



## Full wwPDB EM Validation Report ⓘ

Feb 22, 2025 – 04:23 PM EST

PDB ID : 8VM6  
EMDB ID : EMD-43353  
Title : Composite structure of human FASN with NADPH in State 8  
Authors : Schultz, K.; Marmorstein, R.  
Deposited on : 2024-01-13  
Resolution : 3.50 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

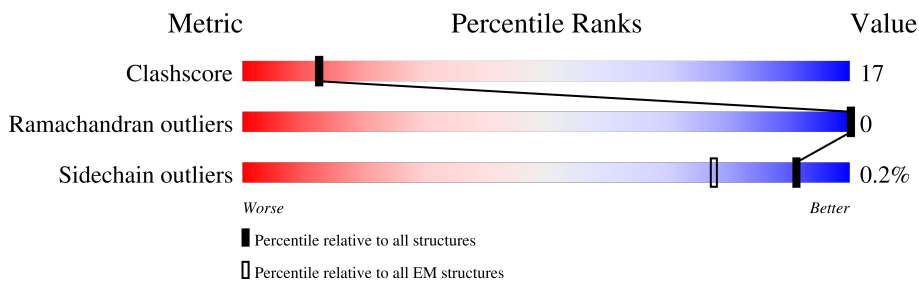
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.50 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	<p>60% 21% 19%</p>
1	B	2553	<p>58% 23% 19%</p>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 50700 atoms, of which 18818 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
			25228	10054	9371	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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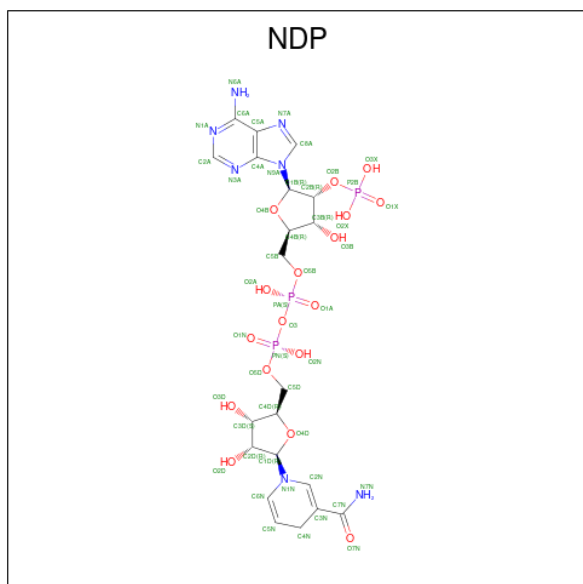
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	ALA	-	expression tag	UNP P49327
A	-4	MET	-	expression tag	UNP P49327
A	-3	GLY	-	expression tag	UNP P49327
A	-2	SER	-	expression tag	UNP P49327
A	-1	GLY	-	expression tag	UNP P49327
A	0	ILE	-	expression tag	UNP P49327
A	1	PRO	-	expression tag	UNP P49327
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).

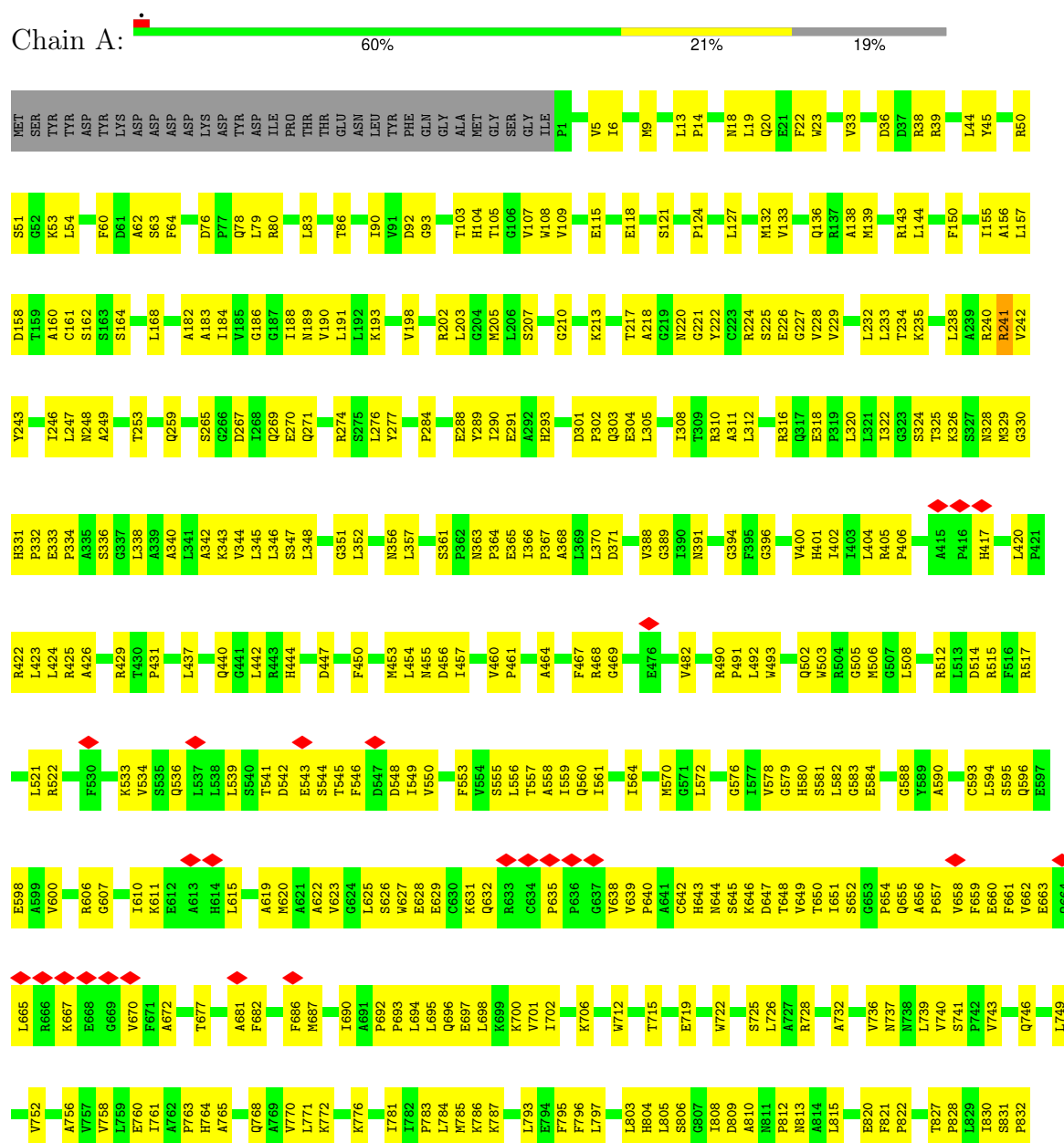


Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
2	A	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
2	B	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
2	B	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	

### 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







R39	R122	R202	Q778	G351	V460	T545	A622	F686	L833	V1052	N1191	S1327
L44	D123	M205	S279	L352	P461	F546	L625	M687	E848	I1055	G1192	N1331
Y45	P124	M206	V282	A354	A464	D547	S626	E688	D849	I1056	N1193	N1332
G46	E125	S207	E285	L357	I366	D548	E627	I690	H852	D1071	Q1195	V1333
L47	T126	S208	S286	I367	R468	I549	E628	A691	GLY	K1072	L1196	L1336
R50	L127	E209	F287	I366	R468	V550	E629	P692	GLY	K1072	L1197	L1343
S51	V128	E209	E288	I366	R468	S552	E630	P693	GLY	K1072	L1198	L1344
D56	M132	C212	F289	I366	R468	F554	E631	P694	GLY	K1072	L1199	H1345
L57	V133	F215	I290	L374	E476	S555	E632	P695	GLY	K1072	L1200	T1356
S58	A138	D216	E291	V376	R477	L556	E633	Q696	GLY	K1072	L1201	V1357
R59	M139	T217	A292	V377	P480	T557	E634	E697	PRO	V1078	L1202	T1361
F60	M142	G221	H293	V377	P480	A558	E635	L698	GLY	V1079	L1203	E1364
D61	N143	Y222	G294	V383	V485	Q560	P636	K699	GLY	V1080	L1204	P1365
A62	R143	Y222	G300	V383	V485	Q560	P636	K699	GLY	V1080	L1205	Q1366
S63	L144	C223	D301	V388	F494	G562	P637	K700	GLY	V1080	L1206	Y1367
F64	S145	R224	E303	V388	F494	L563	P638	K701	GLY	V1080	L1207	G1370
T74	F148	S225	Q302	V388	F494	L563	P639	K702	GLY	V1080	L1208	I1371
M75	D149	E226	Q303	V388	F494	L563	P640	K703	GLY	V1080	L1209	L1372
D76	D149	E226	Q303	V388	F494	L563	P641	K704	GLY	V1080	L1210	W1377
P77	F150	E226	Q303	V388	F494	L563	P642	K705	GLY	V1080	L1211	L1386
Q78	G152	E226	Q303	V388	F494	L563	P643	K706	GLY	V1080	L1212	V1389
L79	A156	E226	Q303	V388	F494	L563	P644	K707	GLY	V1080	L1213	G1390
R80	L157	E226	Q303	V388	F494	L563	P645	K708	GLY	V1080	L1214	L1391
L81	L157	E226	Q303	V388	F494	L563	P646	K709	GLY	V1080	L1215	L1400
L82	D158	E226	Q303	V388	F494	L563	P647	K710	GLY	V1080	L1216	D1410
L83	L159	E226	Q303	V388	F494	L563	P648	K711	GLY	V1080	L1217	V1417
E84	A160	E226	Q303	V388	F494	L563	P649	K712	GLY	V1080	L1218	K1429
V85	C161	E226	Q303	V388	F494	L563	P650	K713	GLY	V1080	L1219	E1435
T86	S162	E226	Q303	V388	F494	L563	P651	K714	GLY	V1080	L1220	D1436
E88	S163	E226	Q303	V388	F494	L563	P652	K715	GLY	V1080	L1221	A1445
V91	S164	E226	Q303	V388	F494	L563	P653	K716	GLY	V1080	L1222	I1446
D92	S165	E226	Q303	V388	F494	L563	P654	K717	GLY	V1080	L1223	V1457
I95	M166	E226	Q303	V388	F494	L563	P655	K718	GLY	V1080	L1224	R1470
N96	A167	E226	Q303	V388	F494	L563	P656	K719	GLY	V1080	L1225	C1471
P97	L168	E226	Q303	V388	F494	L563	P657	K720	GLY	V1080	L1226	L1474
R101	L175	E226	Q303	V388	F494	L563	P658	K721	GLY	V1080	L1227	E1485
H104	A183	E226	Q303	V388	F494	L563	P659	K722	GLY	V1080	L1228	V1486
T105	L184	E226	Q303	V388	F494	L563	P660	K723	GLY	V1080	L1229	D1487
G106	W185	E226	Q303	V388	F494	L563	P661	K724	GLY	V1080	L1230	
V107	G186	E226	Q303	V388	F494	L563	P662	K725	GLY	V1080	L1231	
S112	G187	E226	Q303	V388	F494	L563	P663	K726	GLY	V1080	L1232	
G113	I188	E226	Q303	V388	F494	L563	P664	K727	GLY	V1080	L1233	
S114	N189	E226	Q303	V388	F494	L563	P665	K728	GLY	V1080	L1234	
E115	G190	E226	Q303	V388	F494	L563	P666	K729	GLY	V1080	L1235	
T116	L191	E226	Q303	V388	F494	L563	P667	K730	GLY	V1080	L1236	
S117	L192	E226	Q303	V388	F494	L563	P668	K731	GLY	V1080	L1237	
E118	L193	E226	Q303	V388	F494	L563	P669	K732	GLY	V1080	L1238	
A119	L194	E226	Q303	V388	F494	L563	P670	K733	GLY	V1080	L1239	
L120	L195	E226	Q303	V388	F494	L563	P671	K734	GLY	V1080	L1240	
S121	L196	E226	Q303	V388	F494	L563	P672	K735	GLY	V1080	L1241	
	L197	E226	Q303	V388	F494	L563	P673	K736	GLY	V1080	L1242	
	L198	E226	Q303	V388	F494	L563	P674	K737	GLY	V1080	L1243	
	L199	E226	Q303	V388	F494	L563	P675	K738	GLY	V1080	L1244	
	L200	E226	Q303	V388	F494	L563	P676	K739	GLY	V1080	L1245	
	L201	E226	Q303	V388	F494	L563	P677	K740	GLY	V1080	L1246	
	L202	E226	Q303	V388	F494	L563	P678	K741	GLY	V1080	L1247	
	L203	E226	Q303	V388	F494	L563	P679	K742	GLY	V1080	L1248	
	L204	E226	Q303	V388	F494	L563	P680	K743	GLY	V1080	L1249	
	L205	E226	Q303	V388	F494	L563	P681	K744	GLY	V1080	L1250	
	L206	E226	Q303	V388	F494	L563	P682	K745	GLY	V1080	L1251	
	L207	E226	Q303	V388	F494	L563	P683	K746	GLY	V1080	L1252	
	L208	E226	Q303	V388	F494	L563	P684	K747	GLY	V1080	L1253	
	L209	E226	Q303	V388	F494	L563	P685	K748	GLY	V1080	L1254	
	L210	E226	Q303	V388	F494	L563	P686	K749	GLY	V1080	L1255	
	L211	E226	Q303	V388	F494	L563	P687	K750	GLY	V1080	L1256	
	L212	E226	Q303	V388	F494	L563	P688	K751	GLY	V1080	L1257	
	L213	E226	Q303	V388	F494	L563	P689	K752	GLY	V1080	L1258	
	L214	E226	Q303	V388	F494	L563	P690	K753	GLY	V1080	L1259	
	L215	E226	Q303	V388	F494	L563	P691	K754	GLY	V1080	L1260	
	L216	E226	Q303	V388	F494	L563	P692	K755	GLY	V1080	L1261	
	L217	E226	Q303	V388	F494	L563	P693	K756	GLY	V1080	L1262	
	L218	E226	Q303	V388	F494	L563	P694	K757	GLY	V1080	L1263	
	L219	E226	Q303	V388	F494	L563	P695	K758	GLY	V1080	L1264	
	L220	E226	Q303	V388	F494	L563	P696	K759	GLY	V1080	L1265	
	L221	E226	Q303	V388	F494	L563	P697	K760	GLY	V1080	L1266	
	L222	E226	Q303	V388	F494	L563	P698	K761	GLY	V1080	L1267	
	L223	E226	Q303	V388	F494	L563	P699	K762	GLY	V1080	L1268	
	L224	E226	Q303	V388	F494	L563	P700	K763	GLY	V1080	L1269	
	L225	E226	Q303	V388	F494	L563	P701	K764	GLY	V1080	L1270	
	L226	E226	Q303	V388	F494	L563	P702	K765	GLY	V1080	L1271	
	L227	E226	Q303	V388	F494	L563	P703	K766	GLY	V1080	L1272	
	L228	E226	Q303	V388	F494	L563	P704	K767	GLY	V1080	L1273	
	L229	E226	Q303	V388	F494	L563	P705	K768	GLY	V1080	L1274	
	L230	E226	Q303	V388	F494	L563	P706	K769	GLY	V1080	L1275	
	L231	E226	Q303	V388	F494	L563	P707	K770	GLY	V1080	L1276	
	L232	E226	Q303	V388	F494	L563	P708	K771	GLY	V1080	L1277	
	L233	E226	Q303	V388	F494	L563	P709	K772	GLY	V1080	L1278	
	L234	E226	Q303	V388	F494	L563	P710	K773	GLY	V1080	L1279	
	L235	E226	Q303	V388	F494	L563	P711	K774	GLY	V1080	L1280	
	L236	E226	Q303	V388	F494	L563	P712	K775	GLY	V1080	L1281	
	L237	E226	Q303	V388	F494	L563	P713	K776	GLY	V1080	L1282	
	L238	E226	Q303	V388	F494	L563	P714	K777	GLY	V1080	L1283	
	L239	E226	Q303	V388	F494	L563	P715	K778	GLY	V1080	L1284	
	L240	E226	Q303	V388	F494	L563	P716	K779	GLY	V1080	L1285	
	L241	E226	Q303	V388	F494	L563	P717	K780	GLY	V1080	L1286	
	L242	E226	Q303	V388	F494	L563	P718	K781	GLY	V1080	L1287	
	L243	E226	Q303	V388	F494	L563	P719	K782	GLY	V1080	L1288	
	L244	E226	Q303	V388	F494	L563	P720	K783	GLY	V1080	L1289	
	L245	E226	Q303	V388	F494	L563	P721	K784	GLY	V1080	L1290	
	L246	E226	Q303	V388	F494	L563	P722	K785	GLY	V1080	L1291	
	L247	E226	Q303	V388	F494	L563	P723	K786	GLY	V1080	L1292	
	L248	E226	Q303	V388	F494	L563	P724	K787	GLY	V1080	L1293	
	L249	E226	Q303	V388	F494	L563	P725	K788	GLY	V1080	L1294	
	L250	E226	Q303	V388	F494	L563	P726	K789	GLY	V1080	L1295	
	L251	E226	Q303	V388	F494	L563	P727	K790	GLY	V1080	L1296	
	L252	E226	Q303	V388	F494	L563	P728	K791	GLY	V1080	L1297	
	L253	E226	Q303	V388	F494	L563	P729	K792	GLY	V1080	L1298	
	L254	E226	Q303	V388	F494	L563	P730	K793	GLY	V1080	L1299	
	L255	E226	Q303	V388	F494	L563	P731	K794	GLY	V1080	L1300	
	L256	E226	Q303	V388	F494	L563	P732	K795	GLY	V1080	L1301	
	L257	E226	Q303	V388	F494	L563	P733	K796	GLY	V1080	L1302	
	L258	E226	Q303	V388	F494	L563	P734	K797	GLY	V1080	L1303	
	L259	E226	Q303	V388	F494	L563	P735	K798	GLY	V1080	L1304	
	L260	E226	Q303	V388	F494	L563	P736	K799	GLY	V1080	L1305	
	L261	E226	Q303	V388	F494	L563	P737	K800	GLY	V1080	L1306	
	L262	E226	Q303	V388	F494							



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	167765	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	0.681	Depositor
Minimum map value	-0.155	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.18	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	0.30	0/16198	0.48	0/22023
1	B	0.30	0/16222	0.49	0/22055
All	All	0.30	0/32420	0.49	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	530	0
1	B	15857	9371	15826	542	0
2	A	96	52	52	1	0
2	B	96	52	52	0	0
All	All	31882	18818	31739	1051	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 17.

All (1051) 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:628:GLU:HA	1:A:631:LYS:HE2	1.28	1.12
1:B:717:ILE:HD12	1:B:727:ALA:HB2	1.42	1.00
1:B:569:CYS:SG	1:B:814:ALA:HB1	2.02	0.99
1:A:640:PRO:HA	1:A:651:ILE:HG22	1.43	0.99
1:B:165:LEU:HD11	1:B:402:ILE:HG23	1.41	0.98
1:B:566:LEU:HD22	1:B:815:LEU:HD22	1.45	0.98
1:A:188:ILE:HG22	1:A:228:VAL:HG13	1.46	0.97
1:B:290:ILE:HG23	1:B:322:ILE:HD12	1.44	0.96
1:B:619:ALA:HB3	1:B:658:VAL:HG11	1.48	0.95
1:A:83:LEU:HD23	1:A:144:LEU:HD23	1.49	0.94
1:B:165:LEU:HG	1:B:400:VAL:CG1	1.99	0.93
1:B:164:SER:HB2	1:B:338:LEU:HG	1.50	0.91
1:A:440:GLN:HG3	1:A:833:LEU:HD22	1.51	0.90
1:B:440:GLN:HG3	1:B:833:LEU:HD22	1.52	0.89
1:B:326:LYS:HG2	1:B:331:HIS:HB3	1.52	0.89
1:B:621:ALA:HA	1:B:674:GLU:HA	1.55	0.89
1:A:1212:ASP:OD1	1:A:1213:PRO:HD2	1.71	0.88
1:B:165:LEU:HD11	1:B:402:ILE:CG2	2.05	0.86
1:B:527:VAL:CG2	1:B:600:VAL:CG1	2.53	0.86
1:B:638:VAL:HG13	1:B:651:ILE:HD13	1.57	0.85
1:A:549:ILE:HD11	1:A:611:LYS:HG3	1.59	0.85
1:B:292:ALA:HB2	1:B:322:ILE:HD11	1.58	0.85
1:B:79:LEU:HD21	1:B:143:ARG:HG3	1.59	0.84
1:B:527:VAL:CG2	1:B:600:VAL:HG12	2.08	0.83
1:B:654:PRO:HB2	1:B:657:PRO:HD2	1.61	0.82
1:A:1446:ILE:HG21	1:A:1486:VAL:HG21	1.60	0.82
1:A:164:SER:HB2	1:A:338:LEU:HD13	1.59	0.82
1:A:687:MET:HE3	1:A:690:ILE:HD12	1.61	0.82
1:B:625:LEU:HD21	1:B:670:VAL:HG21	1.60	0.81
1:A:259:GLN:N	1:A:259:GLN:OE1	2.13	0.81
1:B:250:GLY:HA3	1:B:276:LEU:HD21	1.63	0.81
1:B:235:LYS:HG3	1:B:238:LEU:HD13	1.63	0.80
1:A:444:HIS:CD2	1:A:828:PRO:HG2	2.16	0.80
1:B:745:PHE:O	1:B:749:LEU:HG	1.81	0.80
1:A:1275:ARG:NH2	1:A:1321:ALA:O	2.14	0.80
1:A:79:LEU:HD21	1:A:143:ARG:HG3	1.62	0.80
1:A:786:LYS:HB2	1:A:795:PHE:HE2	1.45	0.80
1:B:511:MET:HE1	1:B:520:ILE:HG21	1.64	0.79
1:A:548:ASP:OD1	1:A:550:VAL:N	2.15	0.79
1:B:165:LEU:HG	1:B:400:VAL:HG11	1.64	0.79
1:B:1714:GLN:OE1	1:B:1714:GLN:N	2.16	0.79
1:B:285:GLU:OE1	1:B:285:GLU:N	2.16	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:701:VAL:HG12	1:A:702:ILE:HD12	1.65	0.78
1:B:215:PHE:HZ	1:B:292:ALA:HB3	1.48	0.78
1:B:737:ASN:HA	1:B:740:VAL:HG22	1.65	0.78
1:A:627:TRP:CZ3	1:A:640:PRO:HB2	2.19	0.78
1:B:639:VAL:HG13	1:B:640:PRO:HD2	1.66	0.78
1:A:161:CYS:HB2	1:A:394:GLY:HA2	1.65	0.78
1:A:543:GLU:N	1:A:543:GLU:OE1	2.17	0.78
1:A:1278:GLN:OE1	1:A:1278:GLN:N	2.17	0.78
1:B:556:LEU:HD23	1:B:582:LEU:HD23	1.66	0.78
1:B:47:LEU:HD21	1:B:198:VAL:HG22	1.64	0.77
1:B:1046:LEU:CD1	1:B:1102:ALA:HB3	2.14	0.77
1:A:848:GLU:N	1:A:848:GLU:OE1	2.16	0.77
1:A:274:ARG:HA	1:A:277:TYR:CE2	2.20	0.77
1:A:725:SER:HA	1:A:728:ARG:HH12	1.50	0.77
1:A:1410:ASP:OD1	1:A:1411:SER:N	2.19	0.76
1:A:622:ALA:O	1:A:672:ALA:HA	1.85	0.76
1:A:191:LEU:HD13	1:A:226:GLU:HB3	1.68	0.75
1:B:1071:ASP:OD1	1:B:1072:LYS:N	2.20	0.75
1:B:225:SER:HB2	1:B:330:GLY:O	1.87	0.75
1:B:216:ASP:OD1	1:B:217:THR:N	2.20	0.74
1:B:674:GLU:N	1:B:674:GLU:OE1	2.20	0.74
1:A:549:ILE:HD12	1:A:550:VAL:N	2.03	0.74
1:B:619:ALA:HB3	1:B:658:VAL:CG1	2.18	0.74
1:B:697:GLU:O	1:B:701:VAL:HG23	1.87	0.74
1:B:1046:LEU:HD12	1:B:1046:LEU:O	1.87	0.73
1:B:1197:GLU:OE1	1:B:1197:GLU:N	2.20	0.73
1:B:1046:LEU:HD11	1:B:1102:ALA:HB3	1.69	0.73
1:A:581:SER:OG	1:A:582:LEU:N	2.20	0.73
1:B:1562:GLN:NE2	1:B:1607:ASP:OD1	2.21	0.73
1:B:621:ALA:HB2	1:B:674:GLU:HB3	1.70	0.73
1:A:1145:VAL:HG21	1:A:1356:ILE:HG12	1.72	0.72
1:A:665:LEU:HB3	1:A:670:VAL:CG2	2.20	0.72
1:B:191:LEU:N	1:B:226:GLU:OE2	2.19	0.72
1:B:504:ARG:HD3	1:B:543:GLU:HA	1.72	0.72
1:B:1195:GLN:O	1:B:1199:ALA:N	2.22	0.72
1:A:124:PRO:HA	1:A:127:LEU:HD23	1.71	0.72
1:A:139:MET:HE2	1:A:139:MET:HA	1.71	0.72
1:A:627:TRP:CH2	1:A:640:PRO:HB2	2.25	0.72
1:B:1130:GLU:N	1:B:1130:GLU:OE1	2.21	0.72
1:A:2034:TYR:O	1:A:2038:ASN:ND2	2.23	0.72
1:A:654:PRO:HB2	1:A:657:PRO:HD2	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:LEU:HG	1:B:400:VAL:HG12	1.70	0.71
1:A:644:ASN:HD21	1:A:770:VAL:HG21	1.55	0.71
1:A:719:GLU:HA	1:A:722:TRP:NE1	2.06	0.71
1:B:597:GLU:OE1	1:B:597:GLU:N	2.20	0.71
1:A:198:VAL:HG12	1:B:127:LEU:HD11	1.73	0.71
1:B:1014:GLU:N	1:B:1014:GLU:OE1	2.22	0.71
1:A:456:ASP:OD1	1:A:813:ASN:ND2	2.24	0.71
1:B:2042:GLU:OE2	1:B:2059:GLN:NE2	2.23	0.71
1:A:635:PRO:HD3	1:A:661:PHE:CE1	2.24	0.70
1:A:645:SER:OG	1:A:770:VAL:HG13	1.90	0.70
1:A:1324:ASP:OD2	1:A:1326:ALA:N	2.24	0.70
1:A:584:GLU:OE2	1:A:712:TRP:NE1	2.24	0.70
1:A:642:CYS:CB	1:A:743:VAL:HB	2.22	0.70
1:B:747:GLU:N	1:B:747:GLU:OE1	2.24	0.70
1:B:527:VAL:HG23	1:B:600:VAL:HG11	1.73	0.70
1:A:277:TYR:CE1	1:A:284:PRO:HG3	2.26	0.70
1:A:692:PRO:O	1:A:695:LEU:HG	1.92	0.70
1:A:161:CYS:HA	1:A:333:GLU:O	1.91	0.70
1:B:497:SER:HB3	1:B:762:ALA:HB2	1.74	0.70
1:A:553:PHE:CD2	1:A:582:LEU:HD22	2.26	0.69
1:A:725:SER:HA	1:A:728:ARG:NH1	2.06	0.69
1:B:719:GLU:HA	1:B:722:TRP:CD1	2.27	0.69
1:B:634:CYS:HB2	1:B:638:VAL:O	1.93	0.69
1:A:274:ARG:HA	1:A:277:TYR:CD2	2.27	0.69
1:B:719:GLU:HA	1:B:722:TRP:NE1	2.07	0.69
1:A:132:MET:HE2	1:B:200:PHE:CZ	2.28	0.69
1:A:623:VAL:HG13	1:A:665:LEU:HD13	1.73	0.69
1:B:524:ASP:OD1	1:B:534:VAL:HB	1.92	0.69
1:B:64:PHE:HE1	1:B:464:ALA:HB1	1.58	0.69
1:B:114:SER:O	1:B:117:SER:OG	2.09	0.69
1:B:326:LYS:HG2	1:B:331:HIS:CB	2.21	0.69
1:A:545:THR:HG23	1:A:546:PHE:CD1	2.27	0.68
1:B:47:LEU:HD13	1:B:197:SER:HB2	1.75	0.68
1:B:504:ARG:HA	1:B:546:PHE:CE2	2.28	0.68
1:B:717:ILE:CD1	1:B:727:ALA:HB2	2.22	0.68
1:B:476:GLU:OE2	1:B:477:ARG:NH1	2.25	0.68
1:B:527:VAL:CG2	1:B:600:VAL:HG11	2.22	0.68
1:B:640:PRO:HA	1:B:651:ILE:HG22	1.74	0.68
1:A:324:SER:H	1:A:356:ASN:HD21	1.42	0.68
1:A:694:LEU:O	1:A:698:LEU:HG	1.93	0.68
1:B:343:LYS:HZ3	1:B:354:ALA:HB3	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1327:SER:O	1:B:1331:ASN:ND2	2.25	0.68
1:A:492:LEU:HB2	1:A:808:ILE:CD1	2.24	0.68
1:A:654:PRO:HB2	1:A:657:PRO:CD	2.24	0.68
1:A:786:LYS:HB2	1:A:795:PHE:CE2	2.27	0.68
1:A:1130:GLU:N	1:A:1130:GLU:OE1	2.27	0.68
1:B:82:LEU:HD22	1:B:188:ILE:HG21	1.75	0.68
1:B:556:LEU:HD13	1:B:763:PRO:HG3	1.76	0.67
1:B:1429:LYS:NZ	1:B:1981:GLU:O	2.27	0.67
1:A:139:MET:HE1	1:B:396:GLY:HA3	1.75	0.67
1:A:505:GLY:O	1:A:508:LEU:HD13	1.94	0.67
1:B:527:VAL:HG22	1:B:600:VAL:HG12	1.75	0.67
1:A:168:LEU:HD22	1:A:402:ILE:HD13	1.75	0.67
1:B:326:LYS:CG	1:B:331:HIS:HB3	2.25	0.67
1:B:606:ARG:O	1:B:610:ILE:HG13	1.95	0.67
1:A:631:LYS:HG3	1:A:632:GLN:OE1	1.95	0.67
1:B:343:LYS:NZ	1:B:354:ALA:HB3	2.09	0.67
1:B:51:SER:HA	1:B:223:CYS:SG	2.34	0.67
1:A:557:THR:O	1:A:561:ILE:HG13	1.95	0.66
1:B:658:VAL:O	1:B:662:VAL:HG23	1.95	0.66
1:A:639:VAL:HB	1:A:640:PRO:HD2	1.77	0.66
1:A:1975:LEU:HD12	1:A:1975:LEU:O	1.95	0.66
1:B:293:HIS:N	1:B:304:GLU:OE2	2.15	0.66
1:A:606:ARG:O	1:A:610:ILE:HG13	1.94	0.66
1:A:695:LEU:HD12	1:A:696:GLN:N	2.10	0.66
1:A:115:GLU:OE1	1:A:193:LYS:N	2.28	0.66
1:A:1241:LYS:O	1:A:1311:ASP:N	2.29	0.66
1:A:1286:GLU:OE1	1:A:1286:GLU:N	2.28	0.66
1:B:730:SER:HA	1:B:734:TYR:HD2	1.61	0.66
1:A:38:ARG:HH21	1:A:53:LYS:HE2	1.59	0.66
1:A:213:LYS:HE2	1:A:218:ALA:O	1.96	0.66
1:A:108:TRP:NE1	1:A:155:ILE:HD13	2.10	0.66
1:A:620:MET:HG2	1:A:677:THR:CG2	2.26	0.66
1:A:831:SER:OG	1:A:832:PRO:HD3	1.96	0.66
1:B:79:LEU:O	1:B:83:LEU:HD13	1.95	0.66
1:B:274:ARG:HA	1:B:277:TYR:CE2	2.31	0.66
1:B:618:GLY:N	1:B:679:GLY:O	2.29	0.66
1:B:696:GLN:O	1:B:700:LYS:HG2	1.96	0.65
1:B:157:LEU:O	1:B:157:LEU:HD12	1.96	0.65
1:A:207:SER:HB2	1:A:221:GLY:N	2.11	0.65
1:A:1178:LEU:HB2	1:A:1212:ASP:OD2	1.97	0.65
1:A:1212:ASP:OD1	1:A:1213:PRO:CD	2.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1521:GLU:OE1	1:B:1521:GLU:N	2.29	0.65
1:A:38:ARG:NH2	1:A:53:LYS:HB2	2.11	0.65
1:B:1177:GLU:N	1:B:1177:GLU:OE1	2.29	0.65
1:A:644:ASN:OD1	1:A:770:VAL:HG11	1.97	0.65
1:A:772:LYS:NZ	1:A:781:ILE:HB	2.11	0.65
1:B:597:GLU:O	1:B:601:LEU:HG	1.96	0.65
1:B:344:VAL:HG21	1:B:390:ILE:HD11	1.76	0.65
1:B:557:THR:O	1:B:561:ILE:HG13	1.97	0.65
1:B:627:TRP:CZ3	1:B:640:PRO:HB2	2.32	0.65
1:B:290:ILE:HD12	1:B:389:GLY:O	1.96	0.65
1:B:620:MET:CE	1:B:682:PHE:HB2	2.26	0.65
1:A:291:GLU:OE2	1:A:325:THR:N	2.28	0.65
1:A:655:GLN:OE1	1:A:655:GLN:N	2.26	0.65
1:A:36:ASP:OD2	1:A:38:ARG:NE	2.30	0.64
1:B:1145:VAL:HG21	1:B:1356:ILE:HG12	1.80	0.64
1:A:502:GLN:HE21	1:A:556:LEU:HB2	1.60	0.64
1:B:122:ARG:NH1	1:B:849:ASP:HA	2.13	0.64
1:A:118:GLU:OE2	1:B:118:GLU:HG2	1.97	0.64
1:A:732:ALA:O	1:A:736:VAL:HG23	1.97	0.64
1:A:83:LEU:HD23	1:A:144:LEU:CD2	2.26	0.64
1:B:622:ALA:O	1:B:672:ALA:HA	1.96	0.64
1:A:138:ALA:HB1	1:B:160:ALA:HB2	1.79	0.64
1:A:595:SER:HB3	1:A:598:GLU:HG3	1.78	0.64
1:A:241:ARG:HD3	1:A:243:TYR:CE1	2.32	0.64
1:A:539:LEU:HD23	1:A:539:LEU:O	1.97	0.64
1:A:869:GLU:N	1:A:869:GLU:OE1	2.30	0.64
1:B:209:GLU:N	1:B:209:GLU:OE1	2.31	0.64
1:B:264:PRO:HG3	1:B:300:GLY:HA2	1.80	0.64
1:A:316:ARG:HH21	1:A:318:GLU:HG2	1.63	0.64
1:B:207:SER:HB3	1:B:221:GLY:N	2.13	0.64
1:A:64:PHE:HE1	1:A:464:ALA:HB1	1.63	0.64
1:A:417:HIS:O	1:A:422:ARG:NH2	2.25	0.64
1:A:784:LEU:HD22	1:A:796:PHE:CD2	2.33	0.64
1:A:1176:GLN:N	1:A:1176:GLN:OE1	2.30	0.64
1:B:721:GLN:OE1	1:B:721:GLN:N	2.31	0.64
1:A:908:GLU:OE1	1:A:908:GLU:N	2.31	0.64
1:B:60:PHE:CD1	1:B:80:ARG:HB3	2.33	0.64
1:B:82:LEU:HD22	1:B:188:ILE:CG2	2.27	0.63
1:B:235:LYS:HE3	1:B:238:LEU:HD11	1.80	0.63
1:A:184:ILE:CD1	1:A:232:LEU:HD13	2.28	0.63
1:A:248:ASN:OD1	1:A:249:ALA:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:ARG:NH1	1:B:318:GLU:O	2.31	0.63
1:B:1198:LEU:O	1:B:1202:LEU:N	2.28	0.63
1:A:243:TYR:HB3	1:A:345:LEU:HD22	1.79	0.63
1:B:656:ALA:HB3	1:B:657:PRO:HD3	1.80	0.63
1:A:426:ALA:HB1	1:A:437:LEU:HD13	1.80	0.63
1:B:468:ARG:HD3	1:B:804:HIS:CD2	2.34	0.63
1:B:621:ALA:CA	1:B:674:GLU:HA	2.29	0.63
1:A:749:LEU:O	1:A:752:VAL:HG23	1.99	0.63
1:B:47:LEU:HD21	1:B:198:VAL:CG2	2.29	0.63
1:B:450:PHE:HE1	1:B:830:ILE:HG12	1.63	0.63
1:B:894:ILE:HG22	1:B:935:VAL:HG21	1.81	0.63
1:A:189:ASN:HB2	1:A:334:PRO:HG2	1.81	0.62
1:A:348:LEU:HD13	1:A:406:PRO:HB3	1.81	0.62
1:A:657:PRO:O	1:A:660:GLU:HG2	1.98	0.62
1:B:661:PHE:O	1:B:665:LEU:HG	1.98	0.62
1:B:159:THR:HG21	1:B:166:MET:HG2	1.81	0.62
1:B:322:ILE:CG2	1:B:376:VAL:HG22	2.29	0.62
1:A:78:GLN:HB3	1:A:188:ILE:HD12	1.81	0.62
1:A:1602:GLU:HB3	1:A:1650:VAL:HG23	1.80	0.62
1:B:737:ASN:HA	1:B:740:VAL:CG2	2.30	0.62
1:A:14:PRO:CD	1:A:329:MET:HE3	2.29	0.62
1:A:217:THR:HG23	1:A:361:SER:O	2.00	0.62
1:A:687:MET:CE	1:A:690:ILE:HD12	2.30	0.62
1:B:56:ASP:OD1	1:B:57:LEU:N	2.32	0.62
1:B:426:ALA:HB1	1:B:437:LEU:HD12	1.81	0.62
1:B:654:PRO:HB2	1:B:657:PRO:CD	2.30	0.62
1:A:168:LEU:HD22	1:A:402:ILE:CD1	2.30	0.62
1:A:305:LEU:HD11	1:A:322:ILE:HD11	1.82	0.62
1:A:607:GLY:O	1:A:610:ILE:HB	1.99	0.62
1:B:87:TYR:O	1:B:91:VAL:HG22	2.00	0.62
1:B:662:VAL:O	1:B:666:ARG:HG2	1.99	0.62
1:A:719:GLU:HA	1:A:722:TRP:CE2	2.35	0.62
1:B:290:ILE:O	1:B:322:ILE:HD12	2.00	0.62
1:B:939:GLU:OE1	1:B:939:GLU:N	2.33	0.62
1:B:4:VAL:HG22	1:B:175:ILE:CG2	2.30	0.61
1:B:133:VAL:O	1:B:139:MET:HG3	2.00	0.61
1:B:691:ALA:O	1:B:695:LEU:N	2.23	0.61
1:A:491:PRO:HG2	1:A:756:ALA:CB	2.31	0.61
1:A:9:MET:HG2	1:A:19:LEU:CD1	2.31	0.61
1:A:776:LYS:H	1:A:776:LYS:HD2	1.65	0.61
1:B:501:THR:HG22	1:B:766:LEU:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:HIS:NE2	1:A:828:PRO:HG2	2.14	0.61
1:A:1942:SER:O	1:A:1943:THR:OG1	2.15	0.61
1:A:13:LEU:HB3	1:A:14:PRO:CD	2.30	0.61
1:A:1273:THR:HG21	1:A:1307:LEU:HD11	1.83	0.61
1:B:431:PRO:HG3	1:B:467:PHE:CE2	2.35	0.61
1:B:693:PRO:O	1:B:697:GLU:HG2	2.01	0.61
1:B:432:GLU:N	1:B:432:GLU:OE1	2.32	0.61
1:B:309:THR:HA	1:B:313:CYS:SG	2.41	0.61
1:B:550:VAL:O	1:B:554:VAL:HG23	2.01	0.61
1:B:645:SER:OG	1:B:648:THR:N	2.21	0.61
1:A:646:LYS:HG3	1:A:647:ASP:OD1	1.99	0.61
1:A:1178:LEU:CB	1:A:1212:ASP:OD2	2.49	0.61
1:B:254:ASP:HA	1:B:268:ILE:HG13	1.82	0.61
1:B:1205:GLU:OE1	1:B:1209:LEU:HD12	1.99	0.61
1:A:86:THR:HG23	1:A:184:ILE:HG21	1.82	0.60
1:A:596:GLN:O	1:A:600:VAL:HG23	2.01	0.60
1:B:698:LEU:HD13	1:B:735:ASN:HB2	1.82	0.60
1:A:107:VAL:HG11	1:A:144:LEU:HD12	1.83	0.60
1:A:162:SER:OG	1:A:394:GLY:N	2.34	0.60
1:B:127:LEU:HD12	1:B:127:LEU:O	2.02	0.60
1:B:620:MET:HE1	1:B:682:PHE:HB2	1.83	0.60
1:A:189:ASN:HB2	1:A:334:PRO:CG	2.31	0.60
1:B:25:ASN:HB2	1:B:32:MET:HE2	1.84	0.60
1:B:566:LEU:CD2	1:B:815:LEU:HD22	2.28	0.60
1:B:881:ASP:OD1	1:B:1046:LEU:HD22	2.01	0.60
1:B:1025:ASN:ND2	1:B:1028:SER:OG	2.34	0.60
1:A:425:ARG:HD2	1:A:804:HIS:ND1	2.16	0.60
1:A:772:LYS:HD2	1:A:781:ILE:HD13	1.84	0.60
1:B:112:SER:HB3	1:B:334:PRO:HG3	1.83	0.60
1:B:1274:ASP:OD1	1:B:1275:ARG:N	2.34	0.60
1:A:9:MET:HG2	1:A:19:LEU:HD11	1.84	0.60
1:A:207:SER:HB2	1:A:221:GLY:CA	2.31	0.60
1:A:127:LEU:HD12	1:A:127:LEU:O	2.02	0.60
1:A:623:VAL:HG12	1:A:625:LEU:H	1.67	0.60
1:A:643:HIS:N	1:A:743:VAL:O	2.32	0.60
1:B:1228:LEU:HD21	1:B:1256:ILE:HD12	1.83	0.60
1:B:504:ARG:HA	1:B:546:PHE:HE2	1.67	0.59
1:B:1997:SER:O	1:B:2001:ASN:ND2	2.35	0.59
1:A:431:PRO:HG3	1:A:467:PHE:CE2	2.37	0.59
1:B:31:ASP:OD2	1:B:50:ARG:NH2	2.35	0.59
1:B:495:ILE:CD1	1:B:578:VAL:HB	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:588:GLY:HA2	1:A:712:TRP:CZ3	2.38	0.59
1:A:333:GLU:HB2	1:A:334:PRO:HD3	1.84	0.59
1:A:550:VAL:HG21	1:A:611:LYS:HE2	1.84	0.59
1:A:578:VAL:HG13	1:A:715:THR:CG2	2.33	0.59
1:A:784:LEU:O	1:A:785:MET:HG3	2.00	0.59
1:B:248:ASN:ND2	1:B:279:SER:OG	2.34	0.59
1:B:542:ASP:O	1:B:545:THR:OG1	2.15	0.59
1:A:18:ASN:OD1	1:A:20:GLN:HB3	2.02	0.59
1:B:92:ASP:OD1	1:B:241:ARG:NH2	2.35	0.59
1:B:51:SER:OG	1:B:224:ARG:O	2.15	0.59
1:B:253:THR:HG22	1:B:255:GLY:H	1.67	0.59
1:B:556:LEU:HD23	1:B:582:LEU:CD2	2.31	0.59
1:A:155:ILE:HG22	1:A:156:ALA:N	2.18	0.59
1:A:852:ASN:O	1:A:852:ASN:ND2	2.35	0.59
1:B:290:ILE:HG23	1:B:322:ILE:CD1	2.26	0.59
1:B:291:GLU:OE2	1:B:325:THR:N	2.35	0.59
1:B:654:PRO:HG3	1:B:686:PHE:HZ	1.67	0.59
1:A:93:GLY:O	1:A:240:ARG:HB2	2.02	0.59
1:A:138:ALA:CB	1:B:160:ALA:HB2	2.33	0.59
1:A:293:HIS:CE1	1:A:326:LYS:HE2	2.37	0.59
1:A:396:GLY:HA3	1:B:142:ASN:ND2	2.17	0.59
1:A:1344:LEU:HD21	1:A:1377:TRP:CH2	2.38	0.59
1:B:621:ALA:O	1:B:650:THR:HG23	2.02	0.59
1:B:654:PRO:HG3	1:B:686:PHE:CZ	2.37	0.59
1:B:935:VAL:HG22	1:B:946:VAL:HG22	1.85	0.59
1:A:440:GLN:HG3	1:A:833:LEU:CD2	2.29	0.58
1:A:644:ASN:O	1:A:746:GLN:HB2	2.03	0.58
1:A:642:CYS:SG	1:A:743:VAL:HB	2.43	0.58
1:B:527:VAL:HG21	1:B:600:VAL:CG1	2.31	0.58
1:B:642:CYS:HA	1:B:743:VAL:HB	1.86	0.58
1:A:1246:LEU:HD11	1:A:1299:PRO:HG2	1.83	0.58
1:A:593:CYS:O	1:A:594:LEU:HD23	2.03	0.58
1:A:654:PRO:O	1:A:658:VAL:HG23	2.04	0.58
1:A:1077:ASP:OD1	1:A:1078:VAL:N	2.36	0.58
1:A:514:ASP:OD1	1:A:515:ARG:N	2.36	0.58
1:B:775:LEU:HB3	1:B:779:CYS:SG	2.43	0.58
1:A:301:ASP:HB2	1:A:302:PRO:HD3	1.84	0.58
1:A:491:PRO:HG2	1:A:756:ALA:HB2	1.86	0.58
1:A:492:LEU:HB2	1:A:808:ILE:HD11	1.85	0.58
1:B:652:SER:OG	1:B:684:SER:HB3	2.01	0.58
1:A:737:ASN:HA	1:A:740:VAL:HG22	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:997:ARG:NH2	1:A:1041:SER:O	2.36	0.58
1:B:767:LEU:O	1:B:771:LEU:HD13	2.03	0.58
1:B:881:ASP:OD2	1:B:1046:LEU:HD21	2.03	0.58
1:A:542:ASP:OD1	1:A:544:SER:N	2.37	0.58
1:B:525:GLU:HA	1:B:525:GLU:OE1	2.02	0.58
1:A:772:LYS:HZ3	1:A:781:ILE:HB	1.69	0.58
1:A:83:LEU:CD2	1:A:144:LEU:HD23	2.30	0.58
1:A:2042:GLU:OE2	1:A:2059:GLN:NE2	2.37	0.58
1:B:333:GLU:HB2	1:B:334:PRO:HD3	1.85	0.58
1:A:184:ILE:HD13	1:A:232:LEU:HD13	1.86	0.57
1:A:247:LEU:HD13	1:A:405:ARG:HB2	1.85	0.57
1:A:620:MET:HG2	1:A:677:THR:HG21	1.86	0.57
1:B:477:ARG:HH12	1:B:790:ARG:HD2	1.70	0.57
1:A:6:ILE:HG12	1:A:233:LEU:CD2	2.34	0.57
1:A:103:THR:HG22	1:A:104:HIS:H	1.70	0.57
1:B:1860:GLU:OE1	1:B:1860:GLU:N	2.36	0.57
1:A:324:SER:N	1:A:356:ASN:HD21	2.02	0.57
1:A:333:GLU:N	1:A:333:GLU:OE1	2.37	0.57
1:A:5:VAL:HB	1:A:242:VAL:HG13	1.85	0.57
1:B:351:GLY:C	1:B:352:LEU:HD12	2.24	0.57
1:B:1031:ASP:OD2	1:B:1035:GLN:NE2	2.37	0.57
1:A:533:LYS:HB2	1:A:536:GLN:HB3	1.86	0.57
1:A:1415:LEU:HD22	1:A:1443:LEU:HD22	1.87	0.57
1:B:189:ASN:HB2	1:B:334:PRO:HD2	1.87	0.57
1:A:133:VAL:O	1:A:139:MET:HG3	2.05	0.57
1:A:768:GLN:HG3	1:A:781:ILE:HG21	1.86	0.57
1:A:1725:ASP:OD1	1:A:1726:THR:N	2.38	0.57
1:B:348:LEU:HD13	1:B:406:PRO:HB3	1.86	0.57
1:B:741:SER:HB2	1:B:742:PRO:HD2	1.87	0.57
1:B:764:HIS:CD2	1:B:766:LEU:HB2	2.40	0.57
1:B:1370:GLY:O	1:B:1371:ILE:HD13	2.05	0.57
1:B:1552:ARG:O	1:B:1555:GLN:NE2	2.38	0.57
1:B:191:LEU:O	1:B:192:LEU:HD23	2.05	0.57
1:B:1214:LEU:HD12	1:B:1215:LEU:N	2.20	0.57
1:B:81:LEU:O	1:B:85:VAL:HG23	2.05	0.56
1:A:225:SER:O	1:A:332:PRO:HA	2.05	0.56
1:B:322:ILE:HG13	1:B:323:GLY:N	2.20	0.56
1:A:316:ARG:NH1	1:A:320:LEU:HB2	2.20	0.56
1:A:578:VAL:HG13	1:A:715:THR:HG21	1.86	0.56
1:A:635:PRO:HD3	1:A:661:PHE:CD1	2.40	0.56
1:A:687:MET:CE	1:A:739:LEU:HD21	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1195:GLN:N	1:A:1195:GLN:OE1	2.35	0.56
1:A:1446:ILE:HD12	1:A:1447:ASN:N	2.20	0.56
1:B:22:PHE:CE2	1:B:26:LEU:HD11	2.41	0.56
1:B:755:HIS:N	1:B:778:SER:OG	2.28	0.56
1:A:155:ILE:HG22	1:A:156:ALA:H	1.70	0.56
1:A:619:ALA:O	1:A:658:VAL:HG21	2.06	0.56
1:B:344:VAL:CG2	1:B:390:ILE:HD11	2.34	0.56
1:A:198:VAL:CG1	1:B:127:LEU:HD21	2.36	0.56
1:B:737:ASN:CA	1:B:740:VAL:HG22	2.35	0.56
1:A:642:CYS:HA	1:A:743:VAL:HB	1.87	0.56
1:B:499:MET:HG2	1:B:582:LEU:HD22	1.88	0.56
1:B:1446:ILE:HG23	1:B:1474:LEU:HD12	1.87	0.56
1:A:203:LEU:HD12	1:B:132:MET:HE2	1.88	0.56
1:B:574:PRO:HG2	1:B:577:ILE:HD11	1.88	0.56
1:A:124:PRO:HG3	1:B:195:ASN:OD1	2.06	0.55
1:B:83:LEU:HD12	1:B:144:LEU:HD21	1.88	0.55
1:B:91:VAL:HG12	1:B:97:PRO:HD3	1.88	0.55
1:B:764:HIS:HD2	1:B:766:LEU:HB2	1.71	0.55
1:B:1879:THR:HG23	1:B:2015:TYR:OH	2.06	0.55
1:A:14:PRO:HD3	1:A:329:MET:HE3	1.87	0.55
1:A:698:LEU:HB2	1:A:732:ALA:HB1	1.88	0.55
1:A:1357:VAL:HG23	1:A:1371:ILE:HD13	1.88	0.55
1:B:235:LYS:CG	1:B:238:LEU:HD13	2.34	0.55
1:B:440:GLN:HG3	1:B:833:LEU:CD2	2.32	0.55
1:A:1563:LEU:HD12	1:A:1626:VAL:O	2.06	0.55
1:B:1417:VAL:HG12	1:B:1417:VAL:O	2.06	0.55
1:B:159:THR:OG1	1:B:163:SER:HA	2.07	0.55
1:B:497:SER:HB3	1:B:762:ALA:CB	2.37	0.55
1:B:663:GLU:O	1:B:667:LYS:HG3	2.06	0.55
1:B:713:LEU:HD22	1:B:722:TRP:CZ3	2.41	0.55
1:B:1111:VAL:O	1:B:1111:VAL:HG13	2.07	0.55
1:A:1751:GLU:OE1	1:A:1751:GLU:N	2.37	0.55
1:B:257:LYS:HD3	1:B:265:SER:HB2	1.89	0.55
1:B:421:PRO:HG2	1:B:793:LEU:HD23	1.87	0.55
1:B:1206:ARG:CZ	1:B:1209:LEU:HD13	2.36	0.55
1:A:1535:THR:HG23	1:A:1535:THR:O	2.07	0.55
1:A:1893:LEU:HD12	1:A:1916:SER:OG	2.07	0.55
1:B:124:PRO:HA	1:B:127:LEU:HD23	1.88	0.55
1:B:1228:LEU:HD21	1:B:1256:ILE:CD1	2.37	0.55
1:A:555:SER:O	1:A:559:ILE:HG13	2.07	0.55
1:A:665:LEU:HB3	1:A:670:VAL:HG23	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:LEU:HD21	1:B:512:ARG:HB3	1.88	0.55
1:A:33:VAL:HG13	1:A:51:SER:C	2.26	0.55
1:A:420:LEU:HD22	1:A:512:ARG:HE	1.72	0.55
1:B:527:VAL:HG11	1:B:532:LEU:HD11	1.87	0.55
1:B:1080:VAL:HG22	1:B:1087:THR:HG23	1.89	0.55
1:B:1343:LEU:HD11	1:B:1400:LEU:HD11	1.89	0.55
1:B:1046:LEU:HD12	1:B:1102:ALA:HB3	1.89	0.55
1:A:620:MET:HE2	1:A:650:THR:HG21	1.89	0.54
1:B:721:GLN:HB3	1:B:724:SER:OG	2.07	0.54
1:A:124:PRO:HA	1:A:127:LEU:CD2	2.35	0.54
1:B:14:PRO:CD	1:B:329:MET:HE3	2.36	0.54
1:B:769:ALA:O	1:B:773:ARG:HG2	2.06	0.54
1:A:661:PHE:O	1:A:665:LEU:HG	2.07	0.54
1:A:737:ASN:OD1	1:A:741:SER:HB2	2.07	0.54
1:B:191:LEU:HG	1:B:226:GLU:HG2	1.87	0.54
1:A:253:THR:HG21	1:B:145:SER:HB3	1.89	0.54
1:B:659:PHE:O	1:B:663:GLU:HG3	2.08	0.54
1:A:6:ILE:HA	1:A:233:LEU:CD2	2.38	0.54
1:A:203:LEU:HD12	1:B:132:MET:CE	2.36	0.54
1:A:332:PRO:HG2	1:A:336:SER:HA	1.88	0.54
1:A:628:GLU:CA	1:A:631:LYS:HE2	2.19	0.54
1:B:460:VAL:HG23	1:B:461:PRO:HD2	1.90	0.54
1:A:660:GLU:O	1:A:663:GLU:HG2	2.07	0.54
1:B:687:MET:HA	1:B:690:ILE:HD13	1.90	0.54
1:A:506:MET:HG3	1:A:559:ILE:HD11	1.89	0.54
1:A:622:ALA:HA	1:A:649:VAL:O	2.07	0.54
1:A:655:GLN:O	1:A:659:PHE:HD2	1.90	0.54
1:A:657:PRO:HA	1:A:660:GLU:HG2	1.90	0.54
1:A:1488:PRO:HA	1:A:1493:LEU:HD23	1.88	0.54
1:B:506:MET:HG3	1:B:559:ILE:HD11	1.89	0.54
1:B:1270:TYR:HB3	1:B:1292:VAL:HG12	1.90	0.54
1:A:13:LEU:HB3	1:A:14:PRO:HD2	1.88	0.54
1:A:820:GLU:OE1	1:A:820:GLU:N	2.35	0.54
1:A:1970:ASN:C	1:A:1971:LEU:HD12	2.28	0.54
1:B:615:LEU:HD11	1:B:680:MET:CE	2.37	0.54
1:B:655:GLN:O	1:B:658:VAL:HG12	2.08	0.54
1:A:517:ARG:O	1:A:521:LEU:HG	2.08	0.53
1:A:640:PRO:CA	1:A:651:ILE:HG22	2.27	0.53
1:B:4:VAL:HG22	1:B:175:ILE:HG22	1.89	0.53
1:A:506:MET:CE	1:A:555:SER:HB2	2.37	0.53
1:B:685:TYR:O	1:B:688:GLU:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:MET:HE1	1:A:830:ILE:HD12	1.90	0.53
1:A:1349:ARG:HB2	1:A:1371:ILE:HG22	1.90	0.53
1:B:291:GLU:HG2	1:B:340:ALA:HB1	1.89	0.53
1:A:763:PRO:HA	1:A:785:MET:CE	2.38	0.53
1:B:191:LEU:HG	1:B:226:GLU:CG	2.38	0.53
1:B:276:LEU:CD1	1:B:401:HIS:HB3	2.38	0.53
1:B:577:ILE:N	1:B:577:ILE:HD12	2.23	0.53
1:A:139:MET:HE2	1:A:139:MET:CA	2.39	0.53
1:B:577:ILE:HD13	1:B:591:ASP:OD1	2.08	0.53
1:A:121:SER:HB3	1:B:199:GLN:NE2	2.23	0.53
1:A:235:LYS:HG2	1:A:238:LEU:HD13	1.91	0.53
1:A:318:GLU:OE1	1:A:318:GLU:N	2.32	0.53
1:B:85:VAL:HG12	1:B:230:ALA:HB3	1.91	0.53
1:B:341:LEU:HA	1:B:390:ILE:CD1	2.39	0.53
1:A:793:LEU:O	1:A:797:LEU:HG	2.08	0.53
1:A:460:VAL:HG13	1:A:461:PRO:HD2	1.91	0.53
1:B:294:GLY:HA3	1:B:324:SER:OG	2.09	0.53
1:B:1125:GLU:N	1:B:1125:GLU:OE1	2.42	0.53
1:A:92:ASP:OD1	1:A:241:ARG:NH1	2.41	0.53
1:B:525:GLU:OE1	1:B:528:LYS:HD3	2.08	0.53
1:B:713:LEU:HD22	1:B:722:TRP:HZ3	1.74	0.53
1:B:533:LYS:O	1:B:537:LEU:HG	2.09	0.53
1:A:311:ALA:O	1:A:312:LEU:HD23	2.09	0.52
1:A:447:ASP:OD2	1:A:450:PHE:HB2	2.09	0.52
1:A:580:HIS:CD2	1:A:743:VAL:HG11	2.44	0.52
1:B:191:LEU:H	1:B:226:GLU:CD	2.08	0.52
1:B:311:ALA:C	1:B:312:LEU:HD23	2.28	0.52
1:B:654:PRO:O	1:B:658:VAL:HG12	2.09	0.52
1:B:881:ASP:OD1	1:B:1046:LEU:CD2	2.57	0.52
1:A:606:ARG:HH21	1:A:739:LEU:HD13	1.75	0.52
1:A:687:MET:HE2	1:A:739:LEU:HD21	1.92	0.52
1:B:615:LEU:HD12	1:B:615:LEU:O	2.09	0.52
1:A:692:PRO:HA	1:A:695:LEU:CD2	2.39	0.52
1:A:2018:VAL:HG11	1:A:2041:MET:HB3	1.90	0.52
1:A:342:ALA:O	1:A:346:LEU:HG	2.09	0.52
1:A:351:GLY:C	1:A:352:LEU:HD12	2.30	0.52
1:A:658:VAL:O	1:A:662:VAL:HG23	2.08	0.52
1:A:697:GLU:O	1:A:700:LYS:HB2	2.09	0.52
1:A:1716:ASP:OD1	1:A:1717:SER:N	2.42	0.52
1:B:87:TYR:CE1	1:B:97:PRO:HG2	2.44	0.52
1:B:746:GLN:OE1	1:B:750:TRP:NE1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:ILE:HG12	1:A:233:LEU:HD22	1.92	0.52
1:A:13:LEU:HD12	1:A:22:PHE:CE2	2.44	0.52
1:A:291:GLU:HG2	1:A:340:ALA:HB1	1.92	0.52
1:A:564:ILE:HD13	1:A:590:ALA:HB2	1.92	0.52
1:A:656:ALA:HB3	1:A:657:PRO:HD3	1.92	0.52
1:B:468:ARG:HB2	1:B:485:VAL:CG2	2.39	0.52
1:B:622:ALA:N	1:B:673:LYS:O	2.35	0.52
1:B:1113:ILE:HD11	1:B:2109:PHE:CE1	2.45	0.52
1:A:625:LEU:HA	1:A:629:GLU:OE2	2.10	0.52
1:A:1267:GLN:OE1	1:A:1267:GLN:N	2.43	0.52
1:A:1887:TYR:CD1	1:A:1909:VAL:HG13	2.45	0.52
1:B:13:LEU:HB3	1:B:14:PRO:HD2	1.92	0.52
1:B:516:PHE:CE1	1:B:562:GLY:HA3	2.45	0.52
1:A:60:PHE:CD1	1:A:80:ARG:HB3	2.45	0.52
1:A:505:GLY:C	1:A:508:LEU:HD13	2.30	0.52
1:A:522:ARG:HB2	1:A:596:GLN:HE22	1.75	0.52
1:A:620:MET:SD	1:A:682:PHE:HB2	2.50	0.52
1:A:638:VAL:HG13	1:A:652:SER:O	2.10	0.52
1:A:654:PRO:O	1:A:657:PRO:HD2	2.10	0.52
1:A:781:ILE:N	1:A:781:ILE:HD12	2.24	0.52
1:B:340:ALA:O	1:B:344:VAL:HG23	2.10	0.52
1:B:654:PRO:HD3	1:B:685:TYR:OH	2.10	0.52
1:A:761:ILE:HD13	1:A:784:LEU:HD12	1.90	0.52
1:B:390:ILE:HB	1:B:402:ILE:HD11	1.92	0.52
1:B:47:LEU:HD13	1:B:197:SER:CB	2.39	0.51
1:B:165:LEU:HD23	1:B:400:VAL:HB	1.92	0.51
1:B:694:LEU:CD1	1:B:698:LEU:HG	2.40	0.51
1:A:246:ILE:HG12	1:A:404:LEU:HD21	1.93	0.51
1:B:390:ILE:O	1:B:402:ILE:HG12	2.10	0.51
1:A:302:PRO:HG3	1:A:366:ILE:HD11	1.93	0.51
1:A:105:THR:OG1	1:A:182:ALA:HB3	2.09	0.51
1:B:640:PRO:CA	1:B:651:ILE:HG22	2.38	0.51
1:B:664:GLN:OE1	1:B:667:LYS:HD2	2.11	0.51
1:A:38:ARG:NH2	1:A:53:LYS:HE2	2.25	0.51
1:A:54:LEU:HG	1:A:226:GLU:HG3	1.91	0.51
1:B:194:PRO:O	1:B:198:VAL:HG23	2.11	0.51
1:B:267:ASP:O	1:B:271:GLN:HG3	2.10	0.51
1:B:276:LEU:HD12	1:B:401:HIS:HB3	1.92	0.51
1:B:342:ALA:O	1:B:346:LEU:HG	2.10	0.51
1:B:468:ARG:HB2	1:B:485:VAL:HG21	1.91	0.51
1:A:541:THR:HG22	1:A:541:THR:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:692:PRO:HB2	1:A:693:PRO:CD	2.40	0.51
1:B:39:ARG:NH2	1:B:226:GLU:OE1	2.43	0.51
1:B:235:LYS:HE3	1:B:238:LEU:CD1	2.41	0.51
1:B:704:GLU:HG2	1:B:704:GLU:O	2.11	0.51
1:B:579:GLY:O	1:B:715:THR:HG21	2.11	0.51
1:B:9:MET:HG2	1:B:19:LEU:CD1	2.41	0.51
1:B:105:THR:O	1:B:150:PHE:HB3	2.11	0.51
1:B:1205:GLU:O	1:B:1209:LEU:N	2.43	0.51
1:A:64:PHE:HB2	1:A:429:ARG:CZ	2.40	0.51
1:A:270:GLU:OE1	1:A:310:ARG:NE	2.28	0.51
1:A:606:ARG:NH2	1:A:739:LEU:HA	2.26	0.51
1:A:615:LEU:HD13	1:A:686:PHE:HB3	1.93	0.51
1:A:1214:LEU:O	1:A:1396:TYR:OH	2.20	0.51
1:B:517:ARG:O	1:B:521:LEU:HG	2.10	0.51
1:B:629:GLU:O	1:B:633:ARG:HG2	2.11	0.51
1:B:657:PRO:HA	1:B:660:GLU:OE1	2.11	0.51
1:B:708:ARG:NH2	1:B:714:SER:HB2	2.26	0.51
1:A:821:PHE:HB3	1:A:822:PRO:HA	1.93	0.50
1:B:326:LYS:HE3	1:B:331:HIS:CB	2.41	0.50
1:B:759:LEU:HD23	1:B:782:ILE:HB	1.93	0.50
1:A:289:TYR:OH	1:A:291:GLU:OE1	2.20	0.50
1:A:662:VAL:HG13	1:A:672:ALA:HB1	1.92	0.50
1:A:50:ARG:NH1	1:A:210:GLY:O	2.45	0.50
1:B:534:VAL:HA	1:B:537:LEU:HD12	1.93	0.50
1:A:293:HIS:HB3	1:A:304:GLU:OE1	2.12	0.50
1:A:453:MET:O	1:A:457:ILE:HG23	2.11	0.50
1:A:1909:VAL:HG12	1:A:1911:LYS:H	1.76	0.50
1:B:64:PHE:CE1	1:B:464:ALA:HB1	2.42	0.50
1:B:627:TRP:CD1	1:B:631:LYS:HE2	2.47	0.50
1:B:766:LEU:HD23	1:B:766:LEU:O	2.11	0.50
1:A:808:ILE:HG22	1:A:809:ASP:N	2.27	0.50
1:B:191:LEU:HD22	1:B:224:ARG:NH2	2.27	0.50
1:B:720:ALA:HB3	1:B:721:GLN:OE1	2.12	0.50
1:A:1794:VAL:O	1:A:1795:LEU:HD23	2.11	0.50
1:B:250:GLY:CA	1:B:276:LEU:HD21	2.39	0.50
1:B:450:PHE:CZ	1:B:454:LEU:HD11	2.47	0.50
1:B:620:MET:HE3	1:B:682:PHE:HB2	1.93	0.50
1:A:293:HIS:ND1	1:A:326:LYS:HE2	2.27	0.50
1:B:1371:ILE:C	1:B:1372:LEU:HD12	2.32	0.50
1:A:155:ILE:N	1:A:155:ILE:HD12	2.26	0.50
1:B:44:LEU:HG	1:B:45:TYR:CD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:SER:HB2	1:B:357:LEU:O	2.12	0.50
1:B:498:GLY:O	1:B:556:LEU:HD21	2.12	0.50
1:B:1141:CYS:O	1:B:1145:VAL:HG23	2.12	0.50
1:A:946:VAL:O	1:A:953:VAL:HG12	2.12	0.50
1:B:247:LEU:HD12	1:B:282:VAL:HG21	1.93	0.50
1:B:301:ASP:HB2	1:B:302:PRO:HD3	1.93	0.50
1:B:656:ALA:O	1:B:660:GLU:HG3	2.12	0.50
1:A:468:ARG:HD3	1:A:804:HIS:NE2	2.27	0.49
1:A:697:GLU:O	1:A:701:VAL:HG23	2.12	0.49
1:A:776:LYS:HD2	1:A:776:LYS:N	2.27	0.49
1:B:293:HIS:O	1:B:326:LYS:HD2	2.11	0.49
1:B:511:MET:CE	1:B:520:ILE:HG13	2.42	0.49
1:A:692:PRO:HA	1:A:695:LEU:HG	1.93	0.49
1:A:1125:GLU:N	1:A:1125:GLU:OE1	2.45	0.49
1:B:58:SER:O	1:B:59:ARG:HD3	2.12	0.49
1:B:429:ARG:NH1	1:B:464:ALA:O	2.42	0.49
1:A:168:LEU:HD23	1:A:168:LEU:O	2.11	0.49
1:A:582:LEU:HG	1:A:583:GLY:N	2.27	0.49
1:B:83:LEU:HD12	1:B:144:LEU:CD2	2.41	0.49
1:B:717:ILE:HD12	1:B:727:ALA:CB	2.29	0.49
1:B:756:ALA:HB3	1:B:779:CYS:SG	2.52	0.49
1:A:188:ILE:HG22	1:A:228:VAL:CG1	2.32	0.49
1:A:645:SER:HB2	1:A:648:THR:OG1	2.12	0.49
1:B:270:GLU:HG2	1:B:274:ARG:HH12	1.77	0.49
1:B:732:ALA:O	1:B:736:VAL:HG23	2.12	0.49
1:A:627:TRP:CZ3	1:A:643:HIS:HB2	2.47	0.49
1:B:527:VAL:CG1	1:B:532:LEU:HD11	2.43	0.49
1:B:1837:GLU:OE1	1:B:1837:GLU:N	2.41	0.49
1:A:340:ALA:O	1:A:344:VAL:HG23	2.12	0.49
1:B:126:THR:O	1:B:126:THR:HG22	2.12	0.49
1:A:6:ILE:HA	1:A:233:LEU:HD23	1.95	0.49
1:A:183:ALA:O	1:A:232:LEU:HD12	2.12	0.49
1:A:490:ARG:HD3	1:A:806:SER:O	2.12	0.49
1:A:644:ASN:CG	1:A:770:VAL:HG11	2.33	0.49
1:A:681:ALA:HB3	1:A:686:PHE:HB2	1.95	0.49
1:B:502:GLN:HG2	1:B:552:SER:OG	2.12	0.49
1:B:621:ALA:HB2	1:B:674:GLU:CB	2.42	0.49
1:B:1286:GLU:OE2	1:B:1289:GLN:NE2	2.46	0.49
1:A:184:ILE:HD11	1:A:232:LEU:HD13	1.94	0.49
1:A:442:LEU:HD23	1:A:442:LEU:O	2.13	0.49
1:B:542:ASP:HB2	1:B:545:THR:OG1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:GLU:O	1:A:320:LEU:HD12	2.12	0.49
1:A:429:ARG:NH1	1:A:464:ALA:O	2.46	0.49
1:B:527:VAL:HG13	1:B:530:PHE:CD2	2.48	0.49
1:B:1280:LEU:HD13	1:B:1294:GLN:HG2	1.94	0.49
1:B:1533:VAL:HG13	1:B:1544:ILE:HG23	1.95	0.49
1:B:1487:ASP:N	1:B:1490:SER:OG	2.44	0.48
1:A:158:ASP:O	1:B:138:ALA:HB2	2.13	0.48
1:A:696:GLN:O	1:A:700:LYS:HG2	2.12	0.48
1:B:16:SER:HA	1:B:21:GLU:CD	2.34	0.48
1:B:495:ILE:HB	1:B:760:GLU:OE1	2.13	0.48
1:A:105:THR:O	1:A:150:PHE:HB3	2.13	0.48
1:A:366:ILE:HD12	1:A:366:ILE:N	2.28	0.48
1:A:542:ASP:O	1:A:545:THR:HG22	2.13	0.48
1:B:353:TRP:NE1	1:B:383:VAL:HG22	2.28	0.48
1:B:506:MET:HG3	1:B:559:ILE:CD1	2.43	0.48
1:B:1206:ARG:NH2	1:B:1319:VAL:O	2.46	0.48
1:A:63:SER:OG	1:A:429:ARG:NH2	2.46	0.48
1:A:86:THR:CG2	1:A:184:ILE:HG21	2.44	0.48
1:A:503:TRP:CZ2	1:A:506:MET:HA	2.49	0.48
1:A:760:GLU:OE2	1:A:765:ALA:HA	2.12	0.48
1:A:1603:PHE:CE1	1:A:1626:VAL:HG21	2.48	0.48
1:A:1860:GLU:N	1:A:1860:GLU:OE1	2.45	0.48
1:B:264:PRO:CG	1:B:300:GLY:HA2	2.43	0.48
1:B:309:THR:HG23	1:B:313:CYS:SG	2.53	0.48
1:B:997:ARG:NH2	1:B:1043:LYS:O	2.40	0.48
1:B:2003:ASP:OD1	1:B:2048:ARG:NH1	2.45	0.48
1:A:225:SER:OG	1:A:330:GLY:HA3	2.13	0.48
1:A:642:CYS:CA	1:A:743:VAL:HB	2.42	0.48
1:B:13:LEU:HB3	1:B:14:PRO:CD	2.43	0.48
1:B:426:ALA:HB1	1:B:437:LEU:CD1	2.43	0.48
1:B:1996:TYR:CE1	1:B:2000:LEU:HD11	2.49	0.48
1:A:235:LYS:CG	1:A:238:LEU:HD13	2.43	0.48
1:A:276:LEU:HD12	1:A:401:HIS:CD2	2.49	0.48
1:A:1446:ILE:HG22	1:A:1474:LEU:CD1	2.43	0.48
1:B:1602:GLU:HB3	1:B:1650:VAL:HG23	1.96	0.48
1:B:326:LYS:HE3	1:B:331:HIS:HB2	1.95	0.48
1:B:645:SER:CB	1:B:648:THR:HG1	2.27	0.48
1:A:654:PRO:C	1:A:657:PRO:HD2	2.34	0.48
1:A:1250:GLY:O	1:A:1316:ASN:ND2	2.47	0.48
1:B:527:VAL:HG13	1:B:530:PHE:HD2	1.79	0.48
1:A:698:LEU:HD12	1:A:736:VAL:CG2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2097:LEU:O	1:B:2097:LEU:HD23	2.14	0.48
1:A:570:MET:CE	1:A:815:LEU:HD11	2.44	0.48
1:A:1132:ALA:O	1:A:1135:GLN:N	2.47	0.48
1:B:991:TYR:OH	1:B:1007:GLY:N	2.44	0.48
1:B:460:VAL:CG2	1:B:461:PRO:HD2	2.44	0.47
1:A:276:LEU:HD12	1:A:401:HIS:HD2	1.78	0.47
1:A:424:LEU:HD12	1:A:425:ARG:H	1.79	0.47
1:A:692:PRO:HB2	1:A:693:PRO:HD3	1.96	0.47
1:A:728:ARG:HB2	1:A:728:ARG:CZ	2.44	0.47
1:B:305:LEU:HB2	1:B:366:ILE:HD13	1.96	0.47
1:B:341:LEU:CD1	1:B:390:ILE:HD12	2.44	0.47
1:A:423:LEU:HD12	1:A:424:LEU:H	1.79	0.47
1:A:468:ARG:O	1:A:482:VAL:HG13	2.14	0.47
1:A:1715:LEU:HD22	1:A:1720:PHE:CZ	2.49	0.47
1:B:74:THR:HG21	1:B:128:VAL:HG21	1.95	0.47
1:B:534:VAL:O	1:B:538:LEU:HD13	2.13	0.47
1:B:549:ILE:HD11	1:B:611:LYS:HG3	1.96	0.47
1:A:23:TRP:HB2	1:A:346:LEU:HD13	1.95	0.47
1:A:44:LEU:HG	1:A:45:TYR:CD1	2.49	0.47
1:A:1313:LEU:HD13	1:A:1336:LEU:HD13	1.96	0.47
1:B:503:TRP:CE2	1:B:506:MET:HB3	2.49	0.47
1:B:731:SER:O	1:B:734:TYR:N	2.48	0.47
1:B:811:ASN:OD1	1:B:813:ASN:ND2	2.48	0.47
1:A:324:SER:H	1:A:356:ASN:ND2	2.12	0.47
1:A:506:MET:HE2	1:A:555:SER:HB2	1.97	0.47
1:B:745:PHE:CD2	1:B:749:LEU:HD11	2.49	0.47
1:A:1942:SER:OG	1:A:1958:GLU:OE2	2.19	0.47
1:B:305:LEU:HB3	1:B:366:ILE:HG21	1.95	0.47
1:B:563:LEU:O	1:B:567:LEU:HD13	2.15	0.47
1:B:569:CYS:SG	1:B:814:ALA:CB	2.91	0.47
1:B:1743:LEU:HD23	1:B:1765:ARG:HB2	1.96	0.47
1:A:431:PRO:HG3	1:A:467:PHE:CD2	2.50	0.47
1:A:1913:VAL:C	1:A:1914:LEU:HD12	2.35	0.47
1:B:17:GLU:OE1	1:B:17:GLU:HA	2.14	0.47
1:B:581:SER:CB	1:B:683:HIS:NE2	2.77	0.47
1:B:670:VAL:HG12	1:B:671:PHE:N	2.30	0.47
1:B:801:GLY:O	1:B:804:HIS:HB3	2.14	0.47
1:A:442:LEU:HD23	1:A:442:LEU:C	2.35	0.47
1:A:698:LEU:CB	1:A:732:ALA:HB1	2.45	0.47
1:B:183:ALA:O	1:B:232:LEU:HD12	2.14	0.47
1:B:527:VAL:HG12	1:B:527:VAL:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1391:LEU:C	1:B:1391:LEU:HD23	2.35	0.47
1:A:626:SER:N	1:A:629:GLU:OE2	2.40	0.47
1:A:645:SER:OG	1:A:770:VAL:CG1	2.63	0.47
1:B:205:MET:O	1:B:221:GLY:HA3	2.14	0.47
1:B:745:PHE:CE2	1:B:749:LEU:HD21	2.50	0.47
1:B:1470:ARG:NE	1:B:1500:ASP:OD1	2.48	0.47
1:A:207:SER:OG	1:A:220:ASN:HB2	2.15	0.46
1:A:1219:LEU:HD13	1:A:1255:ARG:HH21	1.80	0.46
1:B:158:ASP:O	1:B:163:SER:HB3	2.15	0.46
1:B:1364:GLU:N	1:B:1365:PRO:HD2	2.31	0.46
1:A:158:ASP:HB2	1:B:156:ALA:HB3	1.96	0.46
1:A:692:PRO:HD2	1:A:693:PRO:HD2	1.97	0.46
1:A:1310:ALA:O	1:A:1336:LEU:HD12	2.14	0.46
1:B:322:ILE:HG21	1:B:374:LEU:HD21	1.98	0.46
1:B:431:PRO:HG3	1:B:467:PHE:CD2	2.50	0.46
1:B:1213:PRO:O	1:B:1217:GLY:N	2.49	0.46
1:A:663:GLU:O	1:A:667:LYS:HG2	2.15	0.46
1:A:1670:THR:C	1:A:1671:LEU:HD12	2.35	0.46
1:B:1457:VAL:HG21	1:B:1471:CYS:HB3	1.97	0.46
1:A:205:MET:HB3	1:A:222:TYR:HE1	1.81	0.46
1:A:1771:LYS:HE3	1:A:1795:LEU:HD22	1.98	0.46
1:B:23:TRP:CZ3	1:B:354:ALA:HB2	2.51	0.46
1:B:198:VAL:O	1:B:202:ARG:HG2	2.15	0.46
1:A:305:LEU:HD23	1:A:366:ILE:HG21	1.97	0.46
1:A:1904:LEU:HB3	1:A:1909:VAL:HG21	1.97	0.46
1:B:711:ARG:NH1	1:B:711:ARG:HB2	2.31	0.46
1:B:1640:TRP:CH2	1:B:1648:VAL:HG21	2.50	0.46
1:B:1909:VAL:HG11	1:B:1912:LEU:HD13	1.98	0.46
1:A:593:CYS:O	1:A:706:LYS:HE2	2.16	0.46
1:A:1909:VAL:HG11	1:A:1912:LEU:HD13	1.96	0.46
1:B:114:SER:HG	1:B:117:SER:CB	2.25	0.46
1:B:619:ALA:CB	1:B:658:VAL:HG11	2.32	0.46
1:B:76:ASP:HA	1:B:116:THR:HG21	1.97	0.46
1:B:322:ILE:HG13	1:B:323:GLY:H	1.81	0.46
1:B:879:THR:C	1:B:880:LEU:HD12	2.36	0.46
1:B:1246:LEU:N	1:B:1246:LEU:HD12	2.31	0.46
1:A:400:VAL:HG12	1:A:401:HIS:N	2.31	0.46
1:A:469:GLY:HA2	1:A:805:LEU:HD21	1.98	0.46
1:A:1287:LEU:O	1:A:1292:VAL:HG22	2.16	0.46
1:B:1209:LEU:CD2	1:B:1215:LEU:HD13	2.46	0.46
1:A:157:LEU:N	1:A:157:LEU:HD12	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:ARG:CZ	1:A:320:LEU:HB2	2.46	0.46
1:A:426:ALA:HB1	1:A:437:LEU:CD1	2.44	0.46
1:B:84:GLU:O	1:B:88:GLU:HG3	2.15	0.46
1:B:468:ARG:HD3	1:B:804:HIS:NE2	2.30	0.46
1:B:524:ASP:O	1:B:527:VAL:N	2.48	0.46
1:B:702:ILE:HD12	1:B:702:ILE:N	2.31	0.46
1:B:556:LEU:CD1	1:B:763:PRO:HG3	2.45	0.45
1:A:160:ALA:O	1:A:394:GLY:HA3	2.17	0.45
1:A:493:TRP:CE3	1:A:576:GLY:HA3	2.51	0.45
1:A:1010:GLU:OE2	1:A:1019:ARG:NH2	2.49	0.45
1:B:766:LEU:HD23	1:B:766:LEU:C	2.37	0.45
1:A:238:LEU:HD12	1:A:238:LEU:N	2.32	0.45
1:A:1417:VAL:HG23	1:A:1424:TRP:CE2	2.52	0.45
1:B:510:LEU:CD1	1:B:563:LEU:HD21	2.46	0.45
1:A:328:ASN:ND2	1:A:357:LEU:HG	2.31	0.45
1:A:514:ASP:HA	1:A:517:ARG:NH1	2.31	0.45
1:A:690:ILE:O	1:A:693:PRO:HG2	2.17	0.45
1:A:694:LEU:CD2	1:A:739:LEU:HD23	2.46	0.45
1:A:1887:TYR:HD1	1:A:1909:VAL:HG13	1.80	0.45
1:B:595:SER:OG	1:B:598:GLU:HG3	2.16	0.45
1:B:651:ILE:C	1:B:651:ILE:HD12	2.37	0.45
1:B:692:PRO:HB2	1:B:693:PRO:HD3	1.97	0.45
1:B:1594:SER:OG	1:B:1596:ASP:O	2.27	0.45
1:A:78:GLN:HG2	1:A:190:VAL:HG13	1.97	0.45
1:A:79:LEU:CD2	1:A:143:ARG:HG3	2.40	0.45
1:B:5:VAL:HG22	1:B:234:THR:O	2.16	0.45
1:B:60:PHE:CE2	1:B:62:ALA:HA	2.52	0.45
1:B:287:PHE:HZ	1:B:403:ILE:HD13	1.82	0.45
1:A:425:ARG:HD2	1:A:804:HIS:CE1	2.51	0.45
1:A:440:GLN:HA	1:A:440:GLN:OE1	2.15	0.45
1:A:549:ILE:HD11	1:A:611:LYS:CG	2.39	0.45
1:A:642:CYS:HB3	1:A:743:VAL:HB	1.98	0.45
1:A:1020:LEU:HD22	1:A:1032:THR:HG22	1.99	0.45
1:B:639:VAL:CG1	1:B:640:PRO:HD2	2.43	0.45
1:A:198:VAL:HG11	1:B:127:LEU:HD21	1.98	0.45
1:A:400:VAL:HG12	1:A:401:HIS:H	1.81	0.45
1:A:693:PRO:O	1:A:697:GLU:HG2	2.17	0.45
1:A:1325:PRO:CG	1:A:1372:LEU:HD11	2.47	0.45
1:A:1417:VAL:HG22	1:A:1417:VAL:O	2.17	0.45
1:A:1617:VAL:HG12	1:A:1628:LEU:HD13	1.99	0.45
1:A:1753:LEU:C	1:A:1753:LEU:HD23	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:ASN:HB2	1:B:32:MET:CE	2.46	0.45
1:A:572:LEU:HD21	1:A:810:ALA:HB2	1.99	0.45
1:B:595:SER:O	1:B:598:GLU:HB2	2.16	0.45
1:B:628:GLU:O	1:B:631:LYS:HB2	2.17	0.45
1:A:138:ALA:HB2	1:B:158:ASP:CG	2.37	0.45
1:A:1327:SER:O	1:A:1331:ASN:ND2	2.48	0.45
1:B:786:LYS:HB2	1:B:795:PHE:CE2	2.52	0.45
1:B:119:ALA:O	1:B:122:ARG:HG2	2.17	0.44
1:B:207:SER:HB3	1:B:221:GLY:CA	2.46	0.44
1:B:730:SER:HA	1:B:734:TYR:CD2	2.47	0.44
1:B:803:LEU:HD11	1:B:808:ILE:HG13	1.99	0.44
1:A:553:PHE:CE2	1:A:582:LEU:HD22	2.51	0.44
1:A:692:PRO:HA	1:A:695:LEU:HD21	1.99	0.44
1:A:1446:ILE:HG22	1:A:1474:LEU:HD12	1.97	0.44
2:A:2601:NDP:P2B	2:A:2601:NDP:HO3A	2.40	0.44
1:A:302:PRO:HA	1:A:366:ILE:CG1	2.48	0.44
1:A:625:LEU:HB3	1:A:629:GLU:HG3	1.99	0.44
1:A:649:VAL:HG12	1:A:650:THR:N	2.32	0.44
1:A:1973:VAL:O	1:A:1973:VAL:HG13	2.17	0.44
1:B:326:LYS:HA	1:B:329:MET:O	2.17	0.44
1:B:1214:LEU:HD12	1:B:1214:LEU:C	2.38	0.44
1:B:1364:GLU:O	1:B:1367:TYR:N	2.51	0.44
1:B:1888:ILE:HD11	1:B:1959:ALA:HB2	1.99	0.44
1:A:502:GLN:HB3	1:A:546:PHE:CD2	2.53	0.44
1:B:425:ARG:CZ	1:B:811:ASN:HA	2.47	0.44
1:B:1445:ALA:O	1:B:1446:ILE:HD13	2.17	0.44
1:A:79:LEU:HD21	1:A:143:ARG:CG	2.43	0.44
1:A:876:VAL:O	1:A:876:VAL:HG12	2.18	0.44
1:A:1274:ASP:OD1	1:A:1275:ARG:N	2.47	0.44
1:B:116:THR:O	1:B:120:LEU:HD13	2.17	0.44
1:B:602:ALA:O	1:B:606:ARG:HG3	2.17	0.44
1:B:671:PHE:CZ	1:B:673:LYS:HD3	2.53	0.44
1:B:1046:LEU:HD12	1:B:1046:LEU:C	2.38	0.44
1:A:1178:LEU:HB3	1:A:1212:ASP:OD2	2.16	0.44
1:B:537:LEU:O	1:B:540:SER:HB3	2.18	0.44
1:A:253:THR:HG21	1:B:145:SER:CB	2.47	0.44
1:A:1245:VAL:C	1:A:1246:LEU:HD12	2.38	0.44
1:A:326:LYS:HE3	1:A:331:HIS:HD2	1.83	0.44
1:A:783:PRO:HG2	1:A:795:PHE:HZ	1.82	0.44
1:B:453:MET:O	1:B:457:ILE:HG23	2.17	0.44
1:B:485:VAL:HG22	1:B:805:LEU:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:754:GLU:HG3	1:B:755:HIS:ND1	2.33	0.44
1:B:1317:CYS:N	1:B:1345:HIS:O	2.50	0.44
1:A:105:THR:HA	1:A:182:ALA:O	2.17	0.44
1:A:207:SER:HB2	1:A:221:GLY:H	1.81	0.44
1:A:1486:VAL:O	1:A:1493:LEU:HD22	2.18	0.44
1:B:125:GLU:HA	1:B:125:GLU:OE1	2.18	0.44
1:B:341:LEU:HA	1:B:390:ILE:HD13	2.00	0.44
1:A:90:ILE:HG12	1:A:232:LEU:HD22	2.00	0.43
1:A:1317:CYS:SG	1:A:1322:LEU:HD12	2.57	0.43
1:B:511:MET:HE2	1:B:520:ILE:HG13	2.00	0.43
1:B:754:GLU:HG3	1:B:755:HIS:N	2.33	0.43
1:B:1275:ARG:NH1	1:B:1298:ASP:OD1	2.50	0.43
1:A:265:SER:O	1:A:269:GLN:HG3	2.17	0.43
1:A:506:MET:HG3	1:A:559:ILE:CD1	2.47	0.43
1:A:690:ILE:HG22	1:A:694:LEU:HB2	2.00	0.43
1:A:991:TYR:CZ	1:A:1006:GLN:HA	2.53	0.43
1:A:1411:SER:O	1:A:1439:ARG:NE	2.46	0.43
1:A:1471:CYS:SG	1:A:1472:VAL:N	2.91	0.43
1:B:627:TRP:NE1	1:B:631:LYS:HE2	2.33	0.43
1:B:848:GLU:H	1:B:848:GLU:CD	2.21	0.43
1:B:1663:GLY:O	1:B:1765:ARG:NH1	2.51	0.43
1:A:328:ASN:HD21	1:A:357:LEU:HG	1.84	0.43
1:A:627:TRP:HB2	1:A:643:HIS:CD2	2.53	0.43
1:A:937:LEU:O	1:A:938:LEU:HD12	2.18	0.43
1:A:2057:ALA:HB3	1:A:2105:VAL:HG22	2.00	0.43
1:B:107:VAL:HG22	1:B:184:ILE:HB	2.00	0.43
1:B:995:ARG:HA	1:B:999:TYR:O	2.18	0.43
1:A:425:ARG:HE	1:A:812:PRO:HD3	1.83	0.43
1:B:1372:LEU:HD13	1:B:1377:TRP:CZ2	2.53	0.43
1:B:1616:LEU:CD1	1:B:1650:VAL:HG22	2.48	0.43
1:A:692:PRO:CD	1:A:693:PRO:HD2	2.49	0.43
1:A:726:LEU:HD12	1:A:726:LEU:N	2.33	0.43
1:A:1974:VAL:HG12	1:A:1994:PRO:HG3	2.01	0.43
1:B:101:ARG:HG2	1:B:148:PHE:O	2.18	0.43
1:A:109:VAL:HA	1:A:186:GLY:O	2.18	0.43
1:A:453:MET:HE2	1:A:453:MET:HB3	1.83	0.43
1:A:1583:LEU:HD11	1:A:1587:ALA:CB	2.48	0.43
1:B:240:ARG:HD2	1:B:821:PHE:CE2	2.53	0.43
1:A:303:GLN:OE1	1:A:303:GLN:HA	2.18	0.43
1:A:391:ASN:HB3	1:A:401:HIS:ND1	2.34	0.43
1:A:891:TYR:OH	1:A:923:THR:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:923:THR:HG23	1:A:923:THR:O	2.19	0.43
1:A:2002:LEU:O	1:A:2006:THR:HG23	2.19	0.43
1:B:95:ILE:HD12	1:B:95:ILE:N	2.33	0.43
1:B:495:ILE:HD13	1:B:578:VAL:HB	1.98	0.43
1:A:160:ALA:O	1:A:161:CYS:HB2	2.19	0.43
1:A:333:GLU:HB2	1:A:334:PRO:CD	2.49	0.43
1:A:763:PRO:HA	1:A:785:MET:HE1	2.01	0.43
1:A:1078:VAL:HG23	1:A:1089:ALA:HB2	2.00	0.43
1:A:1342:LEU:HD23	1:A:1386:LEU:HD21	2.00	0.43
1:A:2020:SER:OG	1:A:2021:SER:N	2.52	0.43
1:B:161:CYS:HA	1:B:333:GLU:O	2.19	0.43
1:B:223:CYS:O	1:B:330:GLY:HA3	2.19	0.43
1:B:265:SER:O	1:B:269:GLN:HG3	2.19	0.43
1:B:1230:THR:O	1:B:1234:ASN:ND2	2.50	0.43
1:A:39:ARG:HG2	1:A:53:LYS:HD2	2.01	0.43
1:A:579:GLY:HA3	1:A:584:GLU:OE1	2.18	0.43
1:B:9:MET:HG2	1:B:19:LEU:HD11	1.99	0.43
1:B:605:TRP:CD1	1:B:701:VAL:HG21	2.54	0.43
1:B:745:PHE:HD2	1:B:749:LEU:HD11	1.84	0.43
1:B:1872:LEU:N	1:B:1872:LEU:HD12	2.33	0.43
1:A:1974:VAL:O	1:A:1974:VAL:HG13	2.19	0.43
1:B:574:PRO:CG	1:B:577:ILE:HD11	2.47	0.43
1:A:222:TYR:HD2	1:A:331:HIS:HB3	1.84	0.42
1:B:6:ILE:HG23	1:B:231:VAL:HG13	2.01	0.42
1:B:692:PRO:N	1:B:693:PRO:HD2	2.34	0.42
1:B:1113:ILE:HD11	1:B:2109:PHE:CZ	2.54	0.42
1:B:1830:VAL:O	1:B:1830:VAL:HG13	2.19	0.42
1:A:13:LEU:HD23	1:A:227:GLY:HA3	2.01	0.42
1:A:76:ASP:OD1	1:A:78:GLN:N	2.36	0.42
1:A:182:ALA:CB	1:A:234:THR:HG22	2.50	0.42
1:A:549:ILE:HD12	1:A:550:VAL:HG23	2.01	0.42
1:A:1148:LEU:HD12	1:A:1148:LEU:N	2.33	0.42
1:A:1336:LEU:HD11	1:A:1340:GLY:HA3	2.01	0.42
1:A:1922:THR:HG22	1:A:1923:GLY:N	2.33	0.42
1:B:9:MET:HE2	1:B:243:TYR:CE2	2.54	0.42
1:B:158:ASP:O	1:B:159:THR:OG1	2.33	0.42
1:B:635:PRO:HD3	1:B:661:PHE:CE1	2.54	0.42
1:B:1487:ASP:O	1:B:1493:LEU:HD23	2.19	0.42
1:B:2033:ASN:OD1	1:B:2034:TYR:N	2.52	0.42
1:A:6:ILE:HG21	1:A:345:LEU:HD11	2.01	0.42
1:A:78:GLN:HE21	1:A:78:GLN:HB2	1.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:VAL:HB	1:A:338:LEU:HB3	2.02	0.42
1:A:267:ASP:O	1:A:271:GLN:HG3	2.19	0.42
1:A:325:THR:HB	1:A:343:LYS:CD	2.49	0.42
1:A:60:PHE:CE2	1:A:62:ALA:HA	2.54	0.42
1:B:160:ALA:O	1:B:394:GLY:HA3	2.18	0.42
1:B:503:TRP:CZ2	1:B:506:MET:HA	2.54	0.42
1:B:1178:LEU:HD11	1:B:1215:LEU:HG	2.01	0.42
1:B:1389:VAL:HG22	1:B:1501:LEU:HD11	2.01	0.42
1:A:333:GLU:CB	1:A:334:PRO:HD3	2.49	0.42
1:A:396:GLY:O	1:B:142:ASN:HB3	2.20	0.42
1:A:1194:LEU:O	1:A:1197:GLU:HG2	2.19	0.42
1:B:168:LEU:O	1:B:168:LEU:HD23	2.19	0.42
1:B:609:CYS:SG	1:B:694:LEU:HA	2.60	0.42
1:B:690:ILE:N	1:B:690:ILE:HD12	2.33	0.42
1:B:912:VAL:HG22	1:B:913:VAL:N	2.34	0.42
1:B:1052:VAL:HG11	1:B:1055:ILE:HG13	2.02	0.42
1:A:454:LEU:HD23	1:A:454:LEU:HA	1.73	0.42
1:A:681:ALA:HB3	1:A:686:PHE:CB	2.49	0.42
1:B:621:ALA:CB	1:B:674:GLU:HA	2.50	0.42
1:B:830:ILE:HG22	1:B:830:ILE:O	2.20	0.42
1:A:549:ILE:O	1:A:553:PHE:HD1	2.02	0.42
1:A:808:ILE:HG22	1:A:809:ASP:H	1.84	0.42
1:A:996:LEU:HD13	1:A:1899:GLU:OE2	2.19	0.42
1:A:189:ASN:HB2	1:A:334:PRO:HD2	2.01	0.42
1:A:246:ILE:HG12	1:A:404:LEU:CD2	2.48	0.42
1:A:302:PRO:CA	1:A:366:ILE:HD11	2.49	0.42
1:A:502:GLN:OE1	1:A:502:GLN:N	2.46	0.42
1:A:502:GLN:HA	1:A:506:MET:SD	2.60	0.42
1:A:772:LYS:HZ2	1:A:781:ILE:HB	1.83	0.42
1:B:322:ILE:HG23	1:B:376:VAL:HG22	2.02	0.42
1:B:608:GLN:OE1	1:B:608:GLN:HA	2.20	0.42
1:B:645:SER:HG	1:B:648:THR:H	1.57	0.42
1:B:694:LEU:HD23	1:B:739:LEU:HD23	2.02	0.42
1:B:1888:ILE:HD11	1:B:1959:ALA:CB	2.50	0.42
1:A:76:ASP:O	1:A:80:ARG:HG3	2.19	0.42
1:A:347:SER:HB3	1:A:352:LEU:O	2.20	0.42
1:A:365:GLU:O	1:A:367:PRO:HD3	2.19	0.42
1:A:783:PRO:O	1:A:784:LEU:HB2	2.18	0.42
1:B:494:PHE:CD2	1:B:761:ILE:HD11	2.55	0.42
1:B:991:TYR:CZ	1:B:1006:GLN:HA	2.55	0.42
1:A:9:MET:HE1	1:A:346:LEU:CD2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:702:ILE:HD12	1:A:702:ILE:N	2.35	0.42
1:B:311:ALA:O	1:B:312:LEU:HD23	2.19	0.42
1:A:425:ARG:HE	1:A:812:PRO:CD	2.33	0.41
1:A:1332:MET:O	1:A:1335:ALA:N	2.53	0.41
1:A:1785:PHE:HB2	1:B:1774:LEU:HD22	2.02	0.41
1:B:424:LEU:HD12	1:B:425:ARG:N	2.35	0.41
1:B:547:ASP:OD1	1:B:548:ASP:N	2.53	0.41
1:B:595:SER:O	1:B:598:GLU:N	2.52	0.41
1:B:758:VAL:HG12	1:B:759:LEU:N	2.35	0.41
1:B:1313:LEU:CD1	1:B:1336:LEU:HB3	2.50	0.41
1:B:2049:ARG:NH1	1:B:2102:PRO:O	2.53	0.41
1:A:124:PRO:HG2	1:B:45:TYR:CZ	2.55	0.41
1:A:139:MET:O	1:A:143:ARG:HG2	2.20	0.41
1:A:189:ASN:HB2	1:A:334:PRO:CD	2.50	0.41
1:A:202:ARG:HA	1:A:202:ARG:HD3	1.84	0.41
1:A:290:ILE:HG23	1:A:290:ILE:O	2.20	0.41
1:A:455:ASN:HB2	1:A:813:ASN:HD21	1.86	0.41
1:A:1561:ALA:HB1	1:A:1627:LEU:HD11	2.03	0.41
1:B:377:VAL:O	1:B:377:VAL:HG23	2.20	0.41
1:A:368:ALA:HA	1:A:371:ASP:OD1	2.21	0.41
1:A:692:PRO:HA	1:A:695:LEU:CG	2.50	0.41
1:A:784:LEU:HD22	1:A:796:PHE:CE2	2.54	0.41
1:B:104:HIS:O	1:B:152:GLY:HA3	2.20	0.41
1:B:200:PHE:CD2	1:B:224:ARG:HD2	2.54	0.41
1:A:457:ILE:O	1:A:457:ILE:HG13	2.19	0.41
1:A:556:LEU:HD11	1:A:560:GLN:NE2	2.36	0.41
1:A:1019:ARG:HD2	1:A:1075:VAL:HG21	2.03	0.41
1:A:1066:LEU:HD23	1:A:1076:ALA:HB2	2.02	0.41
1:A:1877:SER:O	1:A:2100:ASN:ND2	2.53	0.41
1:B:11:GLY:HA2	1:B:85:VAL:CG1	2.51	0.41
1:B:76:ASP:OD1	1:B:78:GLN:N	2.45	0.41
1:B:831:SER:HB3	1:B:832:PRO:HD3	2.03	0.41
1:B:1357:VAL:O	1:B:1361:THR:HG23	2.20	0.41
1:B:1485:GLU:OE1	1:B:1485:GLU:N	2.44	0.41
1:A:1914:LEU:HD12	1:A:1914:LEU:N	2.35	0.41
1:B:692:PRO:HB2	1:B:693:PRO:CD	2.50	0.41
1:B:754:GLU:OE2	1:B:778:SER:HB3	2.21	0.41
1:A:44:LEU:HG	1:A:45:TYR:CG	2.56	0.41
1:A:772:LYS:CE	1:A:781:ILE:HD13	2.50	0.41
1:B:1904:LEU:HB3	1:B:1909:VAL:HG21	2.02	0.41
1:A:304:GLU:O	1:A:308:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1476:ASN:ND2	1:A:1482:HIS:O	2.54	0.41
1:B:388:VAL:HG12	1:B:389:GLY:N	2.34	0.41
1:B:790:ARG:HG3	1:B:791:ASP:N	2.36	0.41
1:B:1246:LEU:HD11	1:B:1299:PRO:HG3	2.02	0.41
1:B:1336:LEU:HD12	1:B:1336:LEU:O	2.21	0.41
1:A:191:LEU:HD21	1:A:224:ARG:CB	2.50	0.41
1:A:302:PRO:HA	1:A:366:ILE:HD11	2.03	0.41
1:A:370:LEU:HD12	1:A:370:LEU:N	2.36	0.41
1:A:764:HIS:ND1	1:A:787:LYS:HB2	2.35	0.41
1:A:803:LEU:HD11	1:A:808:ILE:HD12	2.03	0.41
1:A:1446:ILE:HG21	1:A:1486:VAL:CG2	2.42	0.41
1:A:1968:VAL:O	1:A:1968:VAL:HG23	2.21	0.41
1:B:212:CYS:SG	1:B:222:TYR:HA	2.61	0.41
1:B:438:LEU:HD13	1:B:480:PRO:CB	2.51	0.41
1:B:625:LEU:HD21	1:B:670:VAL:CG2	2.41	0.41
1:B:816:PHE:HB3	1:B:817:PRO:HD2	2.02	0.41
1:B:881:ASP:CG	1:B:1046:LEU:HD21	2.41	0.41
1:B:1018:GLY:O	1:B:1078:VAL:HG12	2.21	0.41
1:B:1333:VAL:HG12	1:B:1386:LEU:HD11	2.01	0.41
1:B:2097:LEU:HD23	1:B:2097:LEU:C	2.40	0.41
1:A:290:ILE:HD12	1:A:389:GLY:C	2.41	0.41
1:A:420:LEU:CD2	1:A:512:ARG:HE	2.33	0.41
1:A:447:ASP:OD2	1:A:827:THR:HG23	2.20	0.41
1:A:758:VAL:HG11	1:A:771:LEU:HD13	2.03	0.41
1:B:321:LEU:HD23	1:B:321:LEU:HA	1.95	0.41
1:B:437:LEU:HD23	1:B:833:LEU:HB3	2.02	0.41
1:B:528:LYS:HB3	1:B:529:PRO:HD3	2.03	0.41
1:B:1885:LYS:O	1:B:1911:LYS:HG3	2.21	0.41
1:A:38:ARG:HE	1:A:53:LYS:HE2	1.86	0.40
1:A:628:GLU:O	1:A:631:LYS:HG2	2.20	0.40
1:A:1080:VAL:HG22	1:A:1087:THR:HG23	2.02	0.40
1:A:1493:LEU:HA	1:A:1496:VAL:HG22	2.03	0.40
1:B:18:ASN:ND2	1:B:832:PRO:HB3	2.36	0.40
1:B:476:GLU:HG3	1:B:477:ARG:HG3	2.02	0.40
1:B:628:GLU:H	1:B:628:GLU:CD	2.23	0.40
1:B:731:SER:H	1:B:734:TYR:HB3	1.85	0.40
1:A:136:GLN:NE2	1:B:112:SER:OG	2.54	0.40
1:A:627:TRP:CE3	1:A:643:HIS:HB2	2.56	0.40
1:A:1304:PRO:HD2	1:A:1307:LEU:HD12	2.03	0.40
1:A:1415:LEU:HD22	1:A:1443:LEU:CD2	2.50	0.40
1:A:1889:ILE:HD11	1:A:1904:LEU:HD12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:655:GLN:HA	1:B:658:VAL:HG12	2.03	0.40
1:B:740:VAL:HG23	1:B:741:SER:N	2.37	0.40
1:A:388:VAL:HG12	1:A:389:GLY:N	2.36	0.40
1:B:14:PRO:HD2	1:B:329:MET:HE3	2.03	0.40
1:B:165:LEU:CG	1:B:400:VAL:HG12	2.45	0.40
1:B:215:PHE:CZ	1:B:292:ALA:HB3	2.40	0.40
1:B:532:LEU:C	1:B:532:LEU:HD12	2.41	0.40
1:B:534:VAL:HG12	1:B:538:LEU:HD13	2.02	0.40
1:B:615:LEU:HD12	1:B:615:LEU:C	2.41	0.40
1:B:1206:ARG:NH1	1:B:1209:LEU:HD13	2.36	0.40
1:B:1905:ILE:HD12	1:B:1937:VAL:HG21	2.03	0.40
1:A:363:ASN:OD1	1:A:364:PRO:HD2	2.22	0.40
1:A:534:VAL:HG11	1:A:558:ALA:CB	2.51	0.40
1:A:1669:GLU:OE1	1:A:1765:ARG:NH2	2.54	0.40
1:B:549:ILE:HD12	1:B:610:ILE:CG2	2.52	0.40
1:B:1486:VAL:HG23	1:B:1493:LEU:HB2	2.03	0.40
1:B:1768:GLU:HG2	1:B:1774:LEU:HD21	2.04	0.40
1:A:189:ASN:O	1:A:226:GLU:HB2	2.22	0.40
1:B:186:GLY:HA2	1:B:229:VAL:O	2.21	0.40
1:B:238:LEU:N	1:B:238:LEU:HD12	2.36	0.40
1:B:289:TYR:OH	1:B:291:GLU:OE1	2.18	0.40
1:B:341:LEU:HD12	1:B:390:ILE:HD12	2.03	0.40
1:B:757:VAL:HA	1:B:780:THR:OG1	2.21	0.40
1:B:1389:VAL:CG2	1:B:1501:LEU:HD11	2.51	0.40
1:B:1651:VAL:HG23	1:B:1652:TYR:N	2.36	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2060/2553 (81%)	2001 (97%)	59 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	2063/2553 (81%)	1980 (96%)	83 (4%)	0	100	100
All	All	4123/5106 (81%)	3981 (97%)	142 (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%)	1703 (100%)	2 (0%)	92	97
1	B	1708/2117 (81%)	1703 (100%)	5 (0%)	91	96
All	All	3413/4234 (81%)	3406 (100%)	7 (0%)	91	97

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	241	ARG
1	A	2013	LEU
1	B	331	HIS
1	B	580	HIS
1	B	734	TYR
1	B	1077	ASP
1	B	1896	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	96	ASN
1	A	328	ASN
1	A	356	ASN
1	A	358	HIS
1	A	379	GLN

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Mol	Chain	Res	Type
1	A	399	ASN
1	A	596	GLN
1	A	1044	HIS
1	A	1110	GLN
1	A	1122	HIS
1	A	1139	GLN
1	A	1191	ASN
1	A	1193	ASN
1	A	1290	HIS
1	A	1458	ASN
1	A	1504	ASN
1	A	1562	GLN
1	A	1595	GLN
1	A	1855	GLN
1	A	2101	GLN
1	B	78	GLN
1	B	173	GLN
1	B	199	GLN
1	B	220	ASN
1	B	356	ASN
1	B	375	GLN
1	B	387	ASN
1	B	768	GLN
1	B	804	HIS
1	B	813	ASN
1	B	1025	ASN
1	B	1056	HIS
1	B	1204	GLN
1	B	1278	GLN
1	B	1476	ASN
1	B	1562	GLN
1	B	1595	GLN
1	B	1845	GLN
1	B	1855	GLN
1	B	1983	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	2602	-	47,52,52	0.66	0	61,80,80	0.84	2 (3%)
2	NDP	A	2601	-	47,52,52	0.65	0	61,80,80	0.84	3 (4%)
2	NDP	B	2601	-	47,52,52	0.64	0	61,80,80	0.81	2 (3%)
2	NDP	A	2602	-	47,52,52	0.66	0	61,80,80	0.86	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	-	-	12/30/77/77	0/5/5/5
2	NDP	B	2601	-	-	10/30/77/77	0/5/5/5
2	NDP	A	2602	-	-	6/30/77/77	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	2602	NDP	P2B-O2B-C2B	-4.13	112.40	123.43
2	B	2601	NDP	P2B-O2B-C2B	-3.86	113.12	123.43
2	A	2602	NDP	P2B-O2B-C2B	-3.69	113.57	123.43
2	A	2601	NDP	C4B-O4B-C1B	-2.54	107.59	109.92
2	A	2602	NDP	C5A-C6A-N6A	2.28	123.78	120.31
2	B	2601	NDP	C5A-C6A-N6A	2.25	123.74	120.31
2	B	2602	NDP	C5A-C6A-N6A	2.24	123.72	120.31
2	A	2601	NDP	C5A-C6A-N6A	2.17	123.62	120.31
2	A	2602	NDP	C4B-O4B-C1B	-2.08	108.02	109.92
2	A	2601	NDP	O3B-C3B-C2B	2.06	116.96	111.19

There are no chirality outliers.

All (39) torsion outliers are listed below:

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

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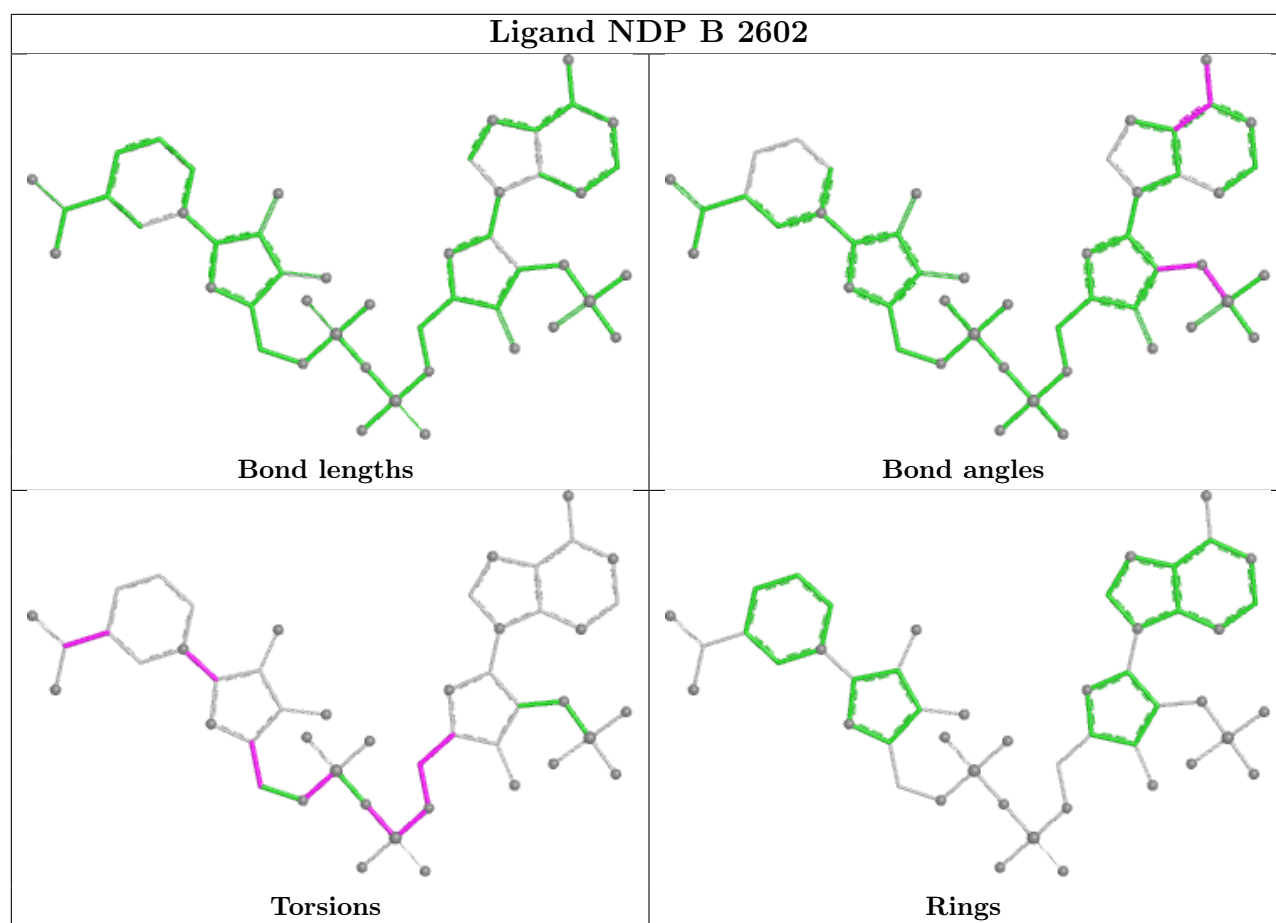
Mol	Chain	Res	Type	Atoms
2	B	2602	NDP	O4D-C1D-N1N-C6N
2	B	2602	NDP	O4D-C4D-C5D-O5D
2	A	2601	NDP	C2N-C3N-C7N-N7N
2	A	2601	NDP	C2B-O2B-P2B-O1X
2	B	2601	NDP	C2B-O2B-P2B-O1X
2	A	2602	NDP	C2B-O2B-P2B-O3X
2	B	2601	NDP	C2B-O2B-P2B-O3X
2	A	2601	NDP	C2N-C3N-C7N-O7N
2	B	2601	NDP	C2N-C3N-C7N-O7N
2	B	2602	NDP	PN-O3-PA-O2A
2	A	2602	NDP	O4B-C4B-C5B-O5B

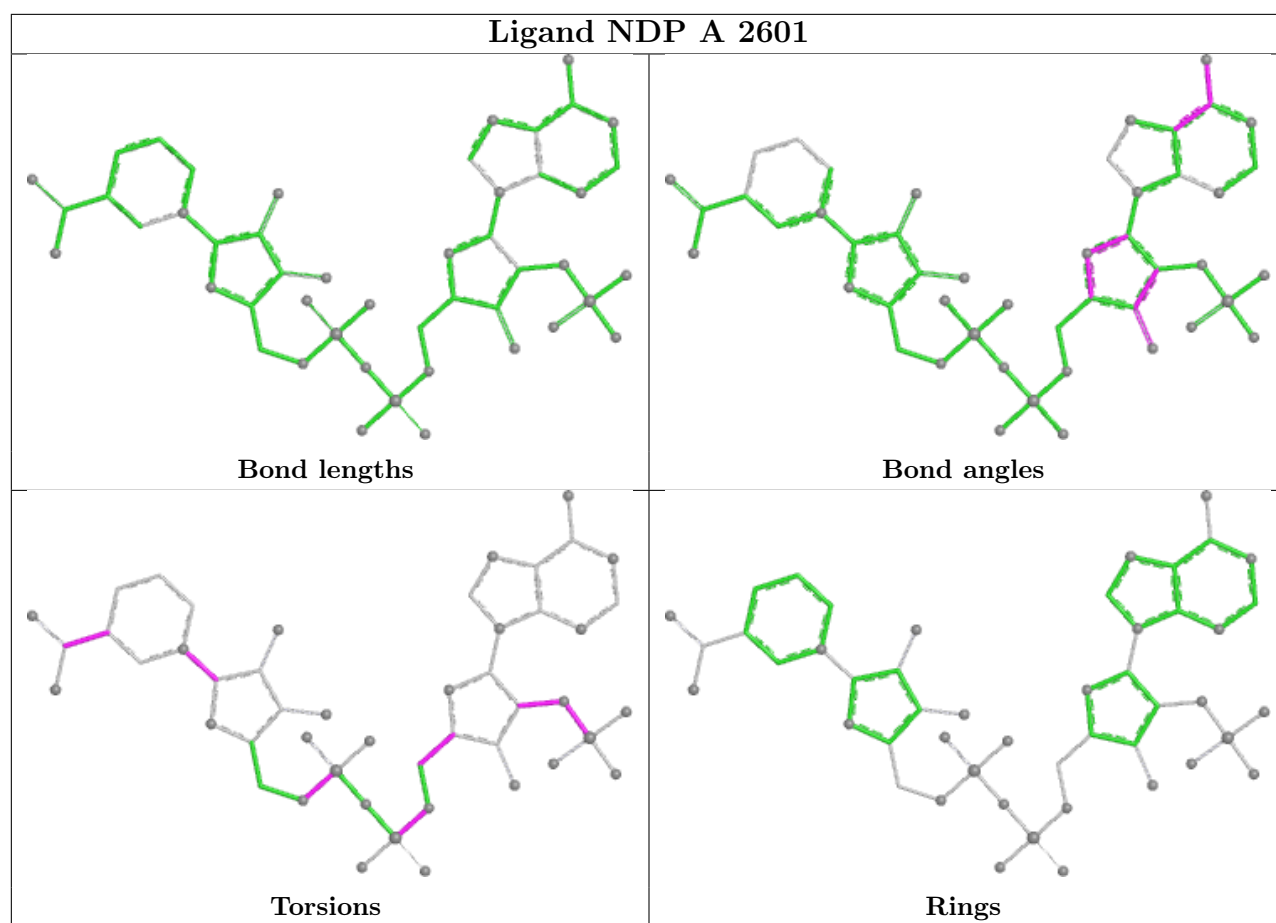
There are no ring outliers.

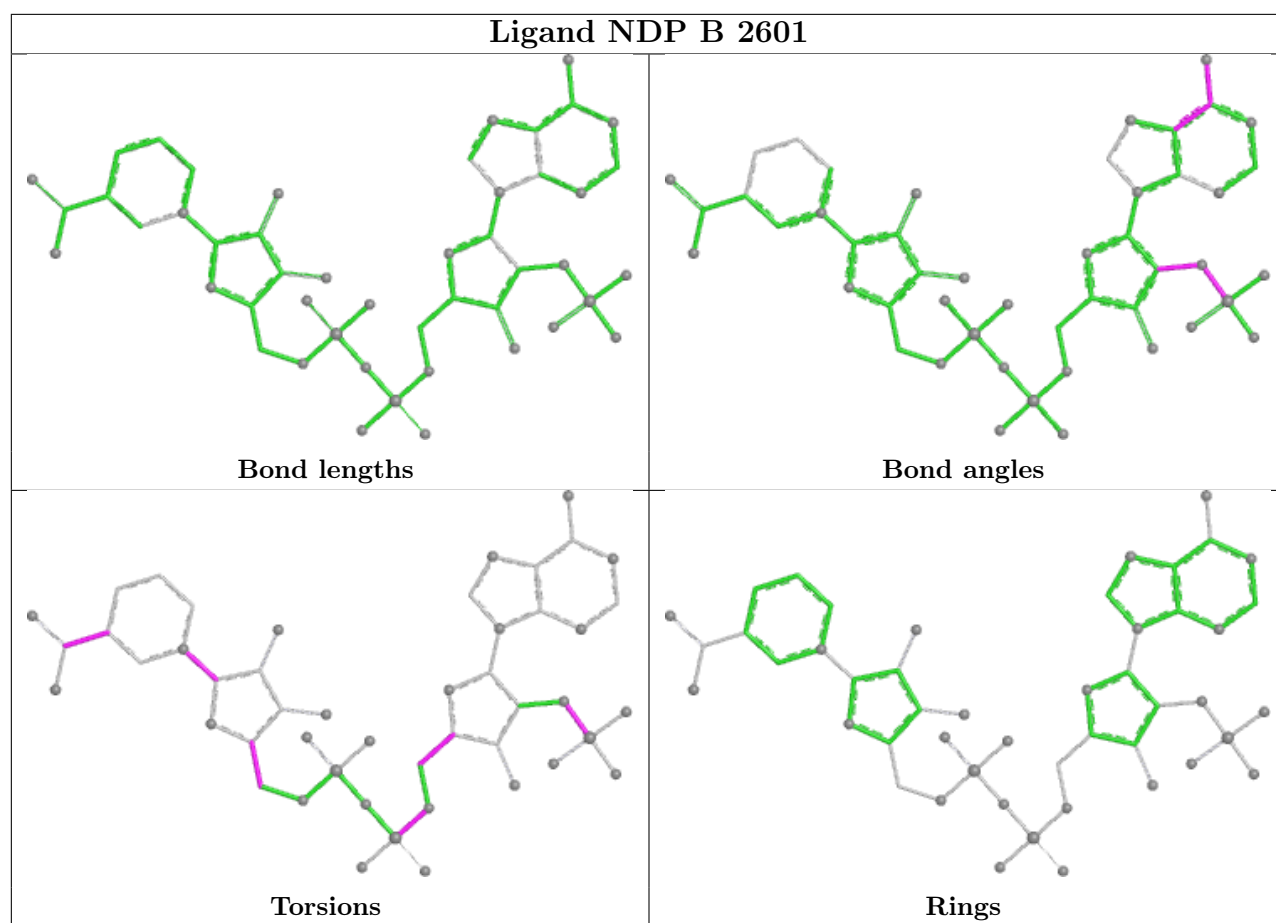
1 monomer is involved in 1 short contact:

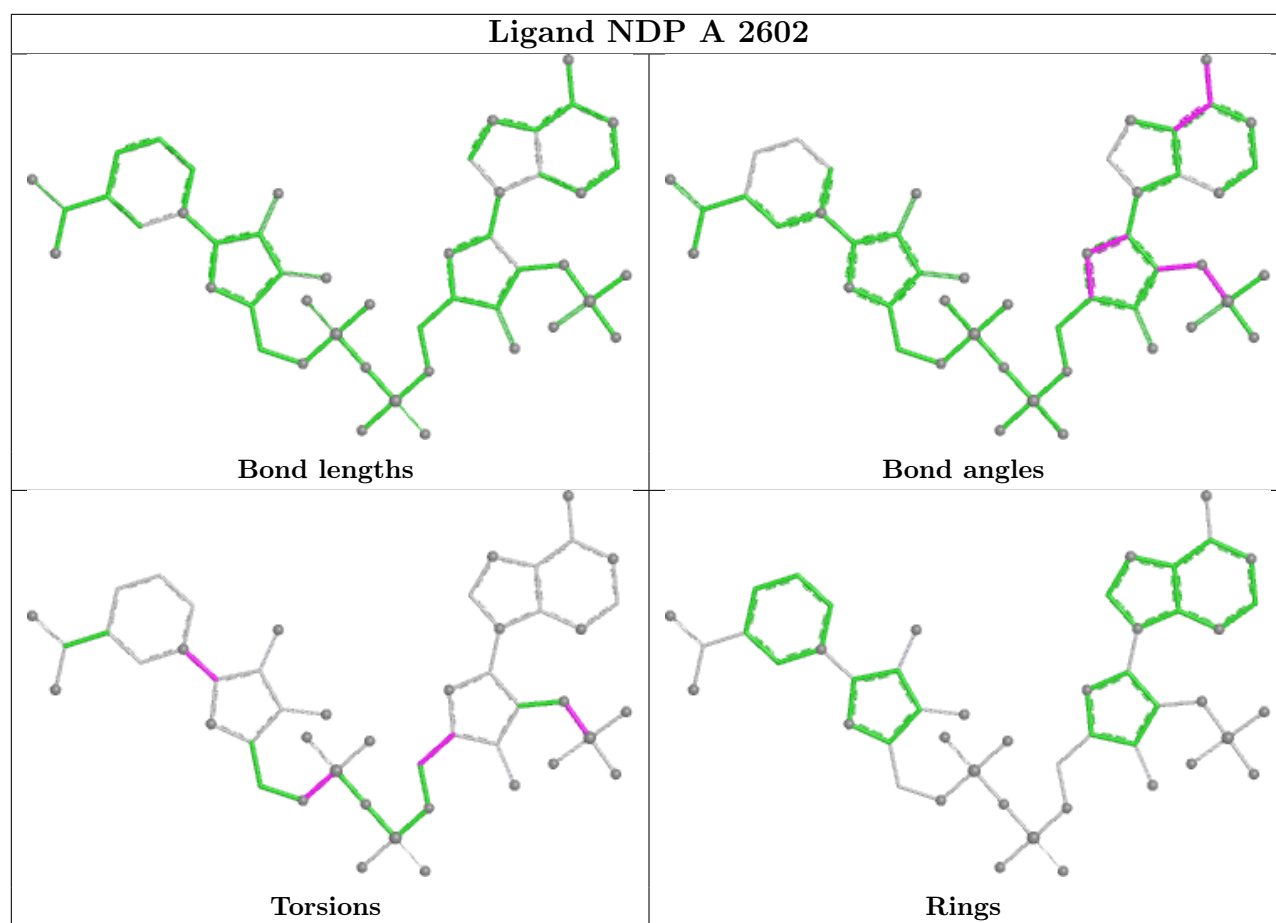
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2601	NDP	1	0

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.

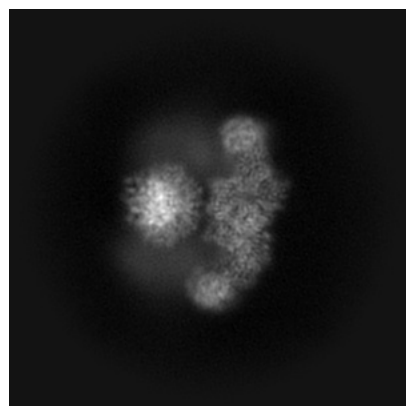
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43353. These allow visual inspection of the internal detail of the map and identification of artifacts.

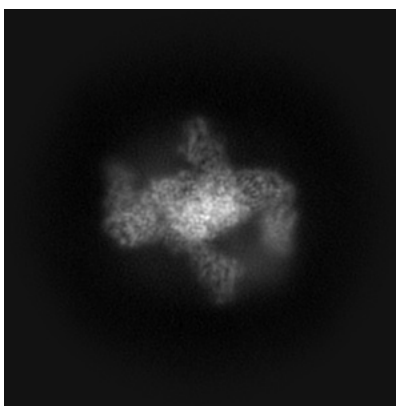
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

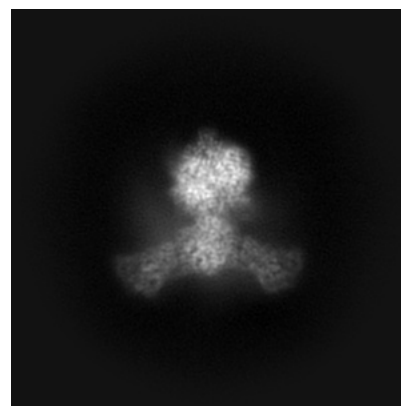
#### 6.1.1 Primary map



X

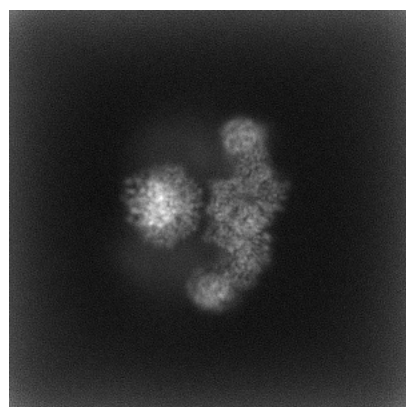


Y

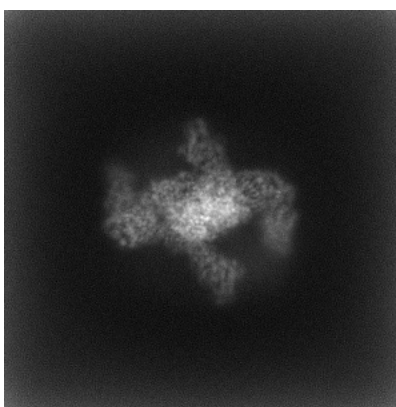


Z

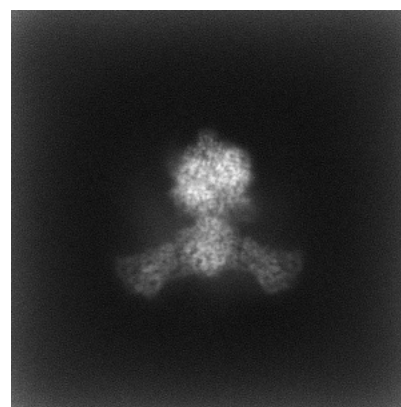
#### 6.1.2 Raw map



X



Y



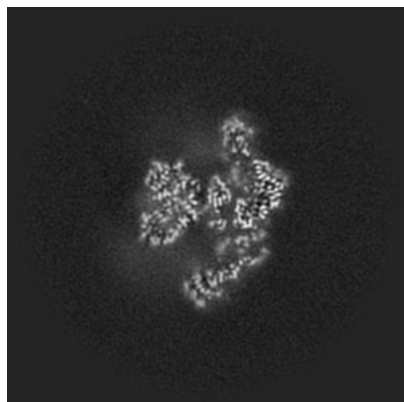
Z

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

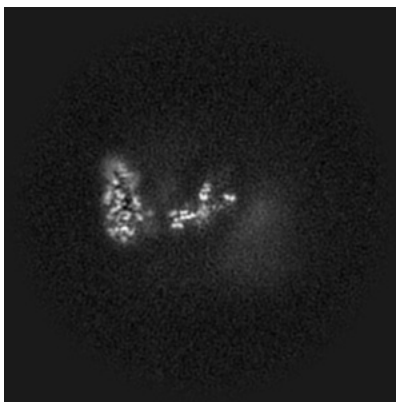


## 6.2 Central slices [i](#)

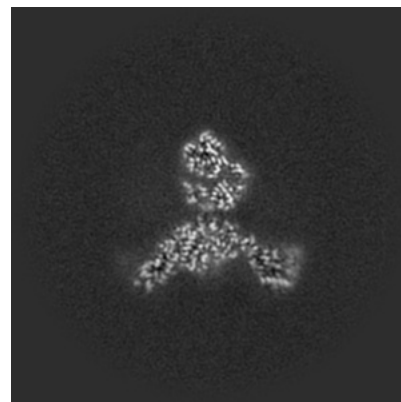
### 6.2.1 Primary map



X Index: 180

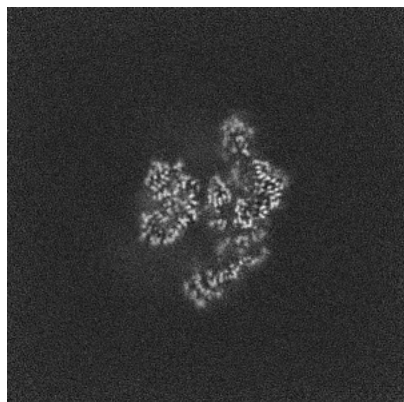


Y Index: 180



Z Index: 180

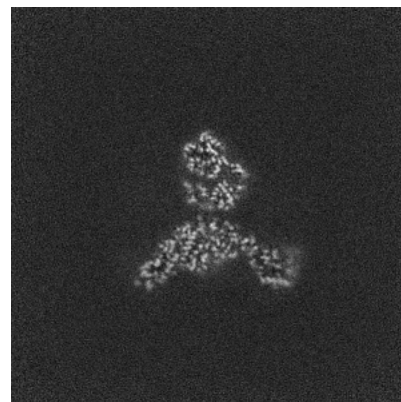
### 6.2.2 Raw map



X Index: 180



Y Index: 180

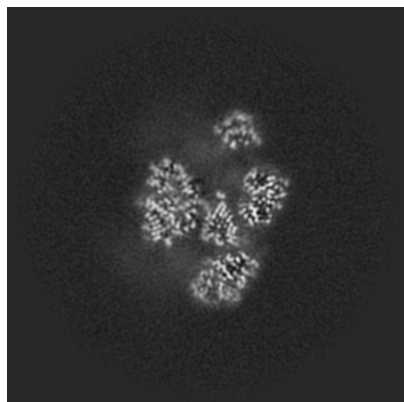


Z Index: 180

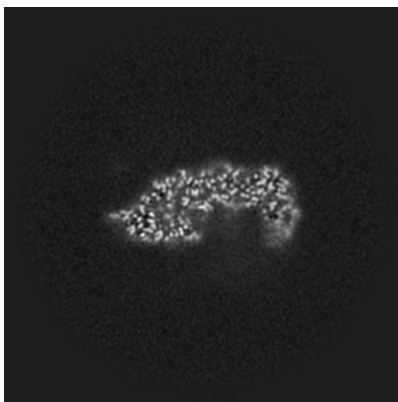
The images above show central slices of the map in three orthogonal directions.

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

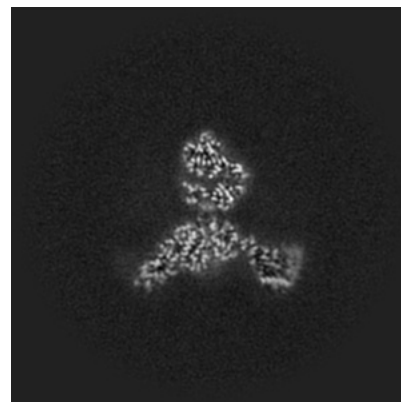
### 6.3.1 Primary map



X Index: 173

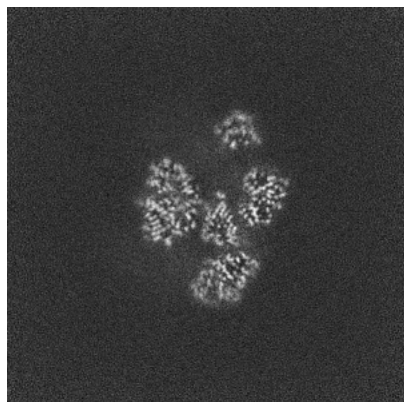


Y Index: 207

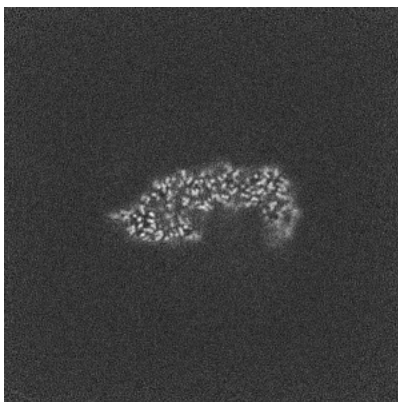


Z Index: 179

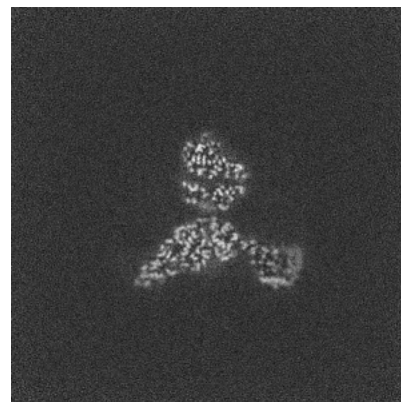
### 6.3.2 Raw map



X Index: 173



Y Index: 207

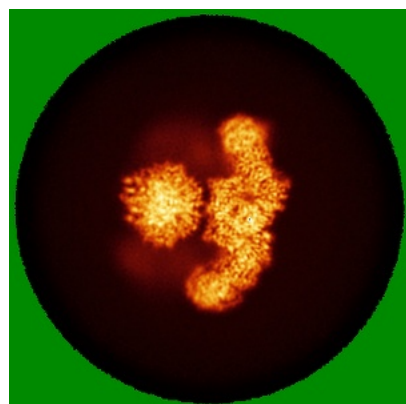


Z Index: 178

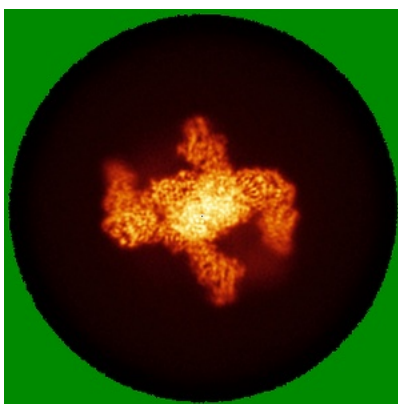
The images above show the largest variance slices of the map in three orthogonal directions.

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

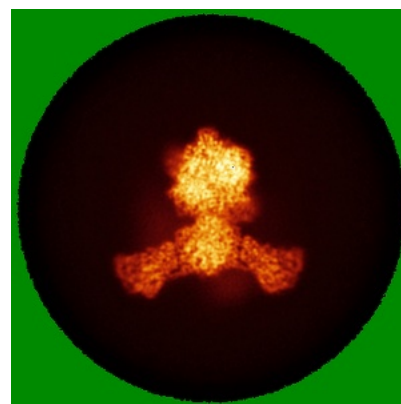
### 6.4.1 Primary map



X

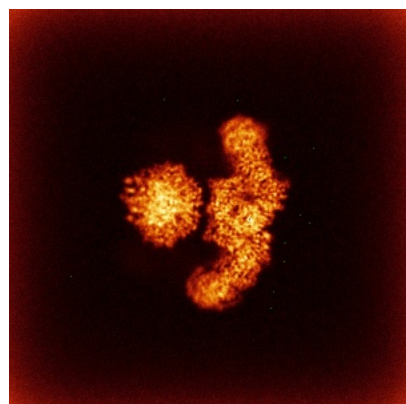


Y

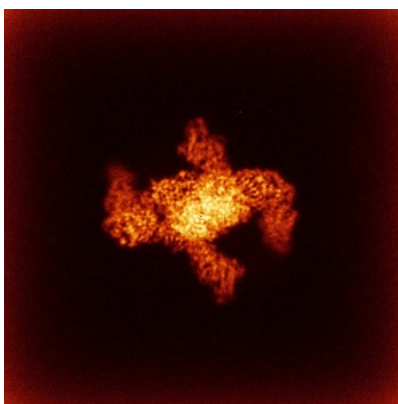


Z

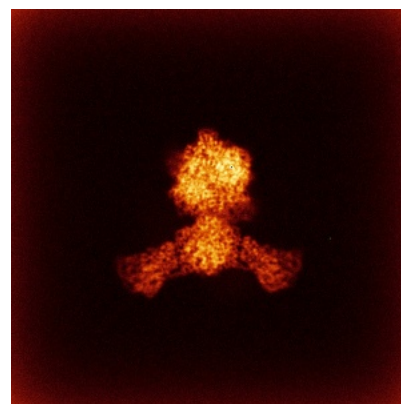
### 6.4.2 Raw map



X



Y

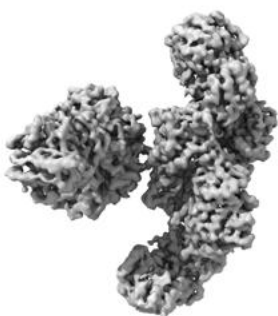


Z

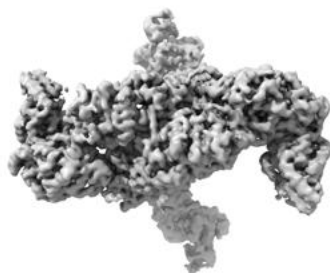
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

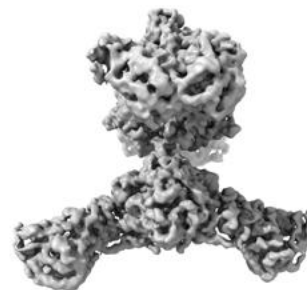
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.18. 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.

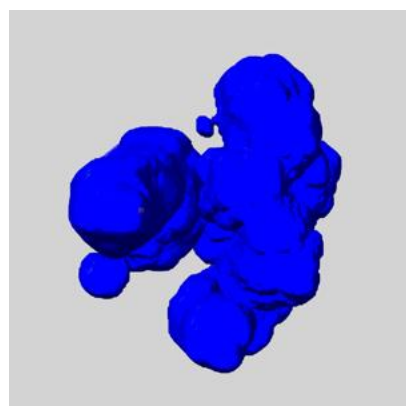
## 6.6 Mask visualisation [i](#)

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

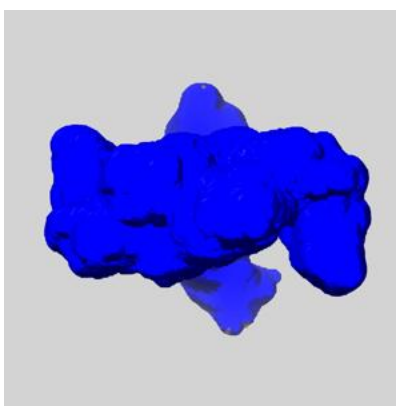
A mask typically either:

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

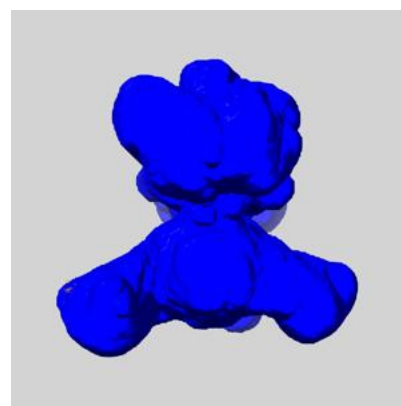
### 6.6.1 emd\_43353\_msk\_1.map [i](#)



X



Y

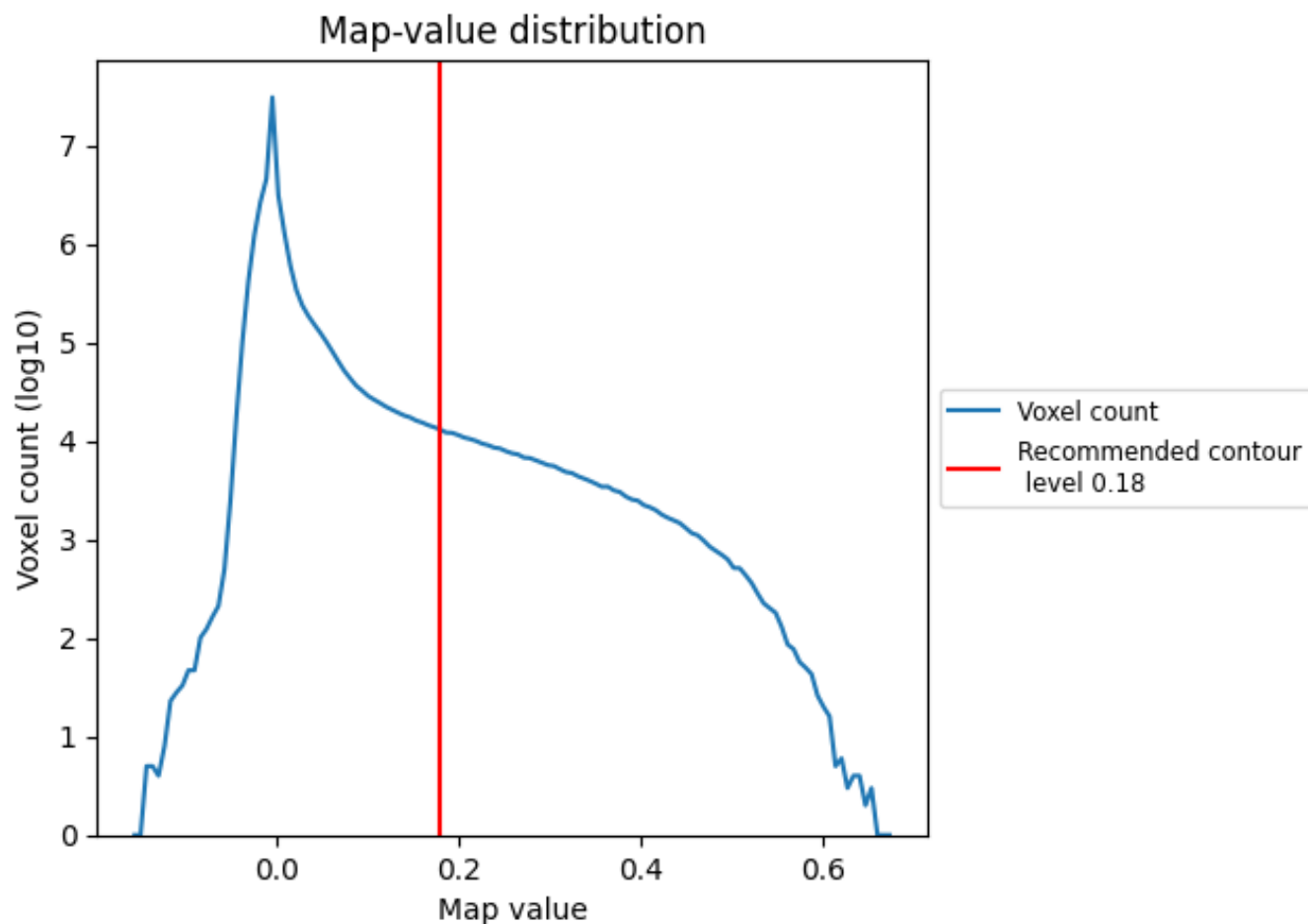


Z

## 7 Map analysis [i](#)

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

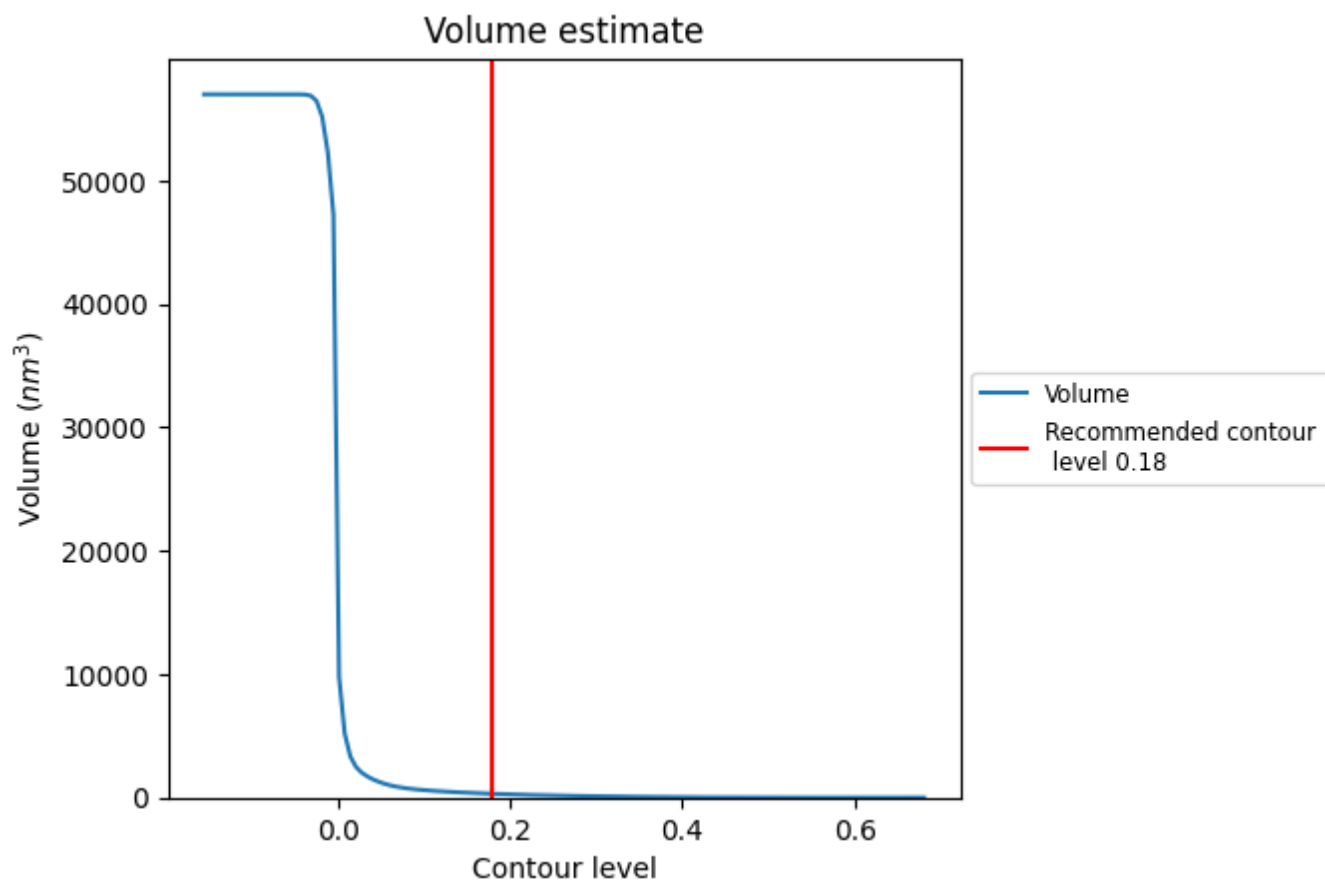
### 7.1 Map-value distribution [i](#)



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.



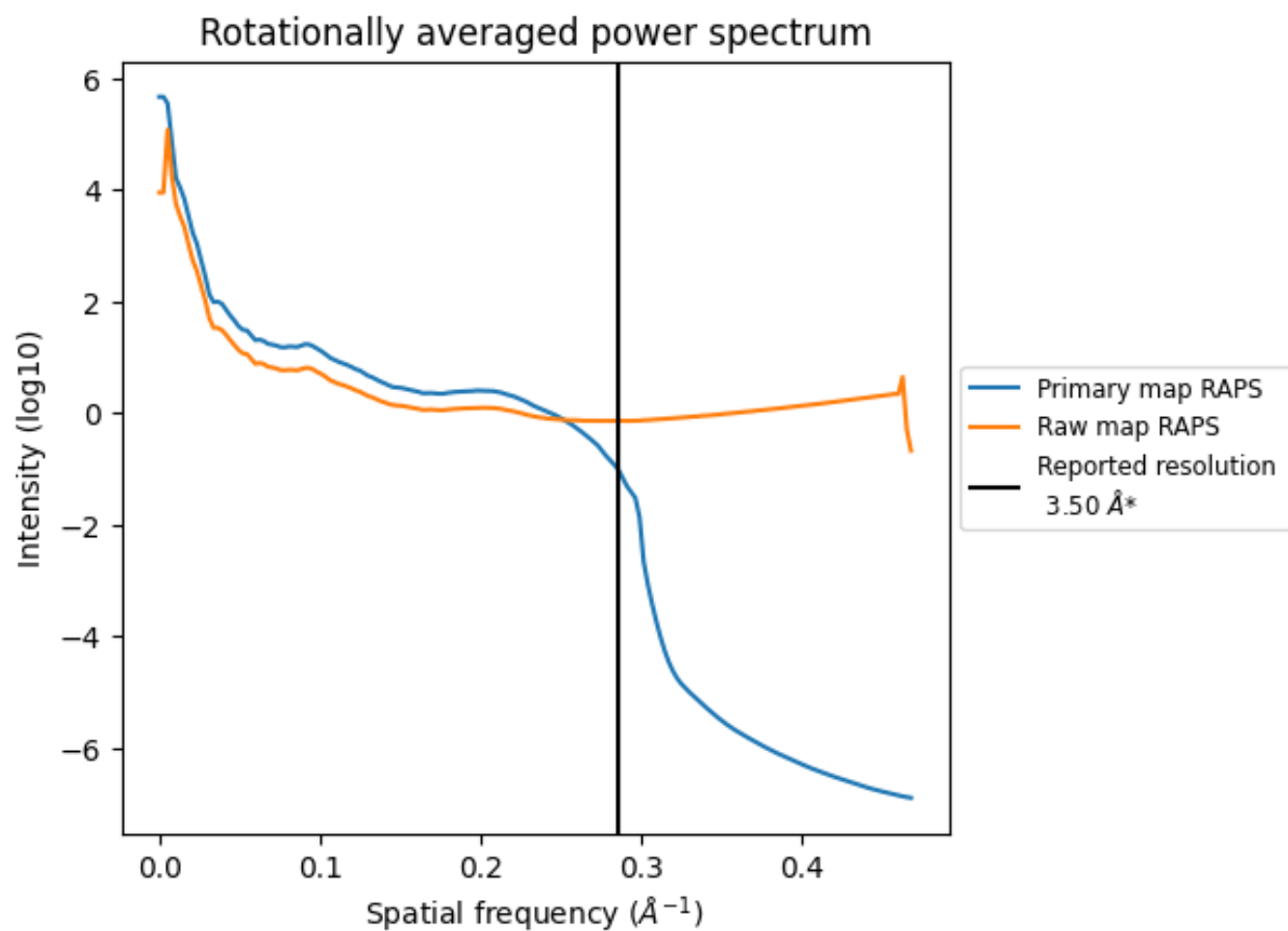
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 307  $\text{nm}^3$ ; this corresponds to an approximate mass of 277 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 ⓘ



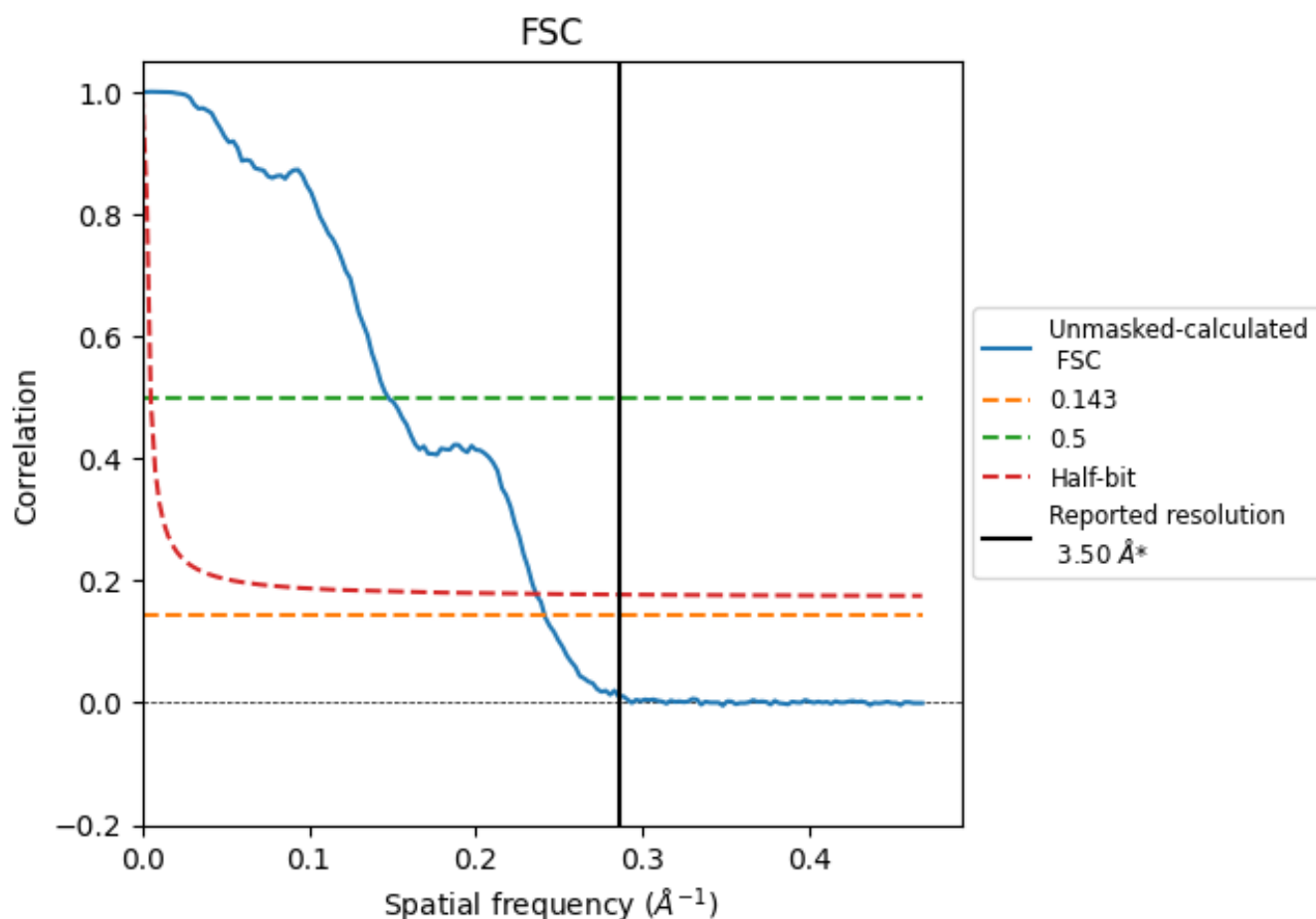
\*Reported resolution corresponds to spatial frequency of  $0.286 \text{ \AA}^{-1}$



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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.286  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

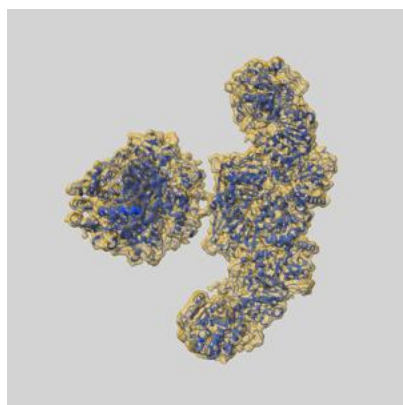
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.14	6.78	4.24

\*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 4.14 differs from the reported value 3.5 by more than 10 %

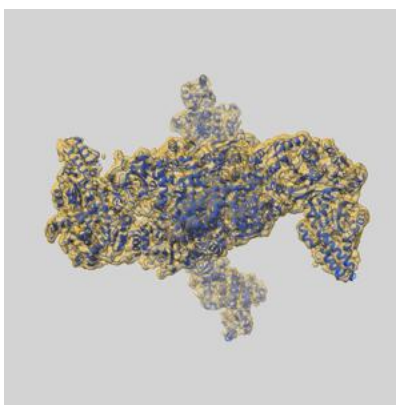
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-43353 and PDB model 8VM6. Per-residue inclusion information can be found in section [3](#) on page [7](#).

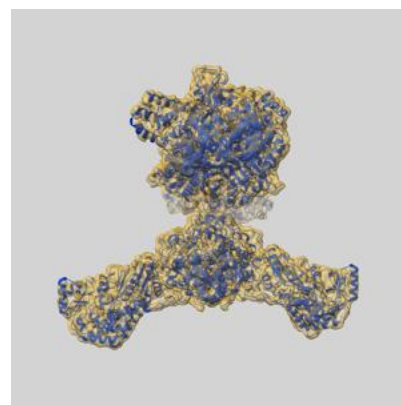
### 9.1 Map-model overlay [i](#)



X



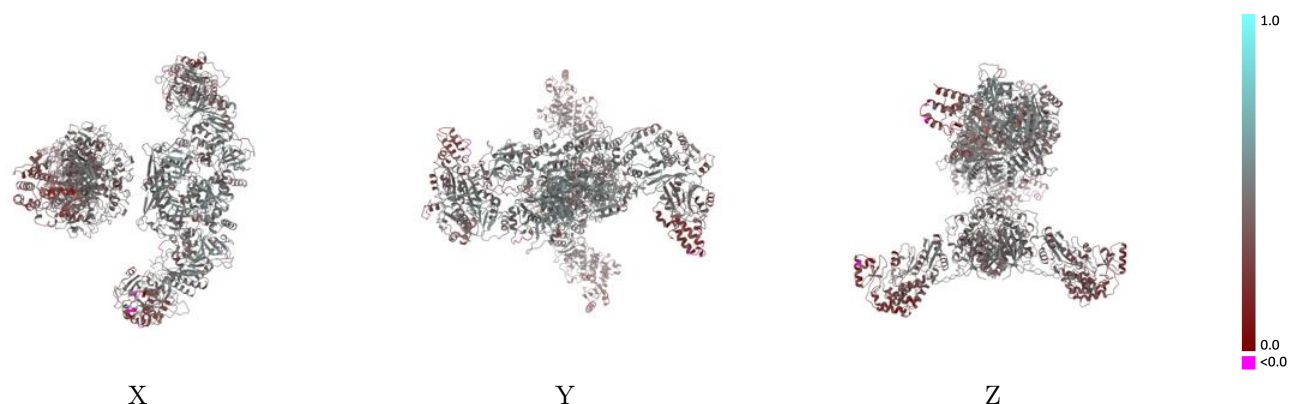
Y



Z

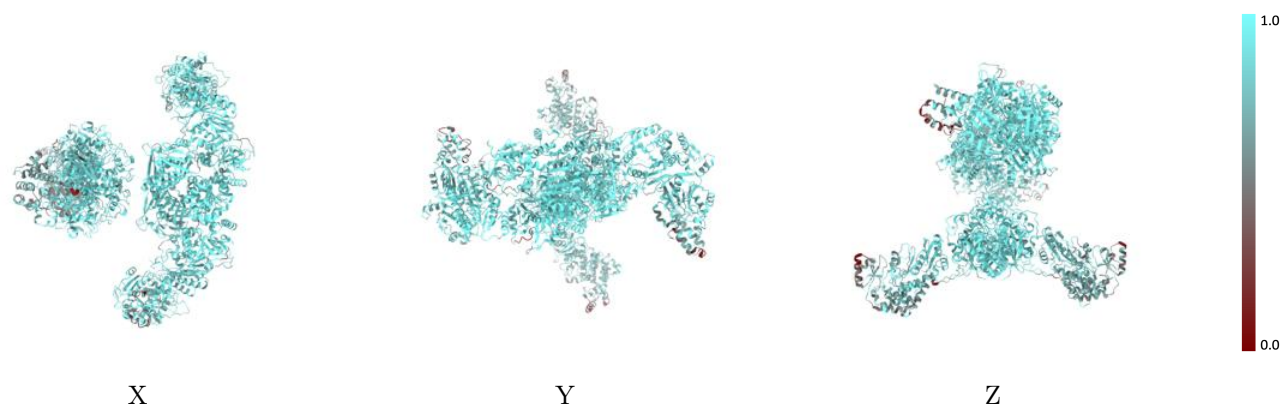
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



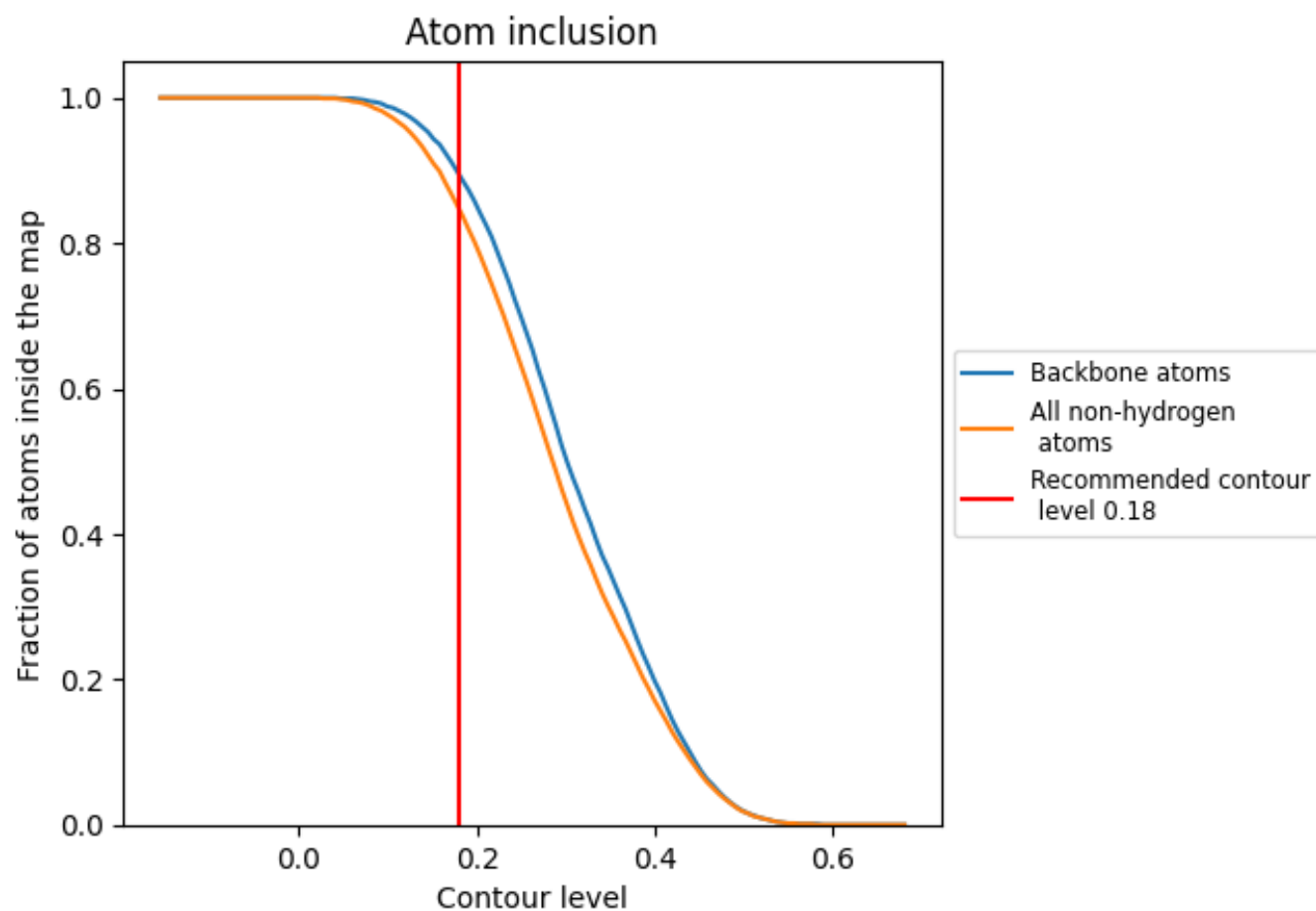
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.18).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 85% 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 (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8470	<div></div> 0.4290
A	<div></div> 0.8510	<div></div> 0.4290
B	<div></div> 0.8460	<div></div> 0.4290

