A:536:GLN:HG3	1.43	1.00
1:A:1446:ILE:HG21	1:A:1486:VAL:HG21	1.39	0.99
1:A:1471:CYS:SG	1:A:1503:MET:HA	2.04	0.98
1:B:654:PRO:HB2	1:B:657:PRO:HD2	1.48	0.94
1:B:682:PHE:HA	1:B:687:MET:HE3	1.47	0.94
1:A:622:ALA:HB2	1:A:650:THR:HG22	1.48	0.94
1:A:501:THR:HG22	1:A:766:LEU:HD13	1.51	0.93
1:B:333:GLU:HB2	1:B:334:PRO:HD3	1.52	0.92
1:A:601:LEU:HD23	1:A:701:VAL:HG13	1.50	0.91
1:A:333:GLU:HB2	1:A:334:PRO:HD3	1.53	0.90
1:B:502:GLN:HB3	1:B:556:LEU:HD11	1.54	0.90
1:A:291:GLU:HG2	1:A:340:ALA:HB1	1.56	0.85
1:A:595:SER:HB3	1:A:598:GLU:HG3	1.59	0.83
1:B:161:CYS:HB2	1:B:394:GLY:HA2	1.61	0.83
1:B:318:GLU:HG2	1:B:319:PRO:HD2	1.62	0.82
1:A:548:ASP:OD1	1:A:549:ILE:N	2.14	0.81
1:B:164:SER:HB3	1:B:338:LEU:HG	1.62	0.81
1:B:1019:ARG:NH1	1:B:1067:TYR:OH	2.14	0.80
1:A:692:PRO:O	1:A:695:LEU:HG	1.82	0.79
1:A:1333:VAL:O	1:A:1405:ARG:NH2	2.15	0.79
1:A:343:LYS:HE2	1:A:354:ALA:HB3	1.64	0.79
1:B:440:GLN:HG2	1:B:833:LEU:HD11	1.64	0.79
1:B:629:GLU:OE1	1:B:629:GLU:N	2.15	0.79
1:A:504:ARG:NH1	1:A:541:THR:O	2.15	0.78
1:A:161:CYS:HB2	1:A:394:GLY:HA2	1.64	0.78
1:A:584:GLU:HG3	1:A:712:TRP:HZ2	1.48	0.78
1:B:628:GLU:O	1:B:632:GLN:HG2	1.82	0.78
1:B:654:PRO:HB2	1:B:657:PRO:CD	2.12	0.78
1:B:654:PRO:HG3	1:B:686:PHE:HZ	1.46	0.77
1:A:21:GLU:O	1:A:25:ASN:ND2	2.17	0.76
1:B:675:VAL:HG23	1:B:677:THR:HG23	1.66	0.76
1:A:654:PRO:HB2	1:A:657:PRO:HD2	1.67	0.76
1:B:432:GLU:N	1:B:432:GLU:OE1	2.19	0.75
1:B:540:SER:HB2	1:B:545:THR:HG21	1.68	0.75
1:A:1617:VAL:HG12	1:A:1628:LEU:HD13	1.67	0.75
1:B:35:ASP:OD1	1:B:49:ARG:HB3	1.87	0.75
1:B:687:MET:O	1:B:690:ILE:HG22	1.85	0.75
1:A:259:GLN:N	1:A:259:GLN:OE1	2.19	0.74
1:B:51:SER:O	1:B:53:LYS:NZ	2.21	0.74
1:A:2034:TYR:O	1:A:2038:ASN:ND2	2.21	0.74
1:B:935:VAL:HG22	1:B:946:VAL:HG22	1.70	0.74
1:A:78:GLN:HB3	1:A:188:ILE:HD12	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:GLU:OE1	1:A:2:GLU:N	2.19	0.73
1:A:763:PRO:O	1:A:785:MET:HB3	1.87	0.73
1:A:112:SER:HB3	1:A:334:PRO:HG3	1.69	0.73
1:A:158:ASP:HB2	1:B:156:ALA:HB3	1.70	0.73
1:A:908:GLU:OE1	1:A:908:GLU:N	2.22	0.73
1:B:137:ARG:NH1	1:B:158:ASP:OD2	2.19	0.73
1:A:136:GLN:OE1	1:A:138:ALA:N	2.22	0.72
1:A:274:ARG:HA	1:A:277:TYR:CD2	2.24	0.72
1:A:654:PRO:HB2	1:A:657:PRO:CD	2.20	0.72
1:B:468:ARG:HD2	1:B:485:VAL:HG21	1.71	0.72
1:B:628:GLU:O	1:B:631:LYS:HG2	1.89	0.72
1:A:3:GLU:HB2	1:A:236:LYS:HG2	1.71	0.72
1:A:1443:LEU:HD11	1:A:1469:LEU:HD22	1.72	0.72
1:B:292:ALA:HB2	1:B:322:ILE:HD11	1.70	0.72
1:A:1016:ASP:OD1	1:A:1017:SER:N	2.23	0.72
1:B:1366:GLN:O	1:B:1370:GLY:N	2.21	0.72
1:A:1617:VAL:HG11	1:A:1626:VAL:HG21	1.72	0.72
1:A:550:VAL:O	1:A:554:VAL:HG22	1.90	0.72
1:A:200:PHE:HD1	1:A:205:MET:HE3	1.55	0.71
1:A:2042:GLU:OE2	1:A:2059:GLN:NE2	2.23	0.71
1:B:1252:LEU:HD11	1:B:1316:ASN:HB2	1.72	0.71
1:B:628:GLU:N	1:B:628:GLU:OE1	2.24	0.71
1:B:319:PRO:HB3	1:B:372:GLY:O	1.91	0.70
1:A:626:SER:HB3	1:A:629:GLU:HG3	1.71	0.70
1:A:635:PRO:HD3	1:A:661:PHE:CE1	2.26	0.70
1:A:657:PRO:HA	1:A:660:GLU:HG2	1.73	0.70
1:A:641:ALA:N	1:A:650:THR:O	2.21	0.70
1:A:1973:VAL:HB	2:A:2602:NDP:H3D	1.72	0.70
1:A:124:PRO:HA	1:A:127:LEU:CD2	2.22	0.70
1:B:274:ARG:HA	1:B:277:TYR:CE2	2.26	0.70
1:A:1365:PRO:O	1:A:1369:GLN:N	2.25	0.70
1:A:708:ARG:NH2	1:A:714:SER:OG	2.25	0.70
1:A:1336:LEU:O	1:A:1405:ARG:NH1	2.25	0.70
1:B:570:MET:HE1	1:B:810:ALA:HB1	1.73	0.70
1:A:787:LYS:HG2	1:A:788:ASP:OD1	1.92	0.69
1:B:640:PRO:HA	1:B:651:ILE:HA	1.73	0.69
1:B:532:LEU:HD21	1:B:604:TYR:HE2	1.55	0.69
1:A:524:ASP:HB2	1:A:534:VAL:HG12	1.74	0.69
1:B:2098:PHE:CD1	1:B:2106:LEU:HD13	2.28	0.69
1:A:1366:GLN:N	1:A:1366:GLN:OE1	2.25	0.69
1:A:1176:GLN:N	1:A:1176:GLN:OE1	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1364:GLU:N	1:A:1364:GLU:OE1	2.25	0.69
1:A:663:GLU:O	1:A:667:LYS:HG2	1.92	0.69
1:B:5:VAL:HB	1:B:242:VAL:HG13	1.74	0.69
1:A:628:GLU:HA	1:A:631:LYS:HE2	1.74	0.68
1:A:124:PRO:HA	1:A:127:LEU:HD23	1.73	0.68
1:B:1571:LEU:HD21	1:B:1622:LEU:HD11	1.75	0.68
1:A:752:VAL:HG21	1:A:775:LEU:CD2	2.23	0.68
1:A:274:ARG:HA	1:A:277:TYR:CE2	2.29	0.68
1:A:620:MET:HG3	1:A:677:THR:HG21	1.74	0.68
1:A:1214:LEU:O	1:A:1396:TYR:OH	2.11	0.68
1:A:1703:GLU:N	1:A:1703:GLU:OE1	2.26	0.67
1:B:1289:GLN:OE1	1:B:1289:GLN:N	2.27	0.67
1:A:706:LYS:O	1:A:729:THR:HG23	1.94	0.67
1:A:9:MET:HG3	1:A:19:LEU:CD1	2.24	0.67
1:A:1725:ASP:OD1	1:A:1726:THR:N	2.27	0.67
1:B:79:LEU:HD21	1:B:143:ARG:HG3	1.77	0.67
1:A:1488:PRO:O	1:A:1494:GLN:NE2	2.26	0.67
1:B:1704:LYS:HG2	1:B:1849:ILE:HD11	1.75	0.67
1:A:290:ILE:HD13	1:A:308:ILE:HD13	1.77	0.66
1:B:543:GLU:N	1:B:543:GLU:OE1	2.27	0.66
1:B:664:GLN:NE2	1:B:668:GLU:OE2	2.28	0.66
1:A:627:TRP:CZ3	1:A:640:PRO:HB2	2.30	0.66
1:A:831:SER:OG	1:A:832:PRO:HD3	1.95	0.66
1:B:216:ASP:OD1	1:B:217:THR:N	2.28	0.66
1:B:752:VAL:HG11	1:B:775:LEU:HD11	1.76	0.66
1:B:674:GLU:N	1:B:674:GLU:OE1	2.29	0.66
1:B:1233:GLU:OE1	1:B:1515:ARG:NH2	2.28	0.66
1:A:155:ILE:HG22	1:A:157:LEU:HD12	1.78	0.66
1:B:1182:LEU:HD21	1:B:1360:LEU:HD11	1.77	0.66
1:A:533:LYS:O	1:A:537:LEU:HD13	1.94	0.65
1:B:1274:ASP:OD1	1:B:1275:ARG:N	2.29	0.65
1:A:138:ALA:HB2	1:B:158:ASP:O	1.97	0.65
1:A:435:GLN:O	1:A:439:GLU:HG2	1.97	0.65
1:A:619:ALA:HB1	1:A:674:GLU:OE2	1.95	0.65
1:A:754:GLU:OE2	1:A:778:SER:OG	2.09	0.65
1:A:763:PRO:HA	1:A:785:MET:SD	2.36	0.65
1:A:1286:GLU:OE1	1:A:1286:GLU:N	2.29	0.65
1:A:1289:GLN:OE1	1:A:1290:HIS:ND1	2.30	0.65
1:A:1410:ASP:OD1	1:A:1411:SER:N	2.30	0.65
1:B:1286:GLU:O	1:B:1289:GLN:NE2	2.30	0.65
1:A:624:GLY:HA2	1:A:647:ASP:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1130:GLU:N	1:A:1130:GLU:OE1	2.30	0.64
1:A:1888:ILE:HD11	1:A:1959:ALA:HB2	1.77	0.64
1:A:548:ASP:OD1	1:A:550:VAL:HG12	1.97	0.64
1:B:1177:GLU:N	1:B:1177:GLU:OE1	2.30	0.64
1:A:620:MET:HB2	1:A:675:VAL:CG2	2.28	0.64
1:A:542:ASP:O	1:A:545:THR:HG22	1.97	0.64
1:A:544:SER:HA	1:A:547:ASP:OD2	1.97	0.64
1:B:1198:LEU:O	1:B:1202:LEU:N	2.31	0.64
1:B:85:VAL:HG12	1:B:230:ALA:HB3	1.80	0.64
1:B:503:TRP:CG	1:B:787:LYS:HG3	2.33	0.64
1:A:631:LYS:HG3	1:A:632:GLN:OE1	1.98	0.64
1:A:689:ALA:O	1:A:692:PRO:HD2	1.98	0.64
1:A:693:PRO:O	1:A:696:GLN:HG3	1.97	0.64
1:B:78:GLN:HB3	1:B:188:ILE:HD12	1.78	0.64
1:A:325:THR:HB	1:A:343:LYS:HD3	1.80	0.64
1:A:428:GLY:HA2	1:A:465:MET:HE1	1.78	0.64
1:A:747:GLU:OE1	1:A:747:GLU:N	2.31	0.64
1:B:708:ARG:HG3	1:B:729:THR:HA	1.80	0.64
1:B:767:LEU:O	1:B:771:LEU:HD13	1.98	0.64
1:A:440:GLN:HG3	1:A:833:LEU:HD22	1.79	0.63
1:A:510:LEU:HD12	1:A:785:MET:CE	2.29	0.63
1:B:304:GLU:HG3	1:B:393:PHE:HE2	1.63	0.63
1:A:615:LEU:HB3	1:A:616:PRO:HD2	1.81	0.63
1:A:1189:GLN:N	1:A:1193:ASN:OD1	2.32	0.63
1:B:570:MET:CE	1:B:810:ALA:HB1	2.28	0.63
1:B:939:GLU:OE1	1:B:939:GLU:N	2.30	0.63
1:A:290:ILE:HG23	1:A:322:ILE:HG13	1.79	0.63
1:A:1997:SER:O	1:A:2001:ASN:ND2	2.30	0.63
1:B:549:ILE:HD11	1:B:553:PHE:CZ	2.34	0.63
1:B:1278:GLN:OE1	1:B:1278:GLN:N	2.30	0.63
1:A:626:SER:O	1:A:630:CYS:N	2.26	0.63
1:B:696:GLN:HG2	1:B:700:LYS:HZ2	1.64	0.62
1:A:137:ARG:HD2	1:B:158:ASP:OD2	1.98	0.62
1:A:189:ASN:HB2	1:A:334:PRO:HD2	1.82	0.62
1:A:621:ALA:O	1:A:651:ILE:HG12	1.99	0.62
1:A:692:PRO:HD2	1:A:693:PRO:HD2	1.79	0.62
1:A:741:SER:HB2	1:A:742:PRO:HD2	1.81	0.62
1:A:1047:TYR:OH	1:A:1586:ASP:OD2	2.14	0.62
1:B:64:PHE:HD2	1:B:429:ARG:HD3	1.64	0.62
1:A:553:PHE:CD2	1:A:582:LEU:HD22	2.33	0.62
1:A:112:SER:CB	1:A:334:PRO:HG3	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:GLN:HG3	1:A:833:LEU:CD2	2.30	0.62
1:A:1773:ASP:OD1	1:A:1778:HIS:ND1	2.32	0.62
1:B:60:PHE:CD1	1:B:80:ARG:HB3	2.34	0.62
1:B:1327:SER:O	1:B:1331:ASN:ND2	2.32	0.62
1:B:1350:GLY:O	1:B:1351:HIS:ND1	2.32	0.62
1:A:620:MET:HE2	1:A:682:PHE:H	1.65	0.62
1:B:258:GLU:OE1	1:B:258:GLU:N	2.31	0.62
1:B:597:GLU:OE1	1:B:597:GLU:N	2.31	0.62
1:B:704:GLU:HB2	1:B:706:LYS:NZ	2.13	0.62
1:B:491:PRO:HG2	1:B:756:ALA:HA	1.81	0.62
1:A:158:ASP:O	1:B:138:ALA:HB2	1.99	0.61
1:A:662:VAL:HG12	1:A:666:ARG:HE	1.63	0.61
1:A:820:GLU:OE1	1:A:820:GLU:N	2.25	0.61
1:B:222:TYR:CD1	1:B:331:HIS:HB3	2.35	0.61
1:B:597:GLU:O	1:B:601:LEU:HD23	2.00	0.61
1:B:717:ILE:CD1	1:B:726:LEU:HD22	2.30	0.61
1:A:713:LEU:HD22	1:A:722:TRP:CZ3	2.35	0.61
1:A:654:PRO:O	1:A:658:VAL:HG23	2.01	0.61
1:A:696:GLN:NE2	1:A:697:GLU:HG2	2.16	0.61
1:A:2065:ASP:OD1	1:A:2087:ARG:NH1	2.33	0.61
1:A:115:GLU:HA	1:A:118:GLU:OE1	2.01	0.61
1:B:51:SER:HA	1:B:223:CYS:SG	2.41	0.61
1:B:1349:ARG:HG2	1:B:1371:ILE:HG22	1.81	0.61
1:A:1200:GLN:OE1	1:A:1200:GLN:N	2.34	0.61
1:A:1570:SER:OG	1:A:1646:ALA:O	2.17	0.61
1:B:477:ARG:HH12	1:B:790:ARG:HD2	1.65	0.61
1:A:915:GLU:OE2	1:A:959:TYR:OH	2.17	0.60
1:B:301:ASP:O	1:B:305:LEU:HD23	2.01	0.60
1:B:1521:GLU:OE1	1:B:1521:GLU:N	2.34	0.60
1:A:663:GLU:HA	1:A:666:ARG:HD2	1.83	0.60
1:B:776:LYS:HB3	1:B:777:PRO:HD2	1.83	0.60
1:A:623:VAL:HG21	1:A:665:LEU:CD1	2.31	0.60
1:A:662:VAL:O	1:A:666:ARG:HG2	2.02	0.60
1:B:23:TRP:HB2	1:B:346:LEU:HD13	1.84	0.60
1:A:235:LYS:CG	1:A:238:LEU:HD13	2.32	0.60
1:A:626:SER:N	1:A:629:GLU:OE2	2.34	0.60
1:A:764:HIS:ND1	1:A:787:LYS:HE3	2.17	0.60
1:B:2022:VAL:HG13	1:B:2060:TRP:O	2.02	0.60
1:A:786:LYS:HE2	1:A:789:HIS:HD2	1.66	0.59
1:B:477:ARG:NH1	1:B:790:ARG:HD2	2.16	0.59
1:A:501:THR:HG22	1:A:766:LEU:CD1	2.29	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:TRP:HB3	1:B:167:ALA:HB1	1.84	0.59
1:B:705:PRO:HG3	1:B:731:SER:HB3	1.85	0.59
1:B:1333:VAL:HG12	1:B:1386:LEU:HD11	1.83	0.59
1:A:657:PRO:O	1:A:660:GLU:HG2	2.01	0.59
1:B:497:SER:OG	1:B:760:GLU:OE2	2.19	0.59
1:B:1613:VAL:CG2	1:B:1633:LEU:HD22	2.32	0.59
1:A:119:ALA:O	1:A:122:ARG:NH1	2.35	0.59
1:A:164:SER:HB2	1:A:338:LEU:HG	1.84	0.59
1:A:759:LEU:HD23	1:A:782:ILE:HB	1.84	0.59
1:A:1492:GLU:O	1:A:1496:VAL:HG23	2.02	0.59
1:B:79:LEU:O	1:B:83:LEU:HD13	2.02	0.59
1:B:532:LEU:HD12	1:B:532:LEU:O	2.02	0.59
1:A:293:HIS:O	1:A:326:LYS:HD2	2.03	0.59
1:B:619:ALA:HB3	1:B:658:VAL:HG11	1.84	0.59
1:A:620:MET:HE2	1:A:682:PHE:HB2	1.84	0.59
1:B:1329:LEU:HB3	1:B:1384:VAL:HG11	1.83	0.59
1:B:654:PRO:O	1:B:658:VAL:HG23	2.03	0.59
1:B:1241:LYS:N	1:B:1311:ASP:OD2	2.35	0.59
1:A:301:ASP:O	1:A:305:LEU:HD23	2.03	0.59
1:B:254:ASP:HA	1:B:268:ILE:HG13	1.85	0.59
1:A:292:ALA:HB2	1:A:322:ILE:HD11	1.84	0.59
1:A:425:ARG:HH21	1:A:811:ASN:HD22	1.49	0.58
1:A:549:ILE:HD13	1:A:610:ILE:HG21	1.84	0.58
1:A:713:LEU:HD22	1:A:722:TRP:HZ3	1.68	0.58
1:B:656:ALA:O	1:B:660:GLU:HG3	2.03	0.58
1:B:717:ILE:HD12	1:B:726:LEU:HD22	1.85	0.58
1:A:530:PHE:HE2	1:A:601:LEU:HD11	1.67	0.58
1:A:665:LEU:HB3	1:A:670:VAL:CG2	2.34	0.58
1:A:786:LYS:HE2	1:A:789:HIS:CD2	2.37	0.58
1:B:95:ILE:HD11	1:B:232:LEU:HD21	1.84	0.58
1:B:343:LYS:NZ	1:B:354:ALA:HB3	2.18	0.58
1:A:784:LEU:HD22	1:A:796:PHE:CD2	2.39	0.58
1:B:314:ALA:O	1:B:315:THR:OG1	2.14	0.58
1:B:696:GLN:HG2	1:B:700:LYS:NZ	2.18	0.58
1:A:585:VAL:HG12	1:A:599:ALA:HB1	1.86	0.58
1:A:1234:ASN:OD1	1:A:1502:VAL:HG23	2.03	0.58
1:B:420:LEU:HD21	1:B:512:ARG:HD2	1.85	0.58
1:A:675:VAL:O	1:A:677:THR:HG23	2.03	0.58
1:B:1795:LEU:HA	2:B:2601:NDP:H72N	1.69	0.58
1:B:1613:VAL:HG22	1:B:1633:LEU:HD22	1.86	0.58
1:A:3:GLU:HB2	1:A:236:LYS:CG	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ILE:HG22	1:A:228:VAL:HG13	1.85	0.58
1:B:694:LEU:O	1:B:698:LEU:HD23	2.03	0.58
1:A:658:VAL:O	1:A:662:VAL:HG23	2.04	0.57
1:A:661:PHE:O	1:A:665:LEU:HG	2.03	0.57
1:A:1419:ASP:OD1	1:A:1421:SER:N	2.37	0.57
1:A:1562:GLN:NE2	1:A:1607:ASP:OD2	2.36	0.57
1:A:123:ASP:OD2	1:A:126:THR:OG1	2.22	0.57
1:B:645:SER:HB3	1:B:648:THR:OG1	2.03	0.57
1:B:972:PRO:HD2	1:B:1079:VAL:HG21	1.85	0.57
1:A:159:THR:O	1:A:163:SER:HB3	2.03	0.57
1:A:2047:LYS:NZ	1:A:2051:GLU:OE2	2.36	0.57
1:B:257:LYS:HE3	1:B:263:PHE:O	2.04	0.57
1:B:689:ALA:O	1:B:692:PRO:HD2	2.03	0.57
1:A:1860:GLU:N	1:A:1860:GLU:OE1	2.38	0.57
1:B:661:PHE:O	1:B:665:LEU:HG	2.05	0.57
1:B:680:MET:HE2	1:B:680:MET:HA	1.85	0.57
1:A:9:MET:HE2	1:A:345:LEU:CD1	2.34	0.57
1:A:124:PRO:HG3	1:B:195:ASN:OD1	2.04	0.57
1:B:1031:ASP:OD2	1:B:1035:GLN:NE2	2.38	0.57
1:A:318:GLU:OE1	1:A:318:GLU:N	2.27	0.57
1:A:620:MET:CE	1:A:682:PHE:H	2.17	0.57
1:B:215:PHE:HZ	1:B:292:ALA:HB3	1.69	0.57
1:A:736:VAL:O	1:A:740:VAL:HG12	2.05	0.57
1:A:745:PHE:CE2	1:A:749:LEU:HD11	2.39	0.57
1:B:1219:LEU:HD12	1:B:1224:LEU:HD22	1.87	0.57
1:A:501:THR:CG2	1:A:766:LEU:HD13	2.30	0.57
1:A:622:ALA:HB2	1:A:650:THR:CG2	2.29	0.57
1:A:692:PRO:CD	1:A:693:PRO:HD2	2.35	0.57
1:A:1313:LEU:HD13	1:A:1336:LEU:CD2	2.34	0.57
1:B:555:SER:O	1:B:559:ILE:HG13	2.05	0.57
1:B:1596:ASP:O	1:B:1597:SER:OG	2.20	0.57
1:B:697:GLU:O	1:B:701:VAL:HG23	2.04	0.56
1:A:627:TRP:HA	1:A:630:CYS:SG	2.45	0.56
1:A:510:LEU:HD12	1:A:785:MET:HE1	1.87	0.56
1:A:1294:GLN:OE1	1:A:1294:GLN:N	2.38	0.56
1:A:1494:GLN:OE1	1:A:1494:GLN:N	2.38	0.56
1:B:209:GLU:N	1:B:209:GLU:OE1	2.39	0.56
1:B:341:LEU:CD1	1:B:404:LEU:HD11	2.36	0.56
1:B:721:GLN:OE1	1:B:721:GLN:N	2.39	0.56
1:B:759:LEU:HD23	1:B:782:ILE:HB	1.87	0.56
1:A:253:THR:HA	1:A:397:GLY:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:PHE:CE2	1:A:601:LEU:HD11	2.39	0.56
1:A:623:VAL:HG12	1:A:624:GLY:H	1.70	0.56
1:A:653:GLY:HA2	1:A:686:PHE:HE1	1.70	0.56
1:B:656:ALA:HB3	1:B:657:PRO:HD3	1.86	0.56
1:B:771:LEU:O	1:B:775:LEU:HB2	2.06	0.56
1:A:524:ASP:CG	1:A:533:LYS:HG3	2.25	0.56
1:A:692:PRO:HA	1:A:695:LEU:HD23	1.87	0.56
1:B:341:LEU:HD11	1:B:404:LEU:HD11	1.87	0.56
1:B:13:LEU:HB3	1:B:14:PRO:HD2	1.88	0.56
1:B:321:LEU:HD11	1:B:384:ARG:NH2	2.21	0.56
1:A:1603:PHE:CE1	1:A:1626:VAL:HG11	2.41	0.56
1:B:291:GLU:HG2	1:B:340:ALA:HB1	1.88	0.56
1:A:13:LEU:HB3	1:A:14:PRO:CD	2.36	0.56
1:A:626:SER:HB3	1:A:629:GLU:CG	2.36	0.56
1:A:1267:GLN:OE1	1:A:1267:GLN:N	2.34	0.56
1:A:1607:ASP:OD1	1:A:1608:ALA:N	2.36	0.56
1:B:556:LEU:O	1:B:560:GLN:HG3	2.06	0.56
1:B:662:VAL:O	1:B:666:ARG:HG2	2.05	0.56
1:B:699:LYS:NZ	1:B:733:GLU:OE2	2.30	0.56
1:A:597:GLU:OE1	1:A:597:GLU:N	2.34	0.56
1:A:1355:ASP:OD1	1:A:1356:ILE:N	2.39	0.56
1:A:1904:LEU:HB3	1:A:1909:VAL:HG21	1.88	0.56
1:B:532:LEU:HD21	1:B:604:TYR:CE2	2.38	0.56
1:A:564:ILE:HG12	1:A:761:ILE:HD13	1.88	0.55
1:A:235:LYS:HG3	1:A:238:LEU:HD13	1.88	0.55
1:A:501:THR:HG22	1:A:766:LEU:HD22	1.87	0.55
1:A:1318:ALA:N	1:A:1345:HIS:O	2.40	0.55
1:A:1940:GLN:NE2	1:A:1958:GLU:OE2	2.39	0.55
1:B:261:VAL:HG13	1:B:262:THR:HG23	1.87	0.55
1:B:290:ILE:O	1:B:322:ILE:HD12	2.05	0.55
1:B:708:ARG:HH22	1:B:714:SER:HB2	1.70	0.55
1:B:749:LEU:O	1:B:752:VAL:HG22	2.06	0.55
1:B:285:GLU:OE1	1:B:285:GLU:N	2.32	0.55
1:B:640:PRO:CB	1:B:651:ILE:HG22	2.37	0.55
1:A:3:GLU:OE1	1:A:3:GLU:N	2.40	0.55
1:A:31:ASP:OD2	1:A:50:ARG:NH2	2.37	0.55
1:A:623:VAL:HG11	1:A:665:LEU:HD13	1.89	0.55
1:A:687:MET:O	1:A:690:ILE:HG22	2.05	0.55
1:A:1973:VAL:HG12	2:A:2602:NDP:O5B	2.06	0.55
1:B:81:LEU:O	1:B:85:VAL:HG23	2.06	0.55
1:A:216:ASP:OD1	1:A:217:THR:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:607:GLY:O	1:A:611:LYS:HG3	2.07	0.55
1:A:1602:GLU:HB3	1:A:1650:VAL:HG23	1.89	0.55
1:B:550:VAL:O	1:B:554:VAL:HG23	2.06	0.55
1:B:642:CYS:HB2	1:B:650:THR:CG2	2.36	0.55
1:A:619:ALA:N	1:A:681:ALA:HB2	2.21	0.55
1:B:194:PRO:O	1:B:198:VAL:HG23	2.06	0.55
1:A:285:GLU:N	1:A:285:GLU:OE1	2.40	0.55
1:A:424:LEU:CD2	1:A:441:GLY:HA3	2.35	0.55
1:B:704:GLU:HB2	1:B:706:LYS:HZ1	1.71	0.55
1:A:241:ARG:HD3	1:A:243:TYR:CZ	2.41	0.55
1:A:424:LEU:HD22	1:A:441:GLY:HA3	1.89	0.55
1:B:654:PRO:HG3	1:B:686:PHE:CZ	2.36	0.55
1:A:623:VAL:HG21	1:A:665:LEU:HD12	1.87	0.55
1:A:986:ALA:O	1:A:990:VAL:HG23	2.06	0.55
1:A:1247:ALA:HB3	1:A:1280:LEU:HD22	1.88	0.55
1:A:1555:GLN:N	1:A:1555:GLN:OE1	2.38	0.55
1:B:658:VAL:O	1:B:662:VAL:HG23	2.07	0.55
1:A:277:TYR:CE1	1:A:284:PRO:HG3	2.42	0.55
1:A:745:PHE:HZ	1:A:771:LEU:HD21	1.72	0.54
1:B:238:LEU:HD23	1:B:238:LEU:O	2.07	0.54
1:B:497:SER:HB2	1:B:762:ALA:CB	2.36	0.54
1:B:1432:LEU:HD11	1:B:1465:GLY:O	2.07	0.54
1:B:252:ASN:ND2	1:B:268:ILE:HG23	2.22	0.54
1:B:619:ALA:HB3	1:B:658:VAL:CG1	2.37	0.54
1:B:1348:LEU:HD11	1:B:1399:THR:HG21	1.88	0.54
1:A:1973:VAL:HG22	1:A:1975:LEU:CD1	2.37	0.54
1:B:13:LEU:HB3	1:B:14:PRO:CD	2.37	0.54
1:B:116:THR:O	1:B:120:LEU:HD23	2.08	0.54
1:B:643:HIS:ND1	1:B:747:GLU:OE2	2.28	0.54
1:A:532:LEU:HD12	1:A:532:LEU:O	2.07	0.54
1:A:1802:GLU:O	1:A:1803:SER:OG	2.23	0.54
1:B:136:GLN:HB3	1:B:139:MET:HG2	1.89	0.54
1:A:527:VAL:HG11	1:A:532:LEU:HD11	1.89	0.54
1:A:1780:LEU:HD13	1:B:1782:MET:HE2	1.89	0.54
1:B:752:VAL:HG21	1:B:775:LEU:CD1	2.38	0.54
1:B:2042:GLU:OE2	1:B:2059:GLN:NE2	2.39	0.54
1:A:391:ASN:HB2	1:A:393:PHE:CZ	2.43	0.54
1:A:708:ARG:HD3	1:A:727:ALA:O	2.08	0.54
1:B:248:ASN:OD1	1:B:249:ALA:N	2.40	0.54
1:A:161:CYS:HA	1:A:333:GLU:O	2.07	0.54
1:A:168:LEU:HD23	1:A:168:LEU:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:GLN:O	1:A:273:ILE:HG13	2.08	0.54
1:A:737:ASN:HA	1:A:740:VAL:HG12	1.90	0.54
1:B:252:ASN:HD21	1:B:268:ILE:HG23	1.73	0.54
1:B:717:ILE:CG2	1:B:721:GLN:HB2	2.37	0.54
1:A:261:VAL:HG13	1:A:262:THR:HG23	1.90	0.54
1:A:607:GLY:O	1:A:610:ILE:HG22	2.06	0.54
1:A:1033:MET:SD	1:A:1089:ALA:HB3	2.48	0.54
1:B:1776:GLN:N	1:B:1776:GLN:OE1	2.41	0.54
1:A:627:TRP:CE3	1:A:643:HIS:HB2	2.44	0.53
1:B:65:PHE:HA	1:B:147:PHE:CE1	2.42	0.53
1:B:110:GLY:CA	1:B:163:SER:HB3	2.38	0.53
1:A:524:ASP:OD1	1:A:533:LYS:HG3	2.08	0.53
1:A:635:PRO:HD3	1:A:661:PHE:CD1	2.43	0.53
1:A:570:MET:HE1	1:A:810:ALA:HB1	1.90	0.53
1:A:752:VAL:O	1:A:752:VAL:HG23	2.08	0.53
1:B:542:ASP:HB2	1:B:545:THR:HG23	1.91	0.53
1:B:50:ARG:HD3	1:B:209:GLU:O	2.09	0.53
1:B:642:CYS:HB2	1:B:650:THR:HG22	1.90	0.53
1:A:59:ARG:HD2	1:A:838:HIS:HB3	1.91	0.53
1:B:552:SER:O	1:B:556:LEU:HD13	2.08	0.53
1:A:57:LEU:HD23	1:A:81:LEU:HD11	1.91	0.53
1:A:620:MET:H	1:A:677:THR:HG21	1.73	0.53
1:A:717:ILE:HD12	1:A:727:ALA:HB2	1.89	0.53
1:A:1286:GLU:O	1:A:1289:GLN:NE2	2.41	0.53
1:B:719:GLU:HA	1:B:722:TRP:CG	2.44	0.53
1:B:1973:VAL:HG11	2:B:2602:NDP:H51N	1.91	0.53
1:A:548:ASP:OD1	1:A:550:VAL:N	2.42	0.53
1:A:642:CYS:N	1:A:650:THR:OG1	2.42	0.53
1:A:1127:CYS:HB2	1:A:1128:LEU:HD12	1.91	0.53
1:B:499:MET:HE1	1:B:682:PHE:CE2	2.44	0.53
1:B:610:ILE:HD13	1:B:682:PHE:HE2	1.73	0.53
1:B:1265:LEU:HD21	1:B:2082:GLY:HA3	1.90	0.53
1:B:1343:LEU:HD11	1:B:1400:LEU:HD11	1.90	0.53
1:A:557:THR:O	1:A:561:ILE:HG13	2.09	0.52
1:B:747:GLU:OE1	1:B:747:GLU:N	2.37	0.52
1:A:521:LEU:O	1:A:525:GLU:HG2	2.09	0.52
1:B:83:LEU:HD12	1:B:144:LEU:HD21	1.90	0.52
1:B:127:LEU:HD12	1:B:127:LEU:O	2.09	0.52
1:B:640:PRO:HG3	1:B:651:ILE:HG22	1.92	0.52
1:B:1606:ARG:NH2	1:B:1862:GLU:O	2.42	0.52
1:B:504:ARG:HH21	1:B:541:THR:HG23	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:LYS:HE3	1:A:44:LEU:HD13	1.89	0.52
1:A:497:SER:HB3	1:A:762:ALA:CB	2.39	0.52
1:A:677:THR:HB	1:A:680:MET:O	2.10	0.52
1:A:1124:GLU:N	1:A:1124:GLU:OE1	2.42	0.52
1:B:95:ILE:HD12	1:B:100:LEU:HD11	1.92	0.52
1:A:242:VAL:HG23	1:A:822:PRO:HB3	1.91	0.52
1:A:692:PRO:HA	1:A:695:LEU:CD2	2.40	0.52
1:A:1795:LEU:HD22	1:B:1786:LEU:O	2.10	0.52
1:B:84:GLU:OE2	1:B:838:HIS:NE2	2.32	0.52
1:B:95:ILE:CD1	1:B:232:LEU:HD21	2.40	0.52
1:B:1417:VAL:HG13	1:B:1424:TRP:CE2	2.44	0.52
1:A:6:ILE:HG23	1:A:231:VAL:CG1	2.38	0.52
1:A:293:HIS:N	1:A:304:GLU:OE2	2.34	0.52
1:A:1458:ASN:ND2	1:A:2025:GLY:O	2.43	0.52
1:A:1888:ILE:HD11	1:A:1959:ALA:CB	2.39	0.52
1:B:625:LEU:HD21	1:B:629:GLU:HB3	1.92	0.52
1:B:682:PHE:HA	1:B:687:MET:CE	2.30	0.52
1:B:703:ARG:HB2	1:B:704:GLU:OE1	2.10	0.52
1:A:694:LEU:O	1:A:698:LEU:HG	2.09	0.52
1:A:705:PRO:HB2	1:A:729:THR:HG21	1.92	0.52
1:A:1893:LEU:HD12	1:A:1916:SER:OG	2.09	0.52
1:B:499:MET:HE1	1:B:682:PHE:CZ	2.44	0.52
1:B:1943:THR:HG22	1:B:1943:THR:O	2.09	0.52
1:B:71:GLN:OE1	1:B:143:ARG:NH2	2.43	0.52
1:B:873:HIS:O	1:B:876:VAL:HG12	2.09	0.52
1:B:1111:VAL:O	1:B:1111:VAL:HG13	2.10	0.52
1:B:663:GLU:O	1:B:667:LYS:HG3	2.10	0.52
1:B:762:ALA:HB1	1:B:763:PRO:HD2	1.92	0.52
1:A:623:VAL:HA	1:A:671:PHE:O	2.10	0.51
1:A:661:PHE:CE2	1:A:665:LEU:HD11	2.44	0.51
1:A:749:LEU:O	1:A:752:VAL:HG22	2.09	0.51
1:A:1220:ASP:OD1	1:A:1255:ARG:NH2	2.39	0.51
1:A:1436:ASP:OD1	1:A:1437:SER:N	2.43	0.51
1:B:503:TRP:CZ2	1:B:506:MET:HA	2.45	0.51
1:B:1197:GLU:O	1:B:1201:VAL:HG23	2.09	0.51
1:B:1453:VAL:O	1:B:1457:VAL:HG23	2.10	0.51
1:B:95:ILE:HG13	1:B:95:ILE:O	2.10	0.51
1:B:424:LEU:HA	1:B:455:ASN:HD21	1.74	0.51
1:B:605:TRP:CD1	1:B:701:VAL:HG21	2.45	0.51
1:B:675:VAL:HG23	1:B:677:THR:CG2	2.38	0.51
1:A:442:LEU:HD23	1:A:442:LEU:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:SER:O	1:A:559:ILE:HG13	2.09	0.51
1:A:620:MET:HB2	1:A:675:VAL:HG22	1.90	0.51
1:A:654:PRO:HD3	1:A:685:TYR:OH	2.11	0.51
1:A:502:GLN:OE1	1:A:502:GLN:N	2.33	0.51
1:B:754:GLU:O	1:B:755:HIS:HB2	2.10	0.51
1:A:460:VAL:CG1	1:A:465:MET:HG3	2.40	0.51
1:A:490:ARG:O	1:A:808:ILE:HD11	2.09	0.51
1:A:698:LEU:HB2	1:A:732:ALA:HB1	1.93	0.51
1:A:1753:LEU:O	1:A:1757:VAL:HG23	2.11	0.51
1:B:110:GLY:HA3	1:B:163:SER:HB3	1.92	0.51
1:B:274:ARG:HA	1:B:277:TYR:CD2	2.46	0.51
1:B:642:CYS:HA	1:B:743:VAL:HB	1.92	0.51
1:B:661:PHE:CE2	1:B:665:LEU:HD21	2.46	0.51
1:B:708:ARG:HG3	1:B:729:THR:CA	2.41	0.51
1:A:552:SER:O	1:A:556:LEU:HG	2.09	0.51
1:B:513:LEU:HD21	1:B:816:PHE:CE1	2.45	0.51
1:B:1113:ILE:HD11	1:B:2109:PHE:CE2	2.46	0.51
1:B:1113:ILE:HD11	1:B:2109:PHE:CZ	2.46	0.51
1:A:13:LEU:HB3	1:A:14:PRO:HD2	1.91	0.51
1:A:305:LEU:HD11	1:A:322:ILE:HD13	1.92	0.51
1:A:1973:VAL:HG22	1:A:1975:LEU:HD13	1.92	0.51
1:A:453:MET:O	1:A:457:ILE:HG23	2.10	0.51
1:A:510:LEU:HD12	1:A:785:MET:HE3	1.93	0.51
1:A:584:GLU:HG3	1:A:712:TRP:CZ2	2.38	0.51
1:A:653:GLY:HA2	1:A:686:PHE:CE1	2.46	0.51
1:A:737:ASN:HA	1:A:740:VAL:CG1	2.40	0.51
1:B:664:GLN:O	1:B:668:GLU:HG3	2.11	0.51
1:A:132:MET:O	1:A:136:GLN:HB2	2.10	0.51
1:A:549:ILE:HD13	1:A:610:ILE:CG2	2.41	0.51
1:B:203:LEU:HD23	1:B:205:MET:SD	2.50	0.51
1:B:563:LEU:O	1:B:567:LEU:HD13	2.11	0.51
1:B:1145:VAL:HG21	1:B:1356:ILE:HG12	1.93	0.51
1:B:1372:LEU:N	1:B:1372:LEU:HD12	2.26	0.51
1:B:1493:LEU:HD23	1:B:1493:LEU:O	2.09	0.51
1:A:1865:LEU:HD23	1:A:1866:LYS:N	2.26	0.51
1:B:705:PRO:CG	1:B:731:SER:HB3	2.41	0.51
1:B:1333:VAL:CG1	1:B:1386:LEU:HD11	2.41	0.51
1:B:1493:LEU:HA	1:B:1496:VAL:HG12	1.93	0.51
1:A:84:GLU:O	1:A:88:GLU:HG3	2.11	0.50
1:A:620:MET:N	1:A:677:THR:HG21	2.26	0.50
1:B:758:VAL:HG21	1:B:775:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1313:LEU:HB3	1:B:1342:LEU:HD12	1.92	0.50
1:A:752:VAL:HG21	1:A:775:LEU:HD22	1.92	0.50
1:B:44:LEU:HD13	1:B:904:GLY:O	2.11	0.50
1:B:243:TYR:HB3	1:B:345:LEU:HD22	1.92	0.50
1:B:304:GLU:O	1:B:308:ILE:HG13	2.10	0.50
1:B:769:ALA:O	1:B:773:ARG:HG2	2.12	0.50
1:A:497:SER:HB3	1:A:762:ALA:HB2	1.93	0.50
1:A:641:ALA:HB3	1:A:650:THR:OG1	2.11	0.50
1:B:577:ILE:N	1:B:577:ILE:HD12	2.27	0.50
1:A:424:LEU:HD12	1:A:455:ASN:OD1	2.12	0.50
1:A:654:PRO:HB2	1:A:657:PRO:HG2	1.94	0.50
1:A:740:VAL:HG13	1:A:741:SER:H	1.77	0.50
1:B:745:PHE:O	1:B:749:LEU:HG	2.12	0.50
1:A:198:VAL:O	1:A:202:ARG:HG2	2.12	0.50
1:B:57:LEU:HD23	1:B:81:LEU:HD11	1.94	0.50
1:B:431:PRO:O	1:B:435:GLN:HG2	2.11	0.50
1:A:1865:LEU:HD22	1:A:1867:GLY:O	2.11	0.50
1:A:1909:VAL:HG12	1:A:1911:LYS:H	1.76	0.50
1:B:412:PRO:HD3	1:B:824:PRO:HG2	1.94	0.50
1:B:595:SER:OG	1:B:598:GLU:HG2	2.12	0.50
1:B:927:LYS:HG2	1:B:928:THR:HG23	1.94	0.50
1:A:460:VAL:HG11	1:A:465:MET:HG3	1.94	0.50
1:B:348:LEU:HD13	1:B:406:PRO:HB3	1.92	0.50
1:B:365:GLU:OE1	1:B:365:GLU:N	2.41	0.50
1:B:702:ILE:HD12	1:B:702:ILE:N	2.27	0.50
1:B:708:ARG:NH2	1:B:714:SER:HB2	2.27	0.50
1:A:133:VAL:HG12	1:A:133:VAL:O	2.11	0.50
1:A:305:LEU:CD1	1:A:322:ILE:HD13	2.42	0.50
1:B:248:ASN:HB2	1:B:280:ALA:HB2	1.94	0.50
1:B:1371:ILE:C	1:B:1372:LEU:HD12	2.33	0.50
1:B:1428:LEU:HD23	1:B:1428:LEU:O	2.12	0.50
1:A:570:MET:CE	1:A:810:ALA:HB1	2.42	0.49
1:B:17:GLU:CG	1:B:55:LYS:HD3	2.42	0.49
1:B:283:ALA:O	1:B:286:SER:OG	2.26	0.49
1:A:9:MET:HE2	1:A:345:LEU:HD13	1.94	0.49
1:A:136:GLN:HB3	1:A:139:MET:HG2	1.94	0.49
1:B:692:PRO:HD2	1:B:693:PRO:HD2	1.94	0.49
1:A:225:SER:O	1:A:332:PRO:HA	2.12	0.49
1:A:664:GLN:O	1:A:667:LYS:HB2	2.12	0.49
1:A:466:PRO:O	1:A:484:GLN:HG3	2.13	0.49
1:B:635:PRO:HD3	1:B:661:PHE:CD1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1411:SER:OG	1:B:1439:ARG:NH1	2.45	0.49
1:B:183:ALA:O	1:B:232:LEU:HD12	2.12	0.49
1:B:1227:CYS:O	1:B:1230:THR:OG1	2.24	0.49
1:A:657:PRO:HA	1:A:660:GLU:CG	2.40	0.49
1:A:705:PRO:HB3	1:A:731:SER:HB3	1.95	0.49
1:A:1250:GLY:O	1:A:1316:ASN:ND2	2.45	0.49
1:A:1280:LEU:HD21	1:A:1287:LEU:HD21	1.95	0.49
1:A:1986:GLU:OE1	1:A:1986:GLU:N	2.43	0.49
1:B:420:LEU:HD22	1:B:512:ARG:HE	1.77	0.49
1:A:1020:LEU:HD22	1:A:1032:THR:HG22	1.94	0.49
1:A:1965:VAL:HG11	1:A:2010:CYS:SG	2.53	0.49
1:B:333:GLU:CB	1:B:334:PRO:HD3	2.32	0.49
1:B:1653:SER:HG	1:B:1807:TRP:HH2	1.57	0.49
1:A:1138:LEU:HD13	1:A:1214:LEU:HD21	1.95	0.49
1:A:155:ILE:N	1:A:155:ILE:HD12	2.28	0.49
1:A:234:THR:CG2	1:A:238:LEU:HB2	2.42	0.49
1:A:564:ILE:HD13	1:A:590:ALA:HB2	1.94	0.49
1:A:759:LEU:CD2	1:A:782:ILE:HB	2.43	0.49
1:A:1617:VAL:HG11	1:A:1626:VAL:CG2	2.41	0.49
1:B:440:GLN:HG2	1:B:833:LEU:CD1	2.39	0.49
1:A:9:MET:HE3	1:A:243:TYR:CZ	2.47	0.48
1:A:759:LEU:HD21	1:A:803:LEU:HD13	1.94	0.48
1:A:2020:SER:OG	1:A:2021:SER:N	2.46	0.48
1:B:435:GLN:O	1:B:439:GLU:HG2	2.13	0.48
1:B:305:LEU:HG	1:B:366:ILE:HD13	1.94	0.48
1:B:365:GLU:O	1:B:367:PRO:HD3	2.12	0.48
1:B:705:PRO:HB3	1:B:730:SER:O	2.12	0.48
1:A:1070:GLN:OE1	1:A:1070:GLN:N	2.45	0.48
1:B:580:HIS:CD2	1:B:743:VAL:HG11	2.48	0.48
1:B:630:CYS:SG	1:B:649:VAL:HB	2.53	0.48
1:A:740:VAL:HG13	1:A:741:SER:N	2.28	0.48
1:B:83:LEU:HD12	1:B:144:LEU:CD2	2.43	0.48
1:B:619:ALA:HB3	1:B:658:VAL:HB	1.96	0.48
1:B:623:VAL:HG13	1:B:665:LEU:HD13	1.94	0.48
1:B:1732:VAL:O	1:B:1736:THR:HG22	2.12	0.48
1:A:744:LEU:N	1:A:744:LEU:HD12	2.29	0.48
1:A:745:PHE:CZ	1:A:771:LEU:HD21	2.48	0.48
1:A:1218:LEU:HD13	1:A:1400:LEU:HB2	1.95	0.48
1:B:504:ARG:HD2	1:B:543:GLU:HG3	1.95	0.48
1:B:1538:ARG:NH2	1:B:1583:LEU:O	2.47	0.48
1:A:630:CYS:O	1:A:634:CYS:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1973:VAL:HG11	2:A:2602:NDP:H52N	1.95	0.48
1:B:524:ASP:OD1	1:B:533:LYS:HA	2.13	0.48
1:B:708:ARG:HD3	1:B:727:ALA:O	2.14	0.48
1:B:1374:GLN:OE1	1:B:1374:GLN:N	2.41	0.48
1:B:62:ALA:HB1	1:B:67:VAL:O	2.13	0.48
1:B:84:GLU:O	1:B:88:GLU:HG3	2.13	0.48
1:B:168:LEU:O	1:B:168:LEU:HD23	2.14	0.48
1:B:503:TRP:CB	1:B:787:LYS:HG3	2.43	0.48
1:B:1628:LEU:N	1:B:1628:LEU:HD23	2.28	0.48
1:A:663:GLU:HA	1:A:666:ARG:CG	2.44	0.48
1:A:1471:CYS:SG	1:A:1502:VAL:O	2.51	0.48
1:B:132:MET:O	1:B:136:GLN:HB2	2.13	0.48
1:B:468:ARG:CD	1:B:485:VAL:HG21	2.41	0.48
1:B:697:GLU:HA	1:B:700:LYS:NZ	2.29	0.48
1:B:1228:LEU:HD11	1:B:1256:ILE:CD1	2.44	0.48
1:A:321:LEU:N	1:A:321:LEU:HD12	2.29	0.48
1:A:656:ALA:HB3	1:A:657:PRO:HD3	1.96	0.48
1:A:692:PRO:HB2	1:A:693:PRO:CD	2.43	0.48
1:B:184:ILE:HD11	1:B:232:LEU:HD13	1.96	0.48
1:B:584:GLU:O	1:B:588:GLY:N	2.41	0.48
1:B:1384:VAL:O	1:B:1385:SER:OG	2.28	0.48
1:A:133:VAL:HG11	1:B:261:VAL:CG1	2.44	0.48
1:A:1446:ILE:CG2	1:A:1486:VAL:HG21	2.28	0.48
1:B:189:ASN:HB2	1:B:334:PRO:HD2	1.96	0.48
1:A:137:ARG:HD3	1:A:158:ASP:OD1	2.14	0.47
1:A:654:PRO:HB2	1:A:657:PRO:CG	2.44	0.47
1:A:776:LYS:HB3	1:A:777:PRO:HD2	1.96	0.47
1:B:506:MET:O	1:B:538:LEU:HD22	2.13	0.47
1:B:717:ILE:O	1:B:722:TRP:NE1	2.44	0.47
1:B:726:LEU:HD23	1:B:726:LEU:C	2.34	0.47
1:A:363:ASN:OD1	1:A:364:PRO:HD2	2.13	0.47
1:A:506:MET:HG3	1:A:559:ILE:HD11	1.96	0.47
1:A:524:ASP:OD1	1:A:533:LYS:HA	2.13	0.47
1:A:720:ALA:HB3	1:A:721:GLN:OE1	2.14	0.47
1:A:1616:LEU:CD1	1:A:1650:VAL:HG22	2.44	0.47
1:B:719:GLU:HA	1:B:722:TRP:CD1	2.49	0.47
1:B:1318:ALA:N	1:B:1345:HIS:O	2.45	0.47
1:B:1699:VAL:HG21	1:B:1705:ARG:HG2	1.96	0.47
1:A:527:VAL:HG12	1:A:527:VAL:O	2.13	0.47
1:A:627:TRP:CE3	1:A:640:PRO:HB2	2.49	0.47
1:A:1198:LEU:HD12	1:A:1198:LEU:C	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:LEU:HD11	1:B:402:ILE:HD13	1.97	0.47
1:B:184:ILE:CD1	1:B:232:LEU:HD13	2.44	0.47
1:B:193:LYS:HE2	1:B:195:ASN:HB2	1.95	0.47
1:A:953:VAL:HG22	1:A:954:VAL:HG23	1.97	0.47
1:B:161:CYS:HA	1:B:333:GLU:O	2.14	0.47
1:A:333:GLU:CB	1:A:334:PRO:HD3	2.34	0.47
1:A:353:TRP:CE2	1:A:383:VAL:HG22	2.49	0.47
1:A:502:GLN:HB3	1:A:556:LEU:HD21	1.96	0.47
1:A:1088:VAL:HG22	1:A:1093:HIS:CD2	2.50	0.47
1:A:2018:VAL:HG11	1:A:2041:MET:HB3	1.97	0.47
1:B:116:THR:HG22	1:B:120:LEU:HD23	1.96	0.47
1:B:196:THR:O	1:B:200:PHE:HD1	1.97	0.47
1:B:1218:LEU:HD13	1:B:1394:SER:HB3	1.96	0.47
1:A:620:MET:HE2	1:A:682:PHE:CB	2.45	0.47
1:A:706:LYS:C	1:A:729:THR:HG23	2.34	0.47
1:A:1826:LEU:HD12	1:A:1826:LEU:N	2.29	0.47
1:B:191:LEU:HD13	1:B:226:GLU:CG	2.45	0.47
1:B:537:LEU:HD22	1:B:551:HIS:CD2	2.50	0.47
1:B:680:MET:HA	1:B:680:MET:CE	2.45	0.47
1:B:894:ILE:HG22	1:B:935:VAL:HG21	1.96	0.47
1:B:1473:LEU:C	1:B:1474:LEU:HD12	2.34	0.47
1:A:549:ILE:CD1	1:A:610:ILE:HG21	2.44	0.47
1:A:663:GLU:HA	1:A:666:ARG:CD	2.45	0.47
1:B:698:LEU:HD12	1:B:702:ILE:HD13	1.97	0.47
1:A:440:GLN:HG3	1:A:833:LEU:CD1	2.45	0.47
1:A:1443:LEU:HD12	1:A:1443:LEU:H	1.79	0.47
1:B:619:ALA:HB3	1:B:658:VAL:CB	2.44	0.47
1:B:728:ARG:O	1:B:728:ARG:HG2	2.15	0.47
1:A:5:VAL:HB	1:A:242:VAL:HG13	1.96	0.47
1:A:517:ARG:O	1:A:521:LEU:HG	2.15	0.47
1:A:657:PRO:CA	1:A:660:GLU:HG2	2.45	0.47
1:A:783:PRO:HB2	1:A:795:PHE:CE2	2.50	0.47
1:A:1071:ASP:OD1	1:A:1072:LYS:N	2.43	0.47
1:A:1628:LEU:HD11	1:A:1632:PHE:HB2	1.97	0.47
1:B:706:LYS:O	1:B:729:THR:OG1	2.29	0.47
1:B:1441:VAL:HG22	1:B:1468:ARG:O	2.15	0.47
1:B:1486:VAL:HG13	1:B:1486:VAL:O	2.15	0.47
1:A:67:VAL:HG13	1:A:71:GLN:HB2	1.97	0.46
1:A:609:CYS:HB3	1:A:690:ILE:HD11	1.96	0.46
1:A:1020:LEU:HD22	1:A:1032:THR:CG2	2.45	0.46
1:A:1128:LEU:HD11	1:A:1218:LEU:HD23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:GLY:O	1:B:223:CYS:HB2	2.15	0.46
1:B:261:VAL:HG22	1:B:261:VAL:O	2.14	0.46
1:A:1471:CYS:SG	1:A:1503:MET:SD	3.13	0.46
1:B:231:VAL:HG12	1:B:233:LEU:HD12	1.96	0.46
1:B:305:LEU:HD12	1:B:374:LEU:HD13	1.97	0.46
1:B:685:TYR:O	1:B:688:GLU:HG3	2.14	0.46
1:B:1280:LEU:HD12	1:B:1281:GLU:N	2.30	0.46
1:A:377:VAL:O	1:A:377:VAL:HG13	2.14	0.46
1:A:661:PHE:CZ	1:A:665:LEU:HD21	2.50	0.46
1:B:585:VAL:HG12	1:B:599:ALA:HB1	1.97	0.46
1:B:1311:ASP:O	1:B:1341:PHE:N	2.48	0.46
1:A:142:ASN:HD22	1:B:396:GLY:HA3	1.80	0.46
1:A:469:GLY:HA2	1:A:805:LEU:HD21	1.97	0.46
1:A:673:LYS:HD2	1:A:674:GLU:H	1.80	0.46
1:A:370:LEU:HD12	1:A:370:LEU:N	2.31	0.46
1:A:523:SER:O	1:A:527:VAL:HG23	2.16	0.46
1:A:655:GLN:HG2	1:A:656:ALA:N	2.31	0.46
1:B:198:VAL:O	1:B:202:ARG:HG2	2.15	0.46
1:B:443:ARG:NH1	1:B:443:ARG:HB3	2.30	0.46
1:B:1457:VAL:HG21	1:B:1471:CYS:HB3	1.98	0.46
1:B:1904:LEU:HB3	1:B:1909:VAL:HG21	1.97	0.46
1:A:440:GLN:HG3	1:A:833:LEU:HD13	1.98	0.46
1:A:680:MET:HG3	1:A:682:PHE:CE1	2.50	0.46
1:A:276:LEU:HD12	1:A:401:HIS:ND1	2.30	0.46
1:A:697:GLU:O	1:A:701:VAL:HG23	2.16	0.46
1:A:989:GLU:OE1	1:A:1924:TYR:N	2.48	0.46
1:A:1973:VAL:HG23	1:A:2034:TYR:HE1	1.80	0.46
1:B:7:ALA:HA	1:B:241:ARG:O	2.16	0.46
1:B:1205:GLU:OE1	1:B:1209:LEU:HD12	2.16	0.46
1:A:288:GLU:HG2	1:A:288:GLU:O	2.15	0.46
1:A:25:ASN:HA	1:A:30:VAL:HG22	1.98	0.46
1:A:39:ARG:HG2	1:A:53:LYS:HD2	1.97	0.46
1:A:127:LEU:HD12	1:A:127:LEU:O	2.16	0.46
1:A:673:LYS:HD2	1:A:674:GLU:N	2.31	0.46
1:A:781:ILE:C	1:A:782:ILE:HD12	2.37	0.46
1:A:1360:LEU:N	1:A:1360:LEU:HD12	2.30	0.46
1:A:2018:VAL:HG13	1:A:2041:MET:CE	2.46	0.46
1:B:1492:GLU:OE1	1:B:1492:GLU:N	2.42	0.46
1:B:1699:VAL:HG11	1:B:1708:LEU:HD12	1.98	0.46
1:A:601:LEU:HD23	1:A:701:VAL:CG1	2.35	0.46
1:A:623:VAL:HG12	1:A:624:GLY:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:783:PRO:O	1:A:784:LEU:HB2	2.16	0.46
1:B:437:LEU:HD22	1:B:454:LEU:HD22	1.98	0.46
1:A:9:MET:HE2	1:A:345:LEU:HD12	1.96	0.45
1:A:12:LYS:HG2	1:A:17:GLU:O	2.15	0.45
1:A:819:VAL:HG23	1:A:821:PHE:CZ	2.51	0.45
1:B:692:PRO:N	1:B:693:PRO:HD2	2.31	0.45
1:B:692:PRO:CD	1:B:693:PRO:HD2	2.46	0.45
1:A:250:GLY:HA3	1:A:276:LEU:HD21	1.97	0.45
1:A:848:GLU:CD	1:A:848:GLU:H	2.20	0.45
1:A:1372:LEU:HG	1:A:1376:ALA:HB3	1.98	0.45
1:A:1902:GLN:OE1	1:A:1932:TRP:NE1	2.45	0.45
1:B:829:LEU:N	1:B:829:LEU:HD12	2.31	0.45
1:A:450:PHE:CE2	1:A:454:LEU:HD11	2.51	0.45
1:A:731:SER:O	1:A:734:TYR:N	2.48	0.45
1:A:946:VAL:O	1:A:953:VAL:HG12	2.15	0.45
1:B:420:LEU:HD22	1:B:512:ARG:NE	2.31	0.45
1:B:503:TRP:NE1	1:B:506:MET:HB3	2.31	0.45
1:B:527:VAL:HG22	1:B:527:VAL:O	2.16	0.45
1:B:733:GLU:O	1:B:736:VAL:HG22	2.16	0.45
1:B:276:LEU:HD12	1:B:401:HIS:HB3	1.99	0.45
1:A:155:ILE:HG21	1:B:157:LEU:HD22	1.96	0.45
1:A:234:THR:HG22	1:A:235:LYS:N	2.32	0.45
1:A:717:ILE:CD1	1:A:727:ALA:HB2	2.46	0.45
1:A:1248:GLY:O	1:A:1251:HIS:NE2	2.49	0.45
1:B:343:LYS:HZ2	1:B:354:ALA:HB3	1.82	0.45
1:B:469:GLY:HA2	1:B:805:LEU:HD21	1.98	0.45
1:A:684:SER:HB2	1:A:686:PHE:HD1	1.82	0.45
1:A:1576:ILE:O	1:A:1580:THR:HG22	2.16	0.45
1:B:1593:THR:HG22	1:B:1593:THR:O	2.16	0.45
1:A:86:THR:O	1:A:90:ILE:HG13	2.17	0.45
1:A:606:ARG:NH1	1:A:739:LEU:HD13	2.31	0.45
1:A:1651:VAL:HG23	1:A:1652:TYR:N	2.31	0.45
1:B:127:LEU:HD12	1:B:127:LEU:C	2.37	0.45
1:B:133:VAL:HG22	1:B:133:VAL:O	2.15	0.45
1:B:1122:HIS:ND1	1:B:1511:TRP:O	2.50	0.45
1:B:1244:GLU:OE2	1:B:1252:LEU:HB2	2.16	0.45
1:B:92:ASP:HA	1:B:830:ILE:HB	1.99	0.45
1:B:619:ALA:CB	1:B:658:VAL:HG11	2.46	0.45
1:A:692:PRO:HB2	1:A:693:PRO:HD3	1.99	0.45
1:B:1650:VAL:HG13	1:B:1651:VAL:N	2.32	0.45
1:B:1973:VAL:HG12	2:B:2602:NDP:H52A	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:THR:HG23	1:A:546:PHE:N	2.33	0.44
1:A:1313:LEU:HD13	1:A:1336:LEU:HD21	1.99	0.44
1:B:126:THR:O	1:B:126:THR:HG22	2.17	0.44
1:B:737:ASN:HA	1:B:740:VAL:HG22	1.98	0.44
1:A:60:PHE:CD2	1:A:80:ARG:HD2	2.53	0.44
1:A:267:ASP:O	1:A:271:GLN:HG3	2.17	0.44
1:A:652:SER:HB3	1:A:681:ALA:HB1	2.00	0.44
1:A:1348:LEU:HD13	1:A:1374:GLN:HB3	1.98	0.44
1:B:301:ASP:HB2	1:B:302:PRO:HD3	1.99	0.44
1:B:610:ILE:HD13	1:B:682:PHE:CE2	2.52	0.44
1:B:793:LEU:O	1:B:797:LEU:HG	2.16	0.44
1:B:995:ARG:HA	1:B:999:TYR:O	2.17	0.44
1:B:1066:LEU:HD23	1:B:1076:ALA:HB2	1.99	0.44
1:B:1624:THR:O	1:B:1624:THR:HG22	2.17	0.44
1:A:133:VAL:HG11	1:B:261:VAL:HG11	1.98	0.44
1:A:556:LEU:O	1:A:560:GLN:HG3	2.18	0.44
1:A:241:ARG:HD3	1:A:243:TYR:CE2	2.52	0.44
1:B:33:VAL:HG12	1:B:50:ARG:HB3	1.99	0.44
1:B:745:PHE:CE2	1:B:749:LEU:HD11	2.53	0.44
1:B:2097:LEU:O	1:B:2097:LEU:HD23	2.17	0.44
1:A:582:LEU:HG	1:A:583:GLY:N	2.32	0.44
1:A:706:LYS:HB3	1:A:707:PRO:HD2	1.98	0.44
1:A:1009:LEU:HD12	1:A:1075:VAL:HG11	1.98	0.44
1:A:1342:LEU:HD11	1:A:1344:LEU:HD21	2.00	0.44
1:A:1743:LEU:HD21	1:A:1767:LEU:CD1	2.48	0.44
1:A:1973:VAL:H	2:A:2602:NDP:H52A	1.81	0.44
1:B:191:LEU:HD13	1:B:226:GLU:HG3	1.98	0.44
1:A:622:ALA:HA	1:A:649:VAL:O	2.16	0.44
1:A:1533:VAL:HG12	1:A:1622:LEU:O	2.18	0.44
1:B:130:TYR:O	1:B:133:VAL:HG12	2.18	0.44
1:B:412:PRO:HD3	1:B:824:PRO:CG	2.47	0.44
1:B:640:PRO:CG	1:B:651:ILE:HG22	2.47	0.44
1:B:1366:GLN:NE2	1:B:1369:GLN:OE1	2.51	0.44
1:A:9:MET:HE1	1:A:345:LEU:HB3	1.98	0.44
1:A:617:PRO:HB2	1:A:655:GLN:CD	2.38	0.44
1:A:878:HIS:CE1	1:A:880:LEU:HD11	2.52	0.44
1:B:347:SER:HB2	1:B:352:LEU:O	2.18	0.44
1:B:528:LYS:N	1:B:529:PRO:HD2	2.33	0.44
1:B:752:VAL:HG21	1:B:775:LEU:HD11	2.00	0.44
1:A:388:VAL:HG12	1:A:389:GLY:N	2.33	0.44
1:A:596:GLN:O	1:A:600:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:THR:HG23	1:B:184:ILE:HG21	2.00	0.44
1:B:155:ILE:HG22	1:B:156:ALA:N	2.33	0.44
1:A:476:GLU:N	1:A:794:GLU:OE2	2.35	0.44
1:A:647:ASP:HB2	1:A:773:ARG:HH11	1.83	0.44
1:B:95:ILE:HD11	1:B:232:LEU:CD2	2.47	0.44
1:B:733:GLU:HA	1:B:736:VAL:HG22	2.00	0.44
1:B:1329:LEU:O	1:B:1333:VAL:HG22	2.18	0.44
1:B:1794:VAL:C	1:B:1795:LEU:HD12	2.38	0.44
1:B:1905:ILE:CD1	1:B:1937:VAL:HG11	2.48	0.44
1:A:654:PRO:C	1:A:657:PRO:HD2	2.37	0.43
1:B:953:VAL:HG12	1:B:954:VAL:HG23	2.00	0.43
1:A:608:GLN:HA	1:A:608:GLN:OE1	2.18	0.43
1:A:695:LEU:HD13	1:A:699:LYS:NZ	2.33	0.43
1:A:1341:PHE:HD2	1:A:1402:LEU:HD11	1.83	0.43
1:B:60:PHE:HB3	1:B:842:TRP:CD1	2.53	0.43
1:B:111:VAL:CG2	1:B:188:ILE:HD11	2.49	0.43
1:B:1206:ARG:NH1	1:B:1209:LEU:HD13	2.32	0.43
1:B:1261:SER:N	1:B:1262:PRO:HD2	2.32	0.43
1:B:1313:LEU:HB2	1:B:1336:LEU:HD21	1.99	0.43
1:A:1343:LEU:O	1:A:1344:LEU:HD23	2.19	0.43
1:A:1454:VAL:HG21	1:A:1514:PHE:HE2	1.82	0.43
1:B:431:PRO:HG3	1:B:467:PHE:CE2	2.53	0.43
1:B:1540:ASP:OD1	1:B:1542:SER:OG	2.30	0.43
1:A:64:PHE:HE1	1:A:464:ALA:HB1	1.84	0.43
1:A:105:THR:O	1:A:150:PHE:HB3	2.17	0.43
1:A:347:SER:HB3	1:A:352:LEU:O	2.19	0.43
1:A:585:VAL:CG1	1:A:599:ALA:HB1	2.49	0.43
1:A:886:PHE:HB2	1:A:925:LEU:HD11	1.99	0.43
1:B:1580:THR:O	1:B:1580:THR:HG22	2.19	0.43
1:A:560:GLN:O	1:A:564:ILE:HG13	2.19	0.43
1:A:1973:VAL:O	1:A:1973:VAL:HG13	2.18	0.43
1:B:1555:GLN:OE1	1:B:1555:GLN:N	2.48	0.43
1:A:341:LEU:O	1:A:345:LEU:HG	2.19	0.43
1:A:550:VAL:HG13	1:A:551:HIS:ND1	2.34	0.43
1:A:663:GLU:HA	1:A:666:ARG:HG2	1.99	0.43
1:A:764:HIS:HB3	1:A:766:LEU:CD1	2.49	0.43
1:A:1261:SER:N	1:A:1262:PRO:HD2	2.34	0.43
1:B:537:LEU:HD22	1:B:551:HIS:HD2	1.84	0.43
1:B:717:ILE:HG22	1:B:721:GLN:HB2	2.00	0.43
1:B:1130:GLU:OE1	1:B:1130:GLU:N	2.46	0.43
1:A:69:PRO:O	1:A:73:HIS:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:LEU:HD12	1:A:157:LEU:N	2.34	0.43
1:A:332:PRO:HB2	1:A:335:ALA:HB3	2.00	0.43
1:A:1699:VAL:HG11	1:A:1708:LEU:HD12	2.01	0.43
1:B:164:SER:OG	1:B:334:PRO:O	2.25	0.43
1:B:503:TRP:HB3	1:B:787:LYS:HG3	2.00	0.43
1:B:520:ILE:HG23	1:B:534:VAL:CG1	2.48	0.43
1:A:695:LEU:HD12	1:A:696:GLN:N	2.33	0.43
1:A:1280:LEU:HD21	1:A:1287:LEU:CD2	2.49	0.43
1:A:1343:LEU:HG	1:A:1400:LEU:HD21	2.01	0.43
1:B:640:PRO:CA	1:B:651:ILE:HG22	2.49	0.43
1:B:720:ALA:HB3	1:B:721:GLN:OE1	2.18	0.43
1:B:764:HIS:ND1	1:B:787:LYS:HB2	2.34	0.43
1:A:760:GLU:OE2	1:A:767:LEU:HB2	2.18	0.43
1:A:2063:ILE:HG12	2:A:2602:NDP:C7N	2.49	0.43
1:B:144:LEU:O	1:B:148:PHE:HD2	2.02	0.43
1:B:293:HIS:N	1:B:304:GLU:OE2	2.28	0.43
1:B:322:ILE:HG22	1:B:375:GLN:O	2.19	0.43
1:B:1025:ASN:ND2	1:B:1028:SER:OG	2.52	0.43
1:A:62:ALA:HB1	1:A:67:VAL:O	2.18	0.43
1:A:468:ARG:HD2	1:A:485:VAL:HG21	2.01	0.43
1:A:491:PRO:HG2	1:A:756:ALA:HA	2.00	0.43
1:B:503:TRP:CD1	1:B:506:MET:HB3	2.54	0.43
1:A:533:LYS:HE3	1:A:536:GLN:CG	2.32	0.42
1:A:879:THR:HG22	1:A:884:VAL:HG22	2.01	0.42
1:A:1443:LEU:HD13	1:A:1457:VAL:HG12	2.01	0.42
1:B:295:THR:CG2	1:B:297:THR:HG23	2.49	0.42
1:B:758:VAL:HB	1:B:781:ILE:HD13	1.99	0.42
1:B:1315:CYS:HB3	1:B:1344:LEU:HD12	1.99	0.42
1:B:524:ASP:OD2	1:B:533:LYS:HB3	2.19	0.42
1:B:1476:ASN:OD1	1:B:1508:ASP:N	2.50	0.42
1:A:495:ILE:HD12	1:A:771:LEU:HD13	2.00	0.42
1:A:595:SER:H	1:A:598:GLU:CD	2.21	0.42
1:A:666:ARG:CZ	1:A:666:ARG:HB3	2.48	0.42
1:A:705:PRO:CB	1:A:729:THR:HG21	2.48	0.42
1:A:891:TYR:O	1:A:895:VAL:HG23	2.19	0.42
1:A:948:GLU:OE2	1:A:949:ASN:ND2	2.52	0.42
1:A:1126:GLY:N	1:A:1393:LYS:O	2.52	0.42
1:B:125:GLU:O	1:B:125:GLU:HG2	2.17	0.42
1:B:732:ALA:O	1:B:736:VAL:HG13	2.20	0.42
1:A:5:VAL:HG11	1:A:236:LYS:HD2	2.01	0.42
1:A:6:ILE:HG23	1:A:231:VAL:HG13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ASP:OD1	1:A:38:ARG:HG3	2.20	0.42
1:A:92:ASP:OD1	1:A:241:ARG:NH1	2.53	0.42
1:A:652:SER:HB2	1:A:684:SER:OG	2.18	0.42
1:A:1225:LYS:HD3	1:A:1259:LEU:HD12	2.01	0.42
1:B:1182:LEU:CD2	1:B:1360:LEU:HD11	2.46	0.42
1:B:1318:ALA:HB1	1:B:1347:LEU:CD1	2.49	0.42
1:B:1699:VAL:HG21	1:B:1705:ARG:CG	2.49	0.42
1:B:2001:ASN:O	1:B:2005:VAL:HG23	2.20	0.42
1:A:1413:ILE:HG21	1:A:1431:ILE:HD12	2.01	0.42
1:B:752:VAL:HG23	1:B:752:VAL:O	2.20	0.42
1:B:1343:LEU:HD12	1:B:1401:PHE:O	2.19	0.42
1:B:1474:LEU:HD12	1:B:1474:LEU:N	2.34	0.42
1:A:661:PHE:CE2	1:A:665:LEU:HD21	2.54	0.42
1:A:673:LYS:HE3	1:A:674:GLU:O	2.19	0.42
1:A:1671:LEU:HD12	1:A:1671:LEU:N	2.35	0.42
1:B:63:SER:OG	1:B:429:ARG:NH2	2.53	0.42
1:B:164:SER:OG	1:B:335:ALA:HA	2.19	0.42
1:B:652:SER:HB3	1:B:681:ALA:HB1	2.00	0.42
1:B:1364:GLU:N	1:B:1365:PRO:HD2	2.35	0.42
1:B:1888:ILE:CD1	1:B:1956:ILE:HD13	2.49	0.42
1:B:1974:VAL:HG13	1:B:1974:VAL:O	2.20	0.42
1:A:18:ASN:OD1	1:A:20:GLN:HB3	2.20	0.42
1:A:151:ARG:NH1	1:B:268:ILE:HD11	2.35	0.42
1:A:263:PHE:CE2	1:A:299:VAL:HG11	2.54	0.42
1:A:353:TRP:NE1	1:A:383:VAL:HG22	2.34	0.42
1:A:1214:LEU:HD23	1:A:1353:LEU:HD22	2.01	0.42
1:A:212:CYS:SG	1:A:222:TYR:HA	2.60	0.42
1:A:252:ASN:HB2	1:B:151:ARG:O	2.20	0.42
1:A:1111:VAL:O	1:A:1111:VAL:HG22	2.19	0.42
1:A:1413:ILE:HG21	1:A:1431:ILE:CD1	2.50	0.42
1:B:65:PHE:CD2	1:B:83:LEU:HD23	2.55	0.42
1:B:701:VAL:HG12	1:B:702:ILE:HD12	2.00	0.42
1:B:717:ILE:HD11	1:B:726:LEU:HD22	2.00	0.42
1:B:1209:LEU:N	1:B:1210:PRO:HD2	2.34	0.42
1:B:1767:LEU:HD23	1:B:1792:HIS:HB2	2.01	0.42
1:A:1246:LEU:N	1:A:1273:THR:O	2.53	0.42
1:A:1313:LEU:HD13	1:A:1336:LEU:HD23	2.01	0.42
1:B:876:VAL:HG13	1:B:877:ASP:OD1	2.19	0.42
1:A:1196:LEU:O	1:A:1200:GLN:NE2	2.52	0.42
1:B:111:VAL:HG22	1:B:188:ILE:HD11	2.01	0.42
1:B:497:SER:HB2	1:B:762:ALA:HB1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:TYR:HA	1:A:321:LEU:O	2.20	0.41
1:A:293:HIS:NE2	1:A:393:PHE:O	2.53	0.41
1:A:497:SER:OG	1:A:501:THR:HG21	2.19	0.41
1:A:784:LEU:O	1:A:785:MET:HG3	2.20	0.41
1:A:802:ARG:NH1	1:A:802:ARG:HB2	2.35	0.41
1:A:1218:LEU:HD21	1:A:1394:SER:HB2	2.01	0.41
1:B:111:VAL:HB	1:B:137:ARG:HD2	2.00	0.41
1:B:325:THR:HB	1:B:343:LYS:HD2	2.02	0.41
1:B:588:GLY:HA2	1:B:712:TRP:CZ3	2.54	0.41
1:A:9:MET:HG3	1:A:19:LEU:HD12	2.01	0.41
1:A:613:ALA:O	1:A:614:HIS:HB2	2.20	0.41
1:A:1314:VAL:HG12	1:A:1343:LEU:HB3	2.01	0.41
1:A:1412:PRO:O	1:A:1439:ARG:NH2	2.53	0.41
1:B:17:GLU:HG3	1:B:55:LYS:HD3	2.01	0.41
1:B:453:MET:O	1:B:457:ILE:HG23	2.20	0.41
1:B:705:PRO:C	1:B:706:LYS:HD2	2.40	0.41
1:A:101:ARG:NH1	1:A:149:ASP:HB2	2.35	0.41
1:A:105:THR:HA	1:A:182:ALA:O	2.20	0.41
1:A:582:LEU:HG	1:A:583:GLY:H	1.85	0.41
1:A:692:PRO:N	1:A:693:PRO:HD2	2.36	0.41
1:B:27:ILE:HG13	1:B:27:ILE:O	2.20	0.41
1:B:233:LEU:HD12	1:B:233:LEU:N	2.35	0.41
1:A:242:VAL:CG2	1:A:822:PRO:HB3	2.49	0.41
1:A:1487:ASP:O	1:A:1490:SER:OG	2.27	0.41
1:B:60:PHE:HB3	1:B:842:TRP:NE1	2.36	0.41
1:B:322:ILE:O	1:B:376:VAL:HA	2.19	0.41
1:A:620:MET:CG	1:A:677:THR:HG21	2.46	0.41
1:A:1128:LEU:HD12	1:A:1128:LEU:N	2.35	0.41
1:A:1483:VAL:O	1:A:1483:VAL:HG13	2.21	0.41
1:A:1519:LEU:HD12	1:A:1519:LEU:O	2.20	0.41
1:B:293:HIS:CD2	1:B:393:PHE:H	2.38	0.41
1:B:1333:VAL:HA	1:B:1336:LEU:HD12	2.03	0.41
1:A:39:ARG:HD3	1:A:39:ARG:HA	1.87	0.41
1:A:476:GLU:HG3	1:A:794:GLU:OE2	2.20	0.41
1:A:708:ARG:NH2	1:A:714:SER:HG	2.19	0.41
1:A:764:HIS:CE1	1:A:787:LYS:HE3	2.55	0.41
1:B:704:GLU:HB2	1:B:706:LYS:HZ2	1.84	0.41
1:B:1138:LEU:C	1:B:1138:LEU:HD23	2.41	0.41
1:B:1905:ILE:HD12	1:B:1937:VAL:HG11	2.03	0.41
1:A:194:PRO:O	1:A:198:VAL:HG23	2.20	0.41
1:A:225:SER:OG	1:A:331:HIS:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:CYS:O	1:A:594:LEU:HD23	2.21	0.41
1:B:54:LEU:HD12	1:B:57:LEU:HD21	2.02	0.41
1:B:808:ILE:HG22	1:B:809:ASP:N	2.36	0.41
1:B:1989:GLN:O	1:B:1993:LYS:HG2	2.20	0.41
1:A:154:SER:C	1:A:155:ILE:HD12	2.41	0.41
1:A:276:LEU:HD12	1:A:401:HIS:HB3	2.03	0.41
1:A:457:ILE:O	1:A:457:ILE:HG13	2.21	0.41
1:A:515:ARG:HB2	1:A:566:LEU:HD23	2.03	0.41
1:A:665:LEU:O	1:A:668:GLU:N	2.53	0.41
1:A:733:GLU:O	1:A:736:VAL:HG12	2.20	0.41
1:A:783:PRO:HB2	1:A:795:PHE:HE2	1.84	0.41
1:A:1329:LEU:HD22	1:A:1380:LEU:CD2	2.51	0.41
1:A:1949:LEU:HD21	1:A:1953:ARG:NH2	2.36	0.41
1:B:52:GLY:O	1:B:225:SER:HA	2.21	0.41
1:B:504:ARG:HH21	1:B:541:THR:CG2	2.34	0.41
1:B:612:GLU:HA	1:B:612:GLU:OE1	2.21	0.41
1:B:622:ALA:HA	1:B:650:THR:HA	2.03	0.41
1:B:625:LEU:HG	1:B:629:GLU:HB2	2.03	0.41
1:B:631:LYS:HA	1:B:634:CYS:SG	2.61	0.41
1:B:687:MET:SD	1:B:739:LEU:HD11	2.61	0.41
1:B:861:ILE:HD13	1:B:934:GLU:HB3	2.03	0.41
1:B:1411:SER:O	1:B:1439:ARG:NH1	2.54	0.41
1:A:64:PHE:CE1	1:A:464:ALA:HB1	2.56	0.41
1:A:655:GLN:OE1	1:A:655:GLN:N	2.36	0.41
1:A:1312:LEU:C	1:A:1313:LEU:HD12	2.41	0.41
1:B:626:SER:HB2	1:B:629:GLU:CD	2.40	0.41
1:B:654:PRO:HB2	1:B:657:PRO:CG	2.49	0.41
1:B:1606:ARG:NH1	1:B:1860:GLU:OE1	2.54	0.41
1:A:1198:LEU:HD12	1:A:1199:ALA:N	2.36	0.40
1:B:549:ILE:HD11	1:B:553:PHE:CE2	2.57	0.40
1:B:605:TRP:CE3	1:B:605:TRP:HA	2.56	0.40
1:A:352:LEU:HD23	1:A:382:PRO:HA	2.03	0.40
1:A:490:ARG:HD3	1:A:806:SER:O	2.21	0.40
1:B:193:LYS:CG	1:B:195:ASN:HD22	2.34	0.40
1:B:293:HIS:HB3	1:B:304:GLU:OE1	2.20	0.40
1:B:593:CYS:SG	1:B:708:ARG:HA	2.62	0.40
1:B:1348:LEU:CD1	1:B:1399:THR:HG21	2.51	0.40
1:B:2063:ILE:HG12	2:B:2602:NDP:C7N	2.52	0.40
1:A:75:MET:CG	1:A:79:LEU:HD23	2.51	0.40
1:B:1141:CYS:O	1:B:1145:VAL:HG23	2.22	0.40
1:A:229:VAL:HG12	1:A:230:ALA:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1780:LEU:HB2	1:B:1782:MET:HE3	2.03	0.40
1:B:371:ASP:OD1	1:B:372:GLY:N	2.48	0.40
1:B:1976:ARG:O	1:B:2033:ASN:ND2	2.53	0.40
1:A:9:MET:HE3	1:A:243:TYR:CE2	2.57	0.40
1:A:47:LEU:HD13	1:A:197:SER:HB2	2.03	0.40
1:A:109:VAL:HG12	1:A:111:VAL:CG2	2.52	0.40
1:A:621:ALA:HA	1:A:673:LYS:O	2.22	0.40
1:A:1593:THR:HG22	1:A:1594:SER:N	2.36	0.40
1:B:132:MET:HB2	1:B:132:MET:HE2	1.99	0.40
1:B:760:GLU:OE2	1:B:767:LEU:HB2	2.21	0.40
1:B:1238:LEU:HD12	1:B:1238:LEU:C	2.42	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2060/2553 (81%)	1989 (97%)	71 (3%)	0	100	100
1	B	2063/2553 (81%)	1996 (97%)	67 (3%)	0	100	100
All	All	4123/5106 (81%)	3985 (97%)	138 (3%)	0	100	100

There are no Ramachandran outliers to report.

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1705/2117 (80%)	1700 (100%)	5 (0%)	91	94
1	B	1708/2117 (81%)	1707 (100%)	1 (0%)	92	96
All	All	3413/4234 (81%)	3407 (100%)	6 (0%)	91	95

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	215	PHE
1	A	277	TYR
1	A	504	ARG
1	A	1123	THR
1	A	1896	PHE
1	B	1896	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1098	HIS
1	A	1296	GLN
1	A	1331	ASN
1	A	1504	ASN
1	A	1553	HIS
1	A	1595	GLN
1	B	170	ASN
1	B	195	ASN
1	B	199	GLN
1	B	455	ASN
1	B	644	ASN
1	B	792	ASN
1	B	1004	HIS
1	B	1366	GLN
1	B	1369	GLN
1	B	1409	GLN
1	B	1494	GLN
1	B	1682	GLN

### 5.3.3 RNA ⓘ

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	0.64	0	61,80,80	0.83	2 (3%)
2	NDP	B	2602	-	47,52,52	0.64	0	61,80,80	0.92	3 (4%)
2	NDP	A	2601	-	47,52,52	0.64	0	61,80,80	0.81	2 (3%)
2	NDP	A	2602	-	47,52,52	0.67	0	61,80,80	0.91	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	-	-	10/30/77/77	0/5/5/5
2	NDP	B	2602	-	-	8/30/77/77	0/5/5/5
2	NDP	A	2601	-	-	8/30/77/77	0/5/5/5
2	NDP	A	2602	-	-	9/30/77/77	0/5/5/5

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2602	NDP	P2B-O2B-C2B	-5.13	109.74	123.43
2	B	2601	NDP	P2B-O2B-C2B	-4.39	111.70	123.43
2	A	2601	NDP	P2B-O2B-C2B	-3.97	112.82	123.43
2	B	2602	NDP	P2B-O2B-C2B	-3.72	113.49	123.43
2	B	2602	NDP	C5A-C6A-N6A	2.33	123.86	120.31
2	A	2602	NDP	C5A-C6A-N6A	2.25	123.74	120.31
2	A	2601	NDP	C5A-C6A-N6A	2.22	123.69	120.31
2	B	2601	NDP	C5A-C6A-N6A	2.18	123.62	120.31
2	B	2602	NDP	C4B-O4B-C1B	-2.12	107.98	109.92

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2601	NDP	C5B-O5B-PA-O2A
2	A	2601	NDP	C5B-O5B-PA-O3
2	A	2601	NDP	C2N-C3N-C7N-N7N
2	A	2602	NDP	C5B-O5B-PA-O1A
2	A	2602	NDP	O4B-C4B-C5B-O5B
2	A	2602	NDP	C2N-C3N-C7N-N7N
2	B	2601	NDP	C5D-O5D-PN-O3
2	B	2601	NDP	C5D-O5D-PN-O2N
2	B	2601	NDP	C2N-C3N-C7N-N7N
2	B	2602	NDP	O4D-C4D-C5D-O5D
2	B	2602	NDP	C3D-C4D-C5D-O5D
2	A	2602	NDP	O4D-C1D-N1N-C6N
2	B	2602	NDP	O4D-C1D-N1N-C6N
2	A	2602	NDP	C3B-C4B-C5B-O5B
2	A	2601	NDP	O4D-C4D-C5D-O5D
2	A	2601	NDP	C3D-C4D-C5D-O5D
2	B	2601	NDP	O4B-C4B-C5B-O5B
2	B	2602	NDP	C3B-C2B-O2B-P2B
2	B	2601	NDP	C3B-C4B-C5B-O5B
2	B	2602	NDP	C1B-C2B-O2B-P2B
2	B	2601	NDP	PA-O3-PN-O1N
2	A	2602	NDP	C4B-C5B-O5B-PA
2	A	2602	NDP	PA-O3-PN-O2N
2	A	2601	NDP	C2N-C3N-C7N-O7N
2	B	2601	NDP	O4D-C1D-N1N-C2N
2	A	2602	NDP	C5B-O5B-PA-O3
2	A	2601	NDP	O4D-C1D-N1N-C2N
2	B	2601	NDP	O4D-C4D-C5D-O5D
2	A	2601	NDP	C2D-C1D-N1N-C2N

*Continued on next page...*



*Continued from previous page...*

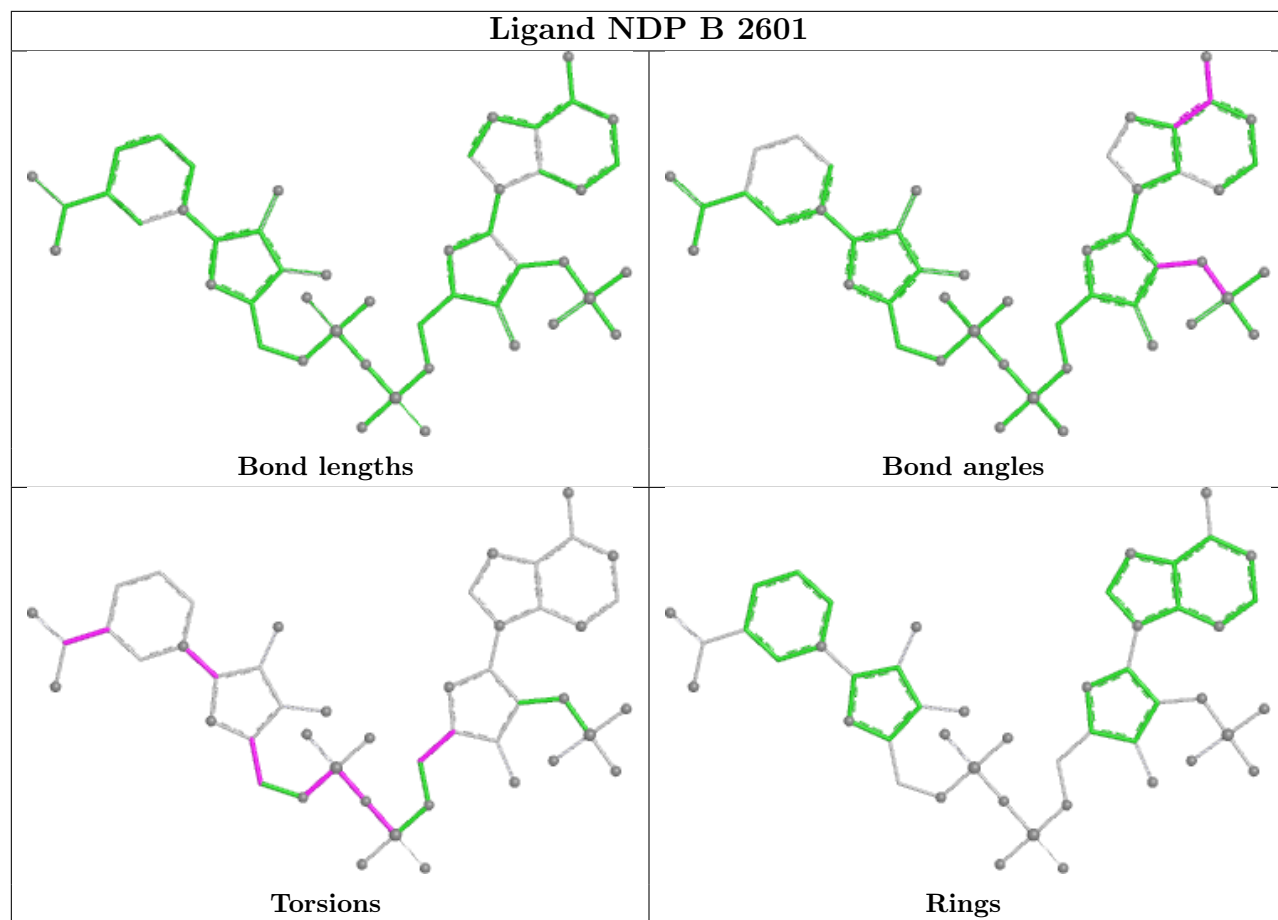
Mol	Chain	Res	Type	Atoms
2	B	2602	NDP	C2B-O2B-P2B-O1X
2	B	2601	NDP	PA-O3-PN-O2N
2	B	2602	NDP	C2B-O2B-P2B-O3X
2	A	2602	NDP	PA-O3-PN-O1N
2	B	2601	NDP	PN-O3-PA-O2A
2	B	2602	NDP	O4B-C4B-C5B-O5B

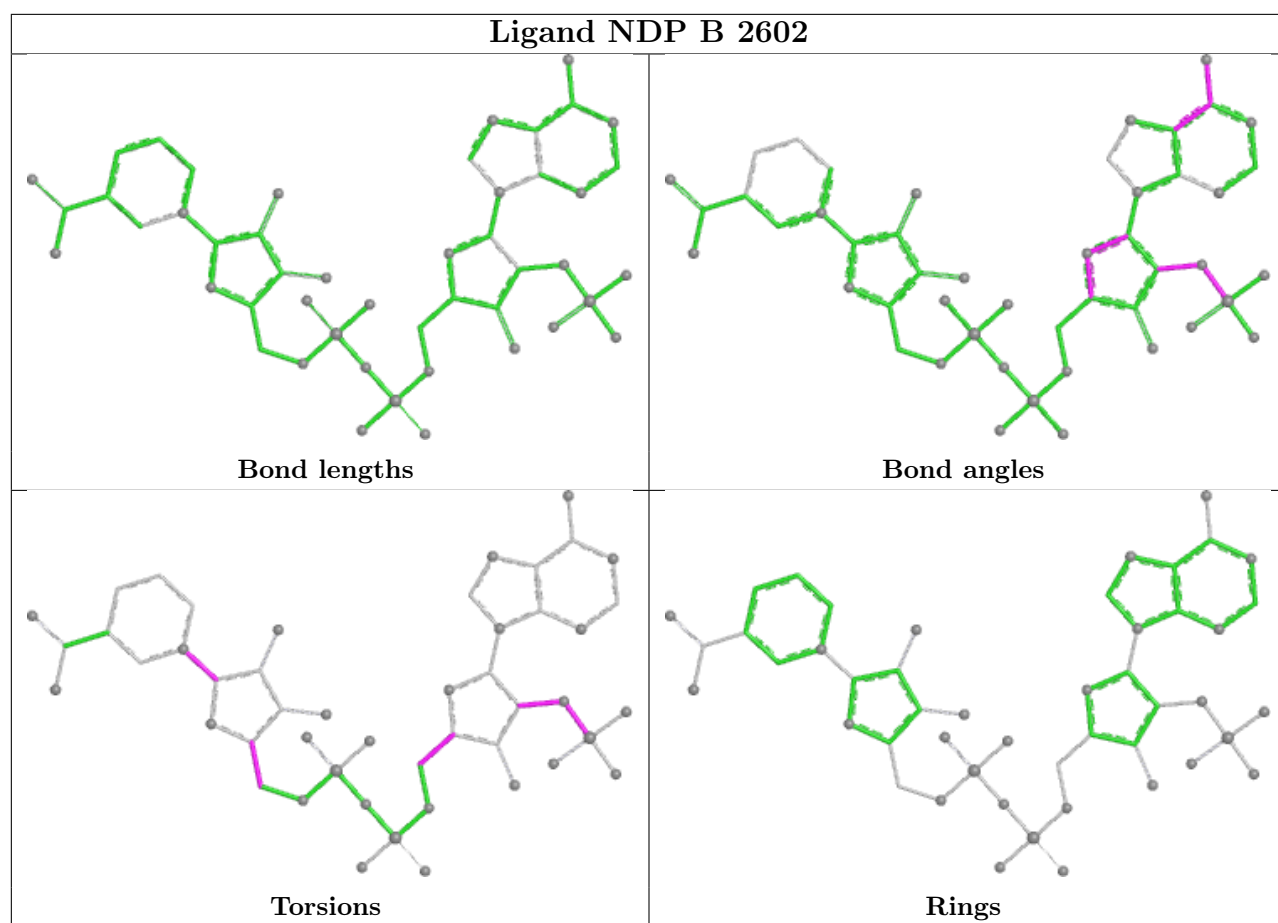
There are no ring outliers.

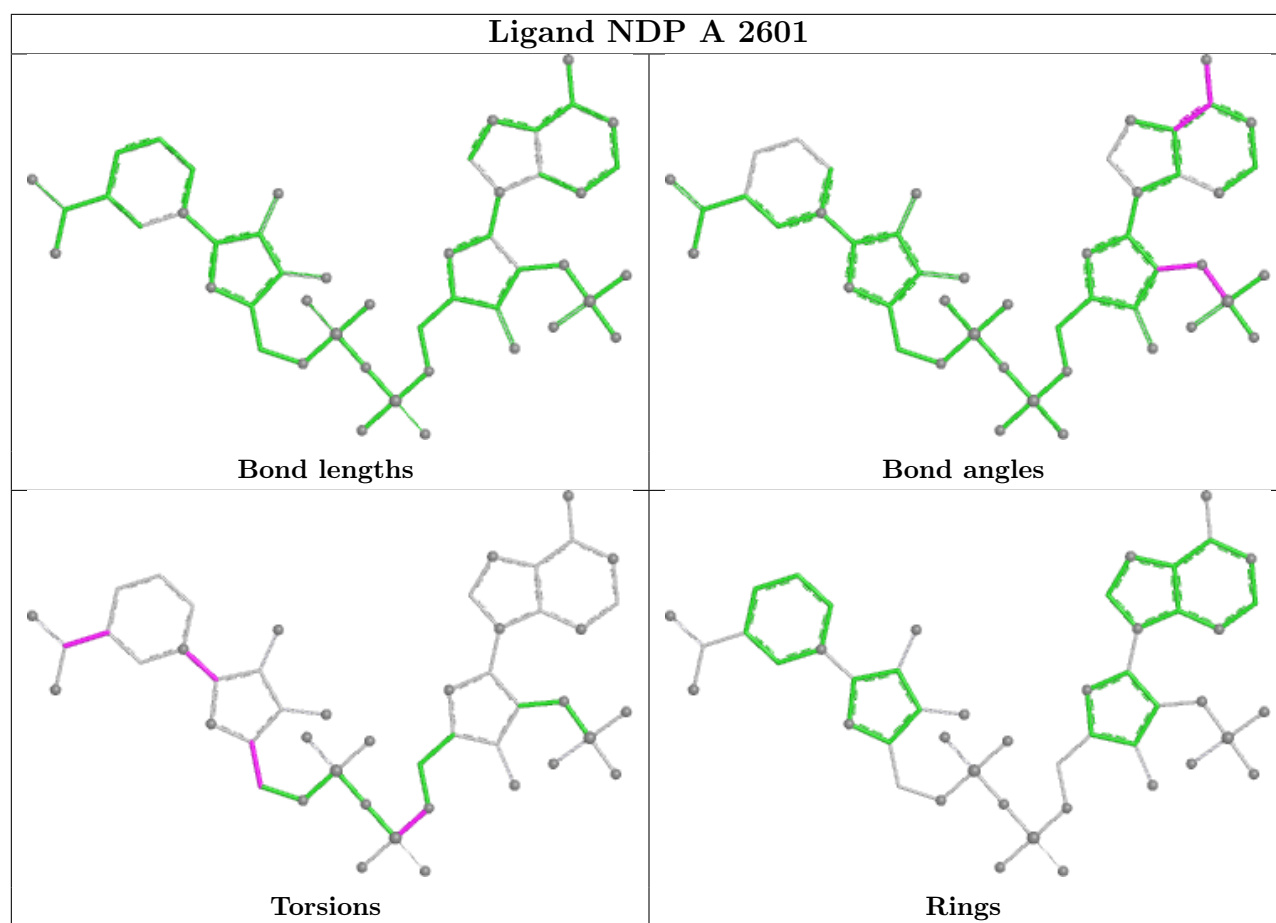
3 monomers are involved in 9 short contacts:

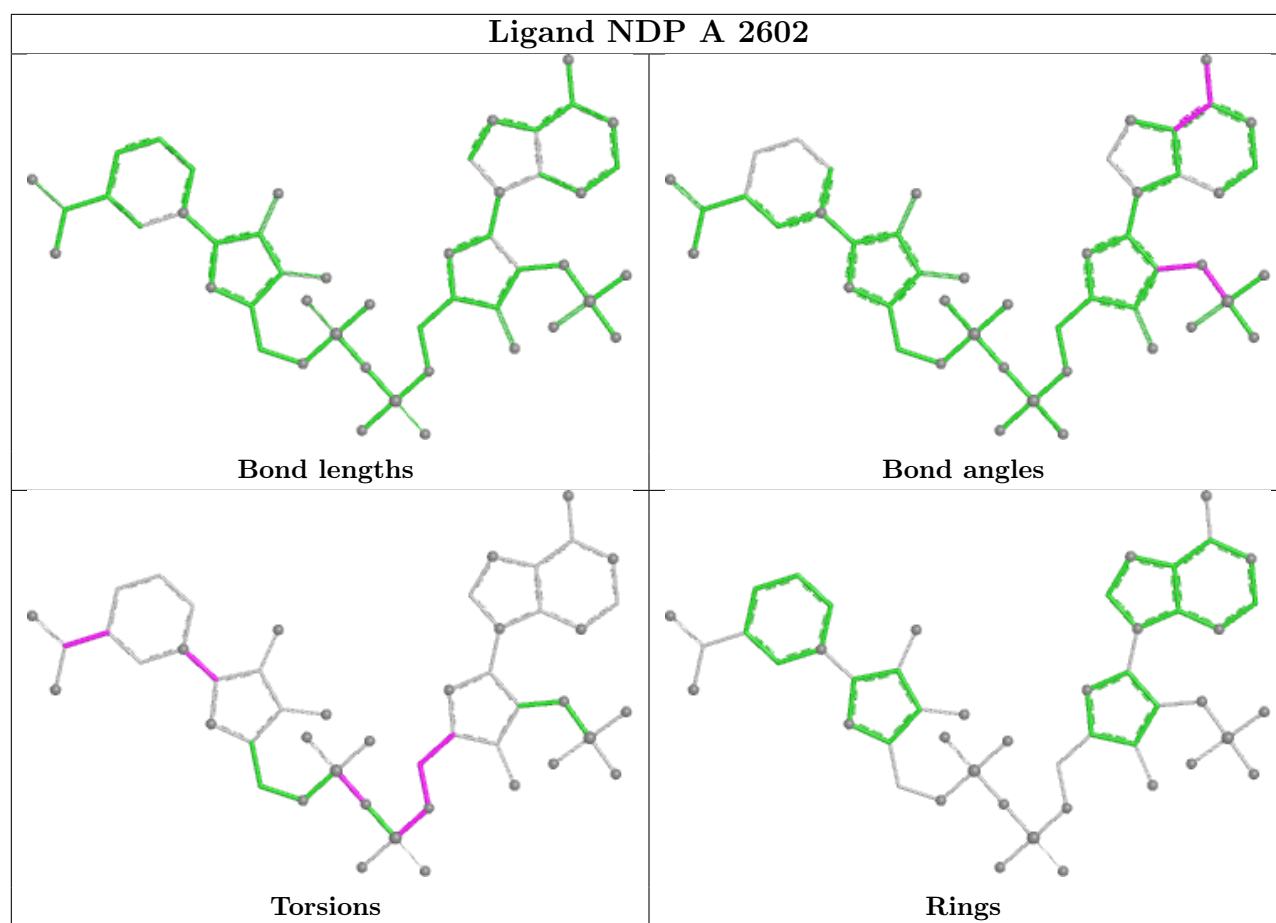
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2601	NDP	1	0
2	B	2602	NDP	3	0
2	A	2602	NDP	5	0

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.

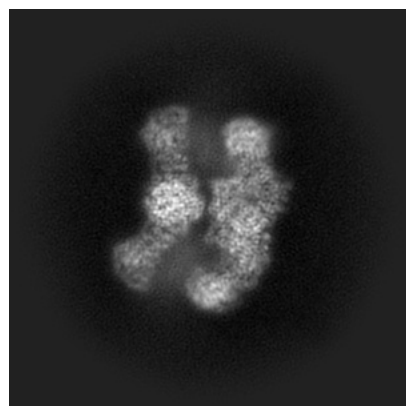
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43340. These allow visual inspection of the internal detail of the map and identification of artifacts.

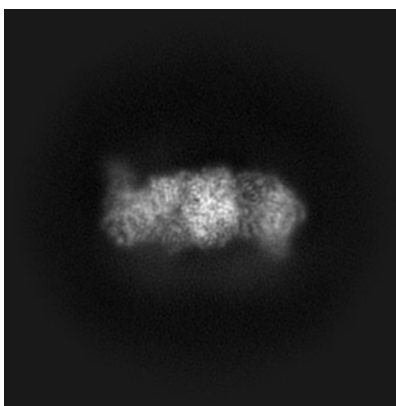
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

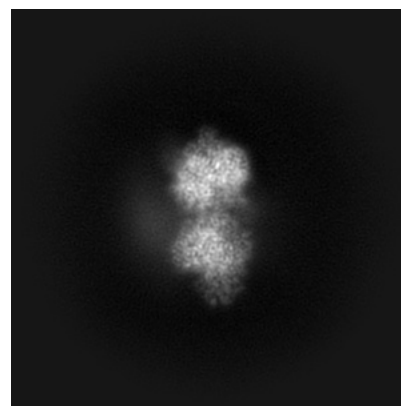
#### 6.1.1 Primary map



X

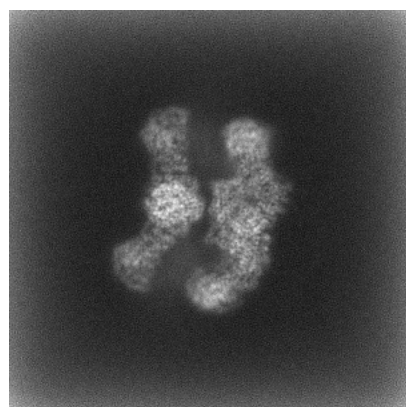


Y

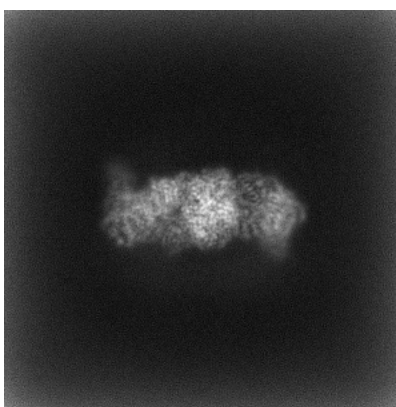


Z

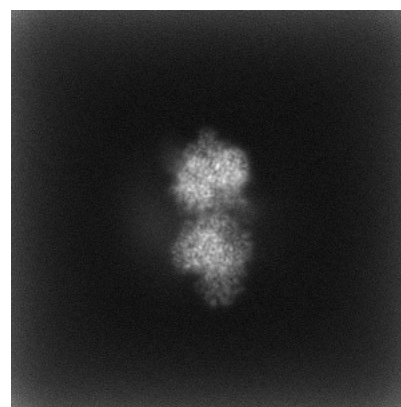
#### 6.1.2 Raw map



X



Y

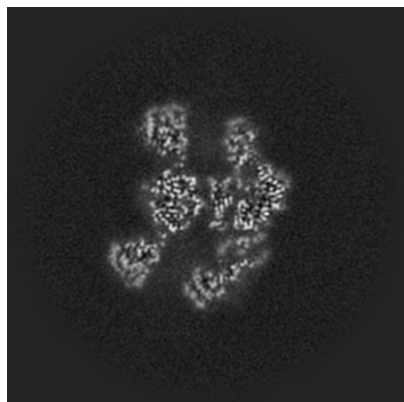


Z

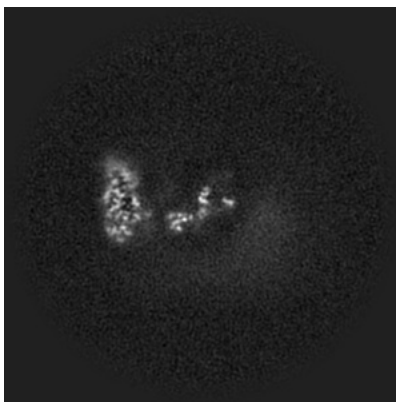
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

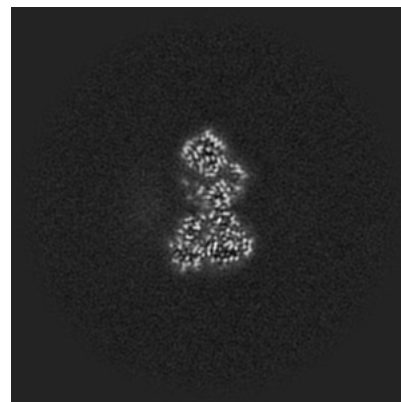
### 6.2.1 Primary map



X Index: 180

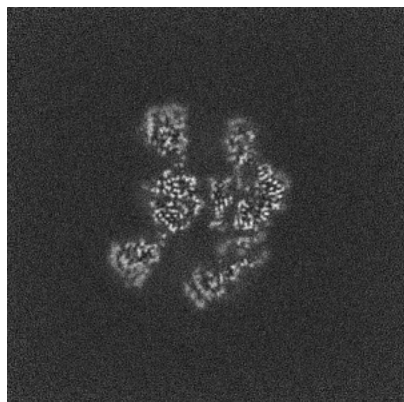


Y Index: 180



Z Index: 180

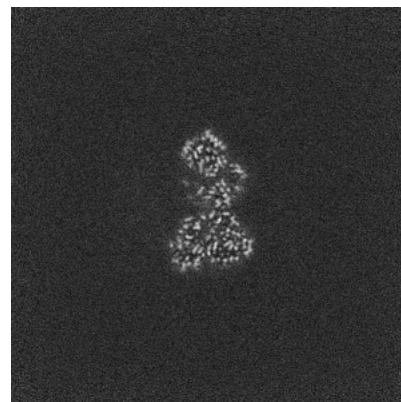
### 6.2.2 Raw map



X Index: 180



Y Index: 180



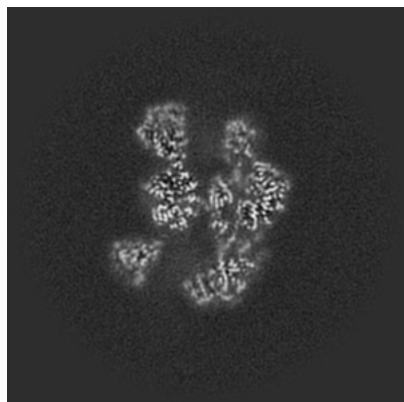
Z Index: 180

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

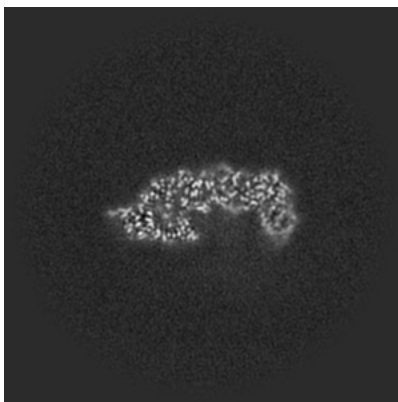


## 6.3 Largest variance slices [i](#)

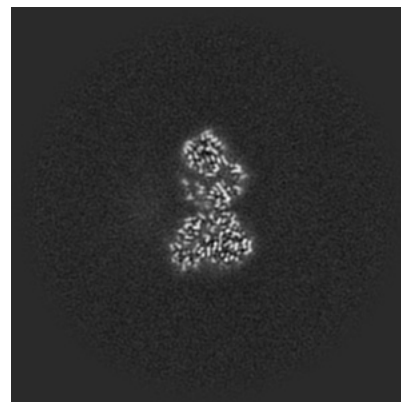
### 6.3.1 Primary map



X Index: 177

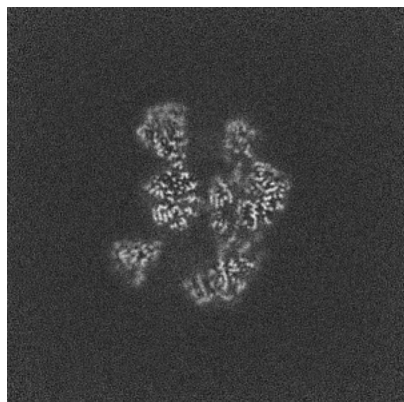


Y Index: 208

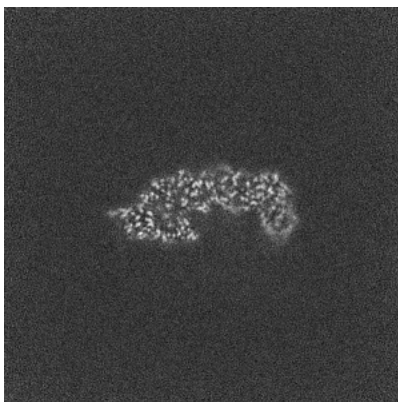


Z Index: 179

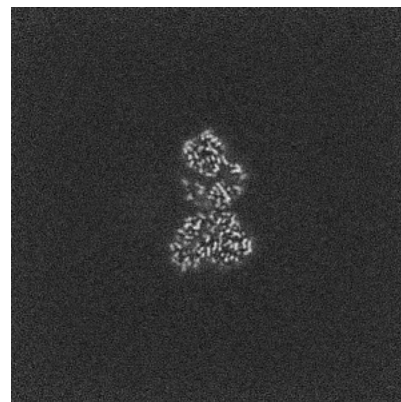
### 6.3.2 Raw map



X Index: 177



Y Index: 208



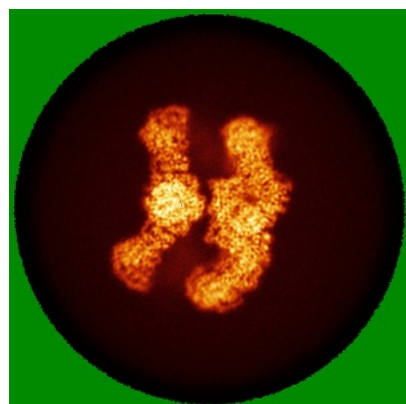
Z Index: 179

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

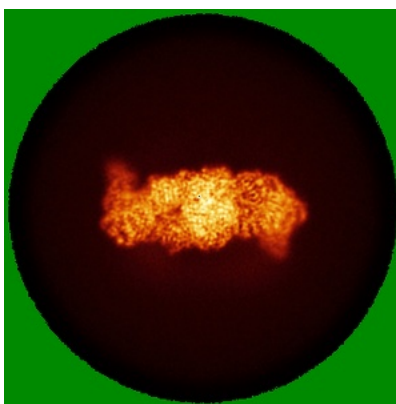


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

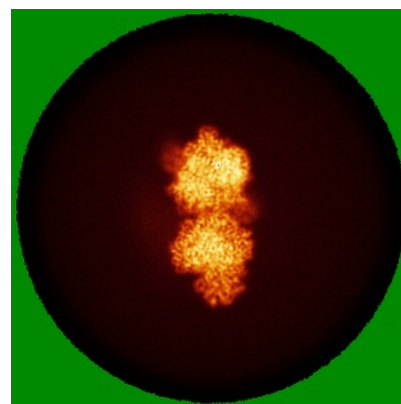
### 6.4.1 Primary map



X

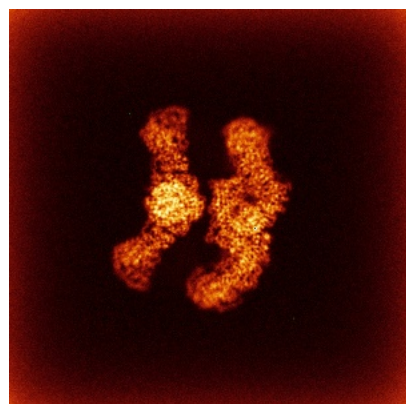


Y

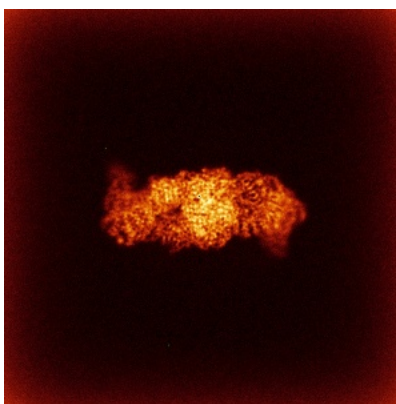


Z

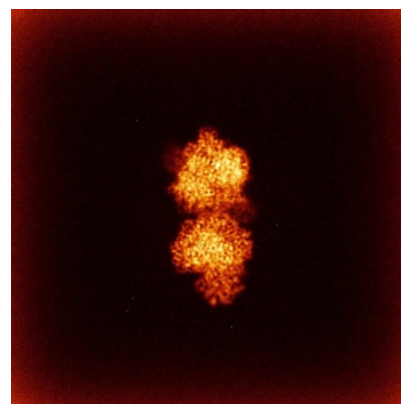
### 6.4.2 Raw map



X



Y

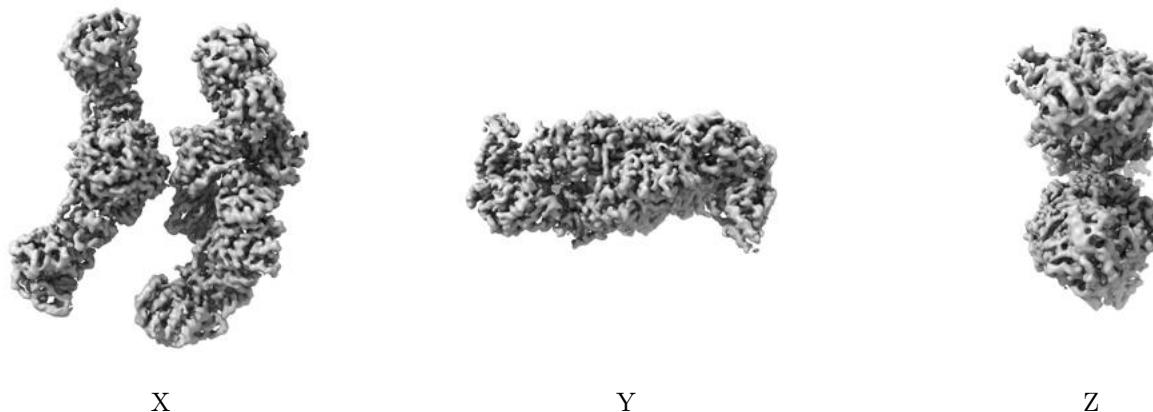


Z

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.

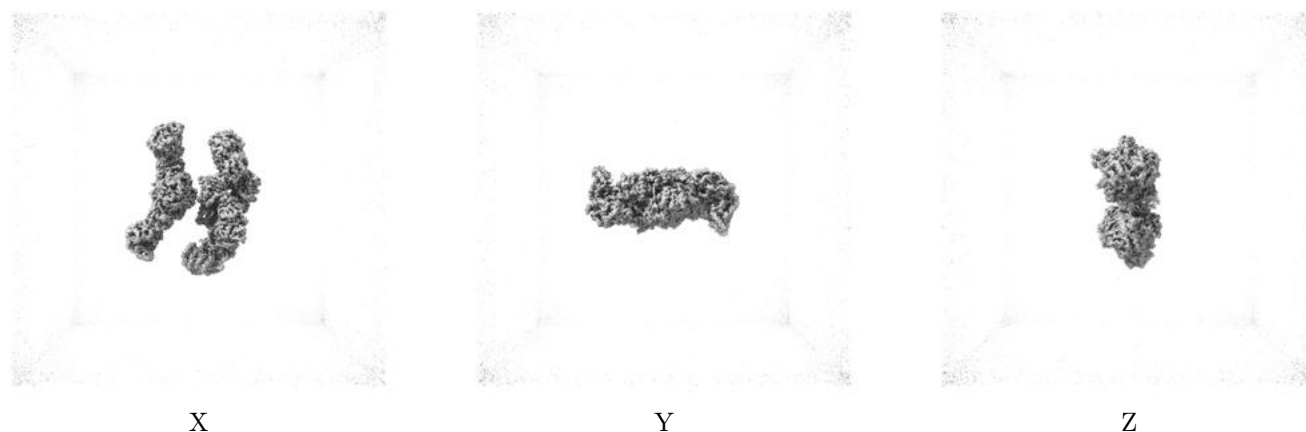
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.213. 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.

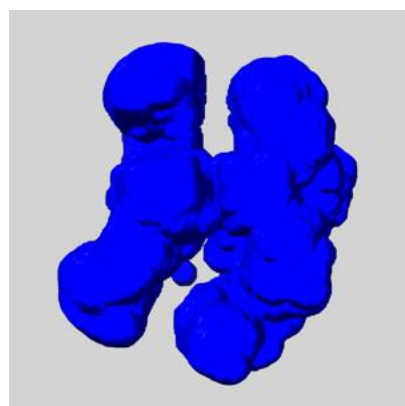
## 6.6 Mask visualisation [i](#)

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

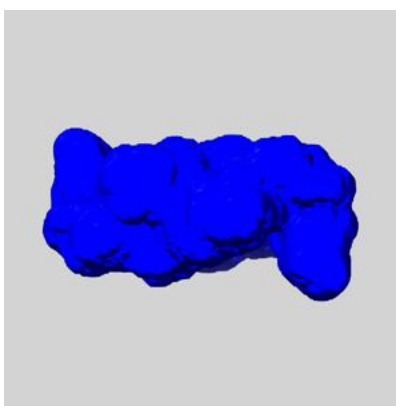
A mask typically either:

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

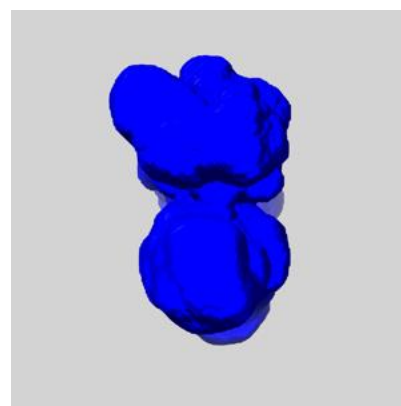
### 6.6.1 emd\_43340\_msk\_1.map [i](#)



X



Y

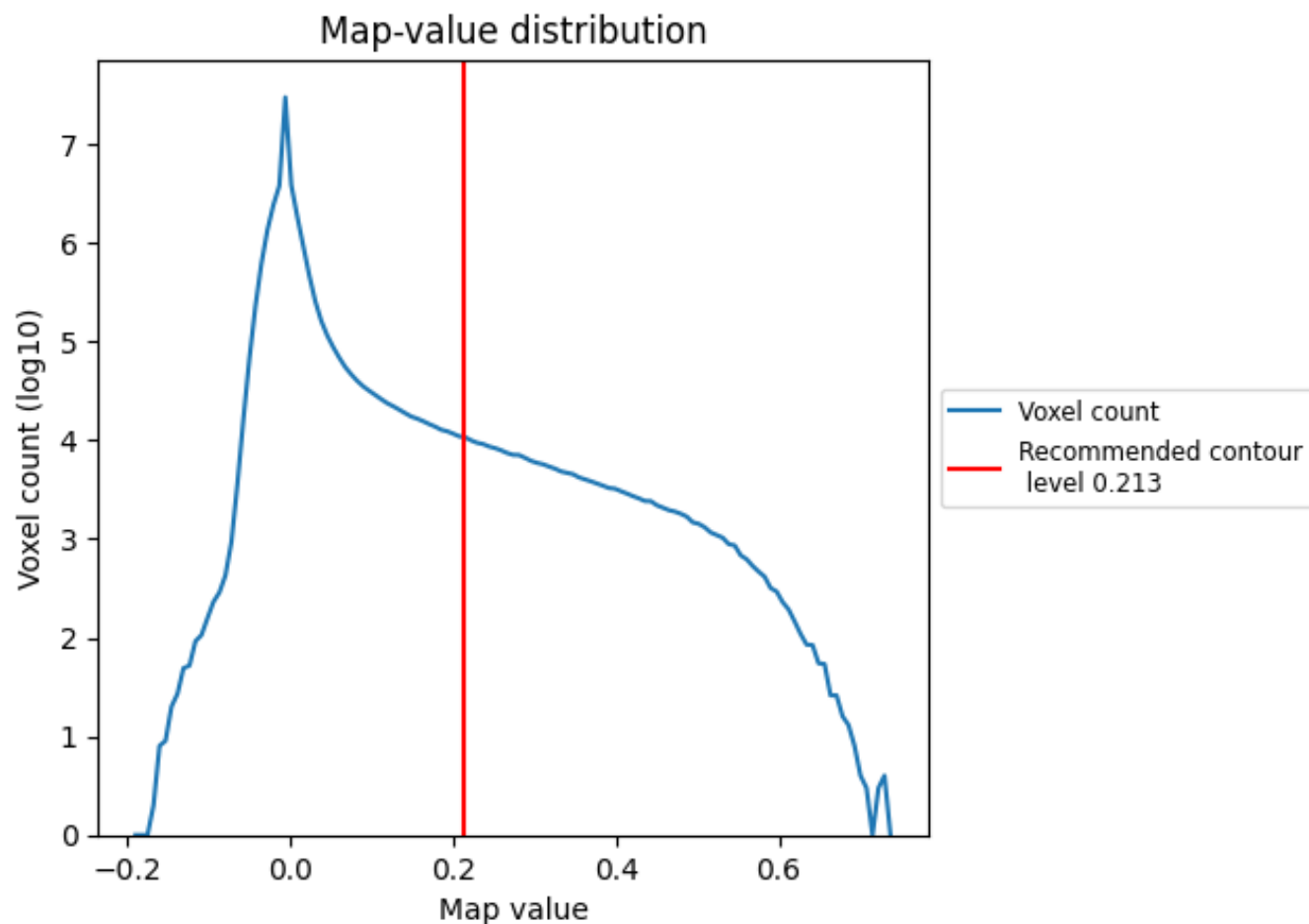


Z

## 7 Map analysis [i](#)

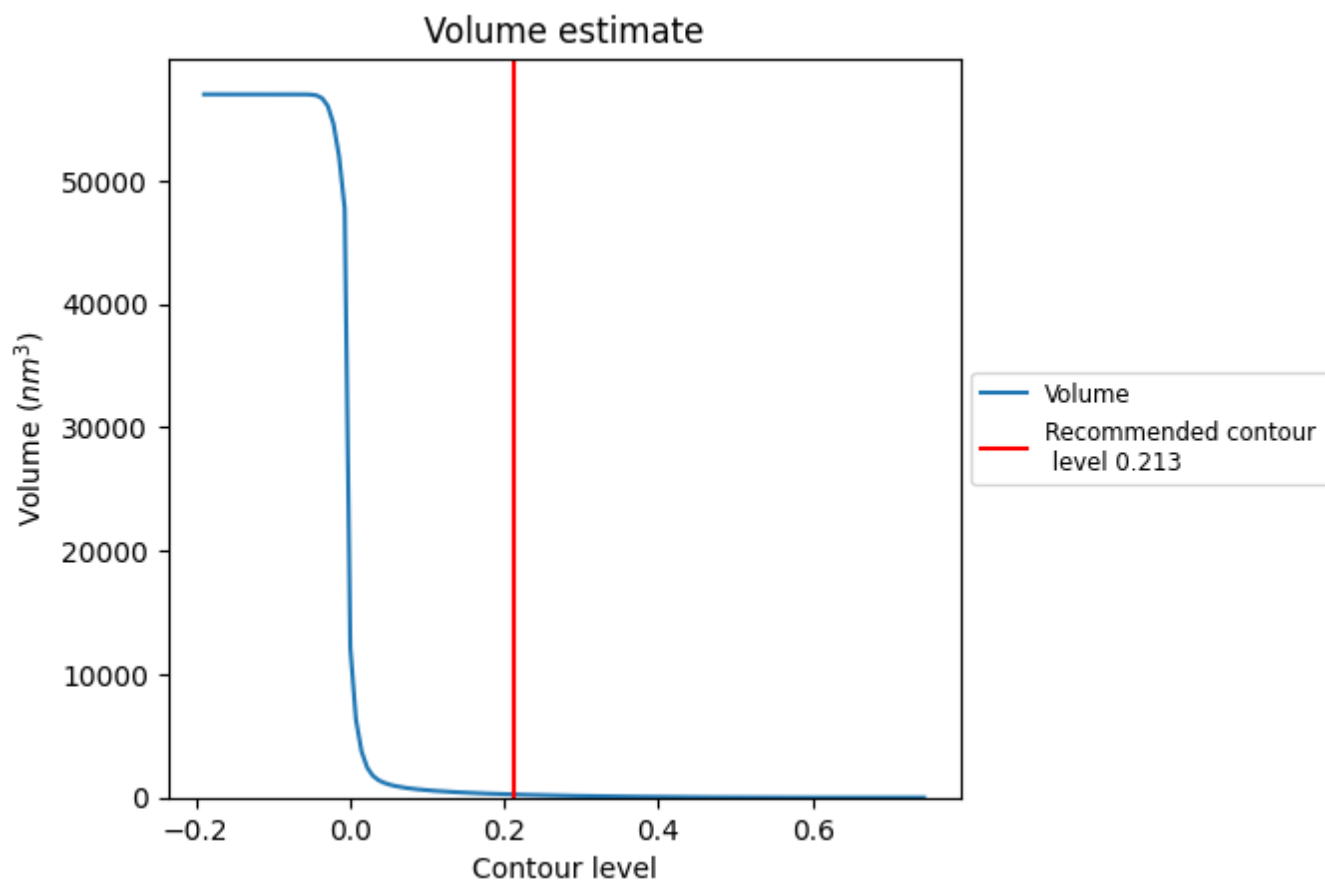
This section contains the results of statistical analysis of the map.

### 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.

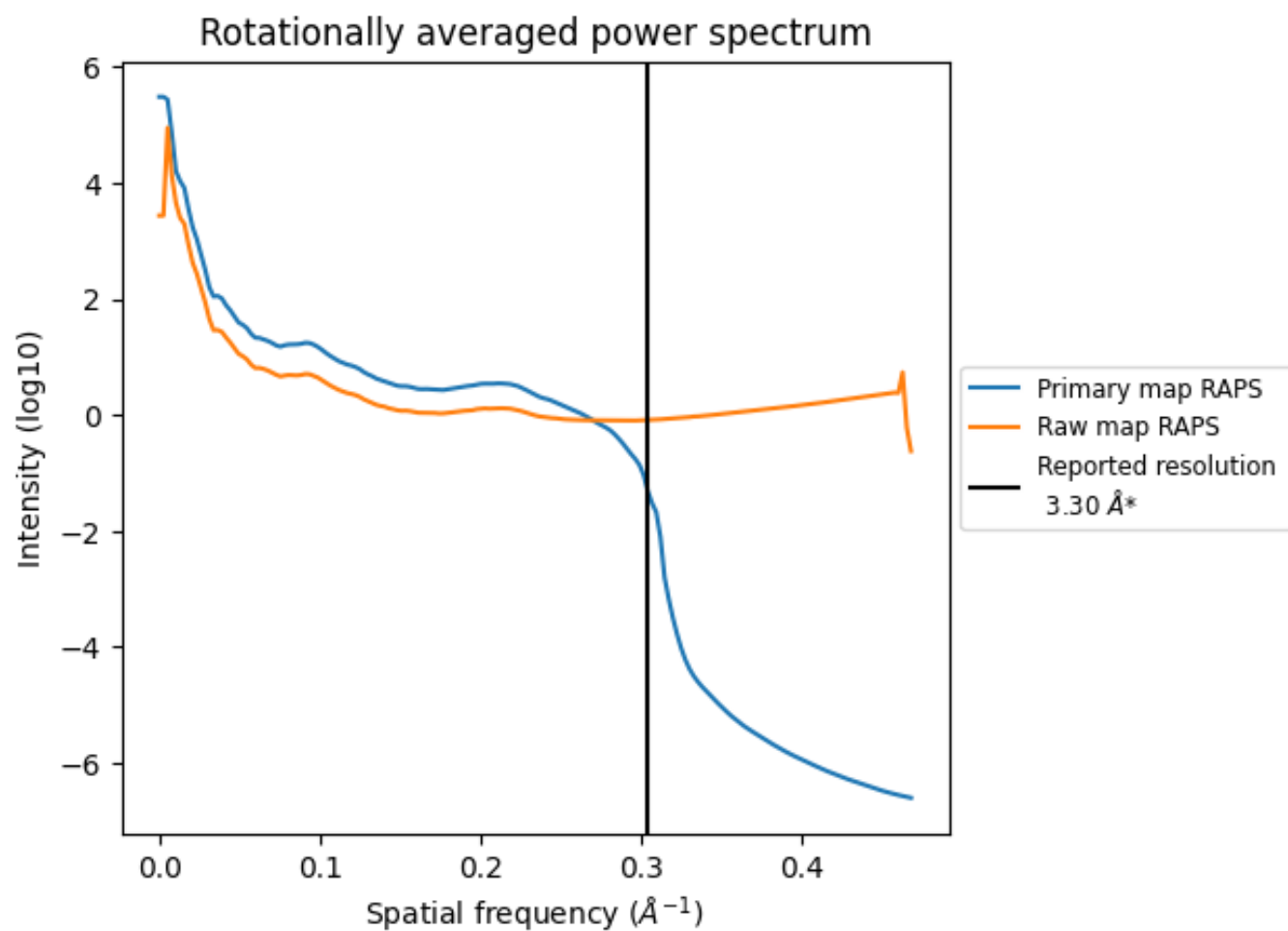
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 250 nm<sup>3</sup>; this corresponds to an approximate mass of 226 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 ⓘ

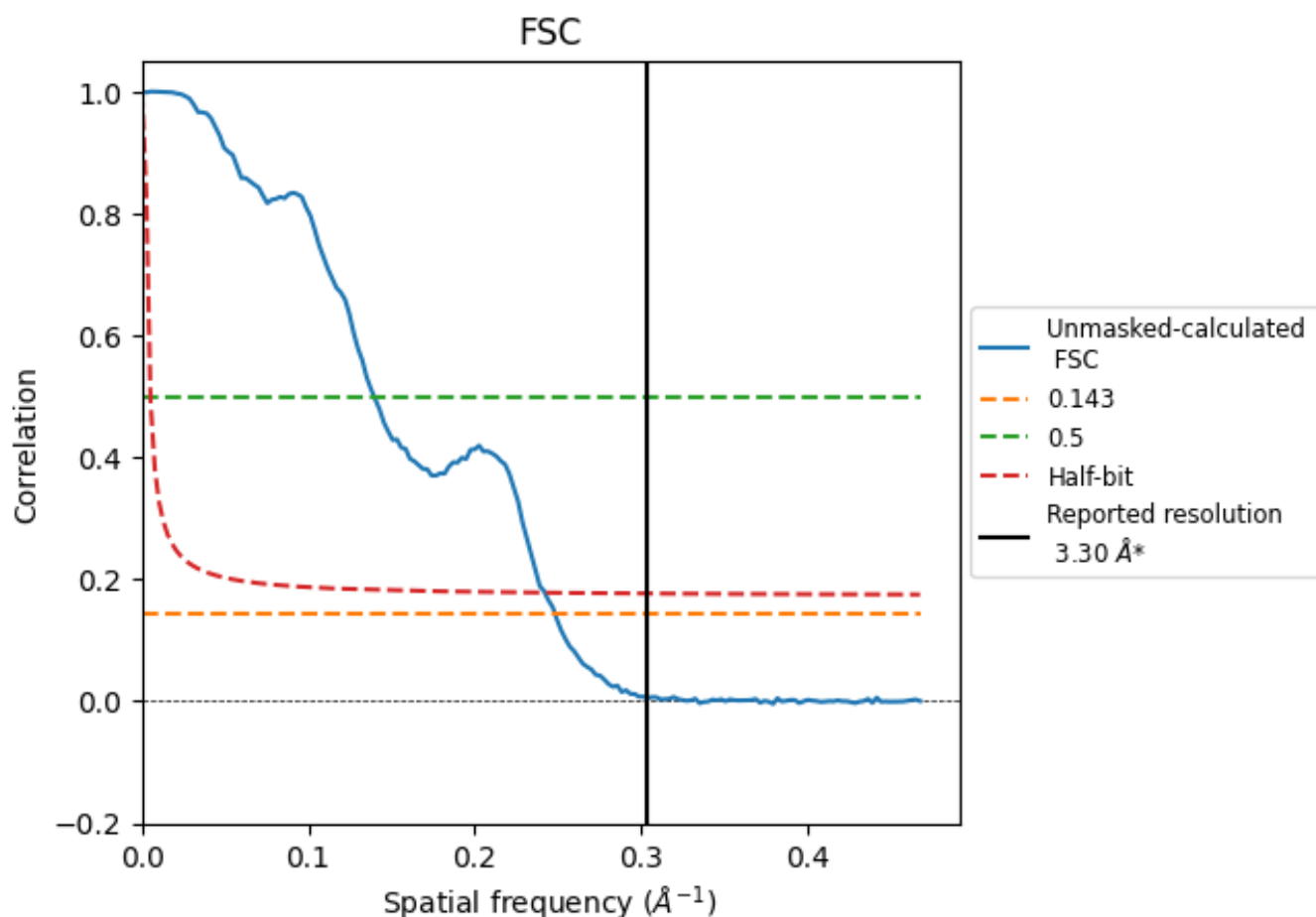


\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

## 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 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*	4.03	7.17	4.13

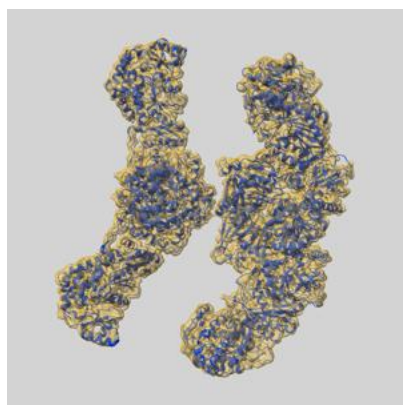
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.03 differs from the reported value 3.3 by more than 10 %



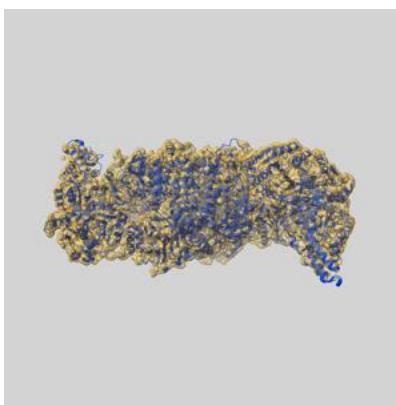
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-43340 and PDB model 8VLO. Per-residue inclusion information can be found in section 3 on page 7.

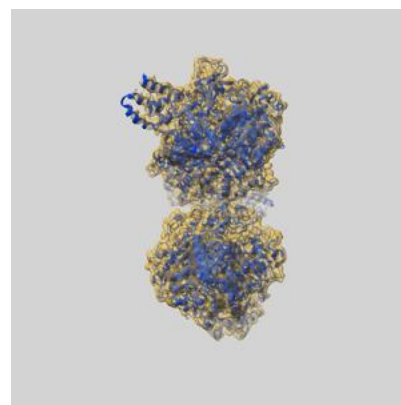
### 9.1 Map-model overlay [i](#)



X



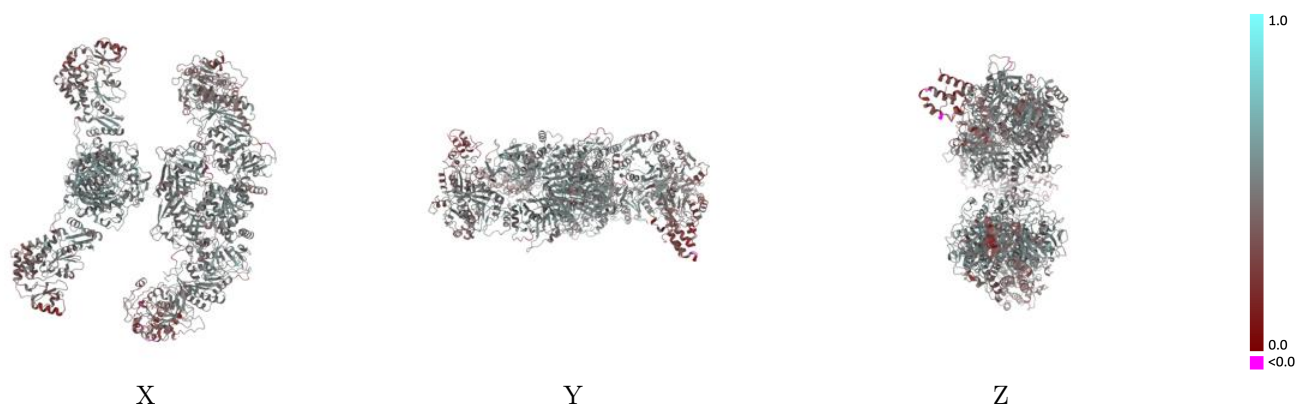
Y



Z

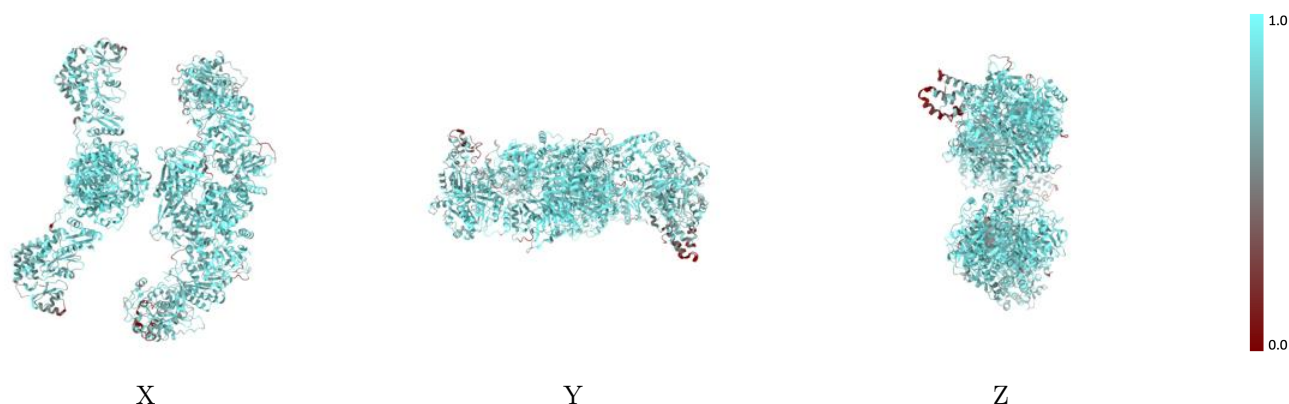
The images above show the 3D surface view of the map at the recommended contour level 0.213 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



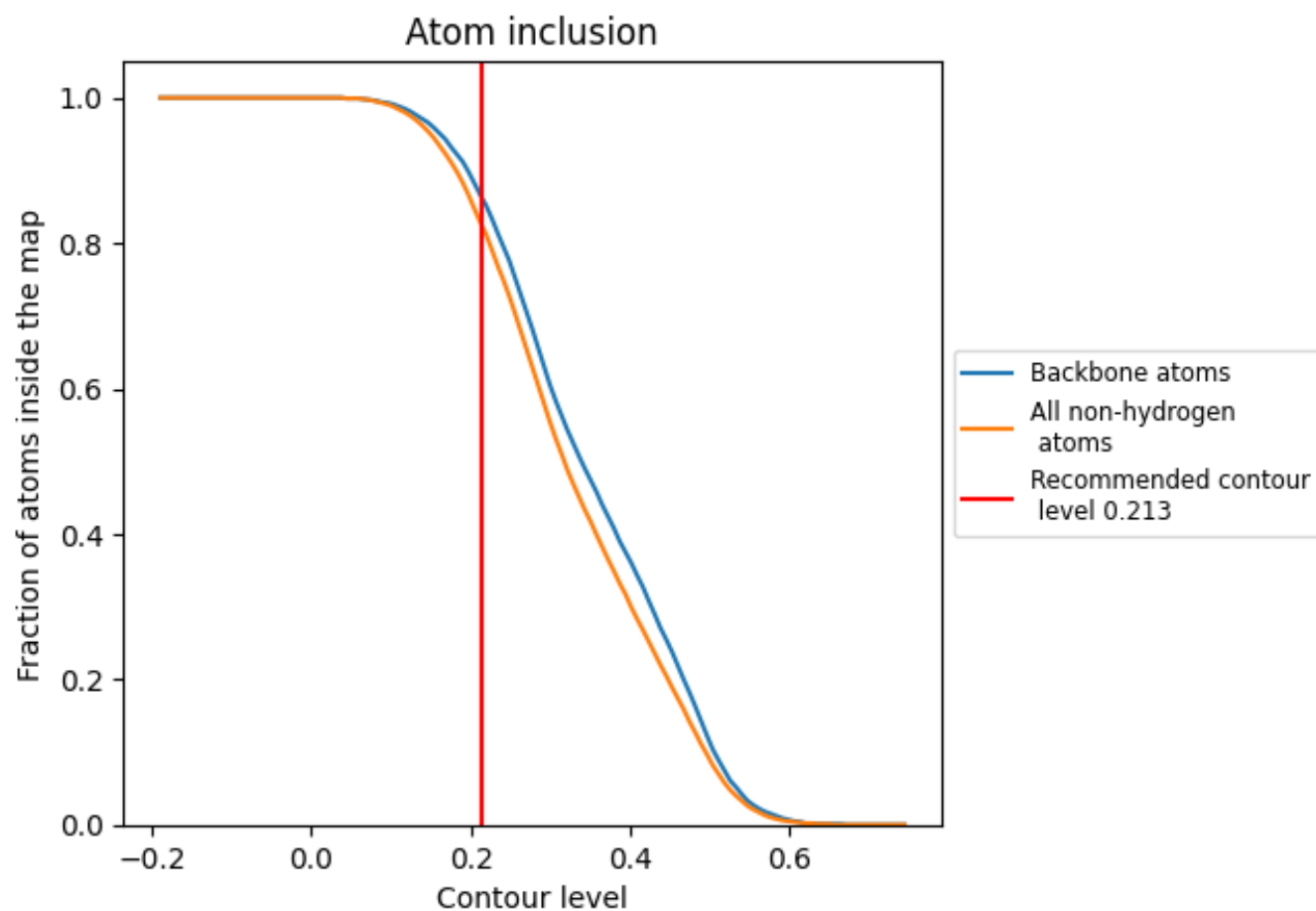
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.213).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 83% 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 (0.213) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8260	<div></div> 0.4660
A	<div></div> 0.8300	<div></div> 0.4670
B	<div></div> 0.8250	<div></div> 0.4650

