



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 06:17 PM UTC

PDB ID : 8VM0 / pdb_00008vm0
EMDB ID : EMD-43350
Title : Composite structure of human FASN with NADPH in State 4
Authors : Schultz, K.; Marmorstein, R.
Deposited on : 2024-01-12
Resolution : 3.30 Å (reported)
Based on initial model : 3HHD

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

We welcome your comments at validation@mail.wwpdb.org

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>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

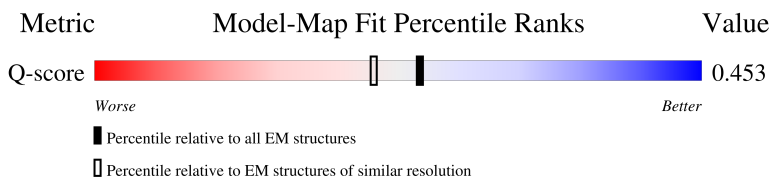
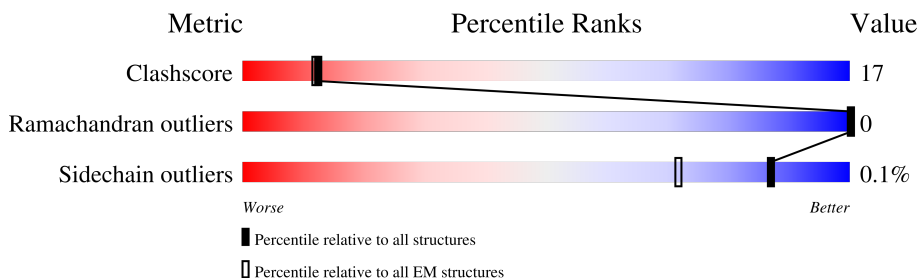
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	 59% 22% 19%
1	B	2553	 58% 23% 19%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 50709 atoms, of which 18827 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Fatty acid synthase.

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

There are 88 discrepancies between the modelled and reference sequences:

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

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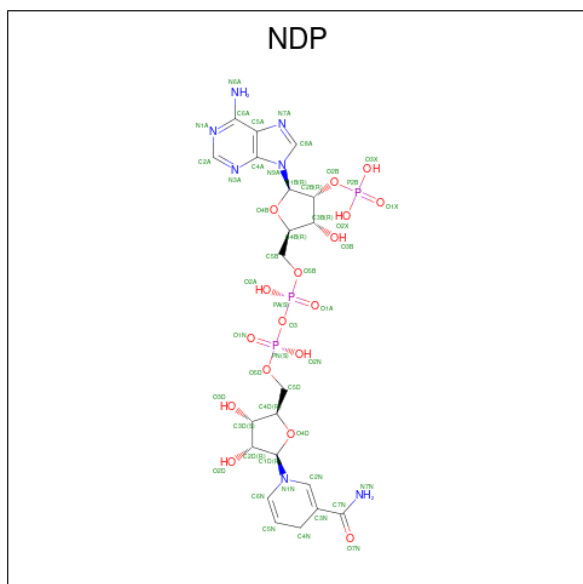
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	ALA	-	expression tag	UNP P49327
A	-4	MET	-	expression tag	UNP P49327
A	-3	GLY	-	expression tag	UNP P49327
A	-2	SER	-	expression tag	UNP P49327
A	-1	GLY	-	expression tag	UNP P49327
A	0	ILE	-	expression tag	UNP P49327
A	1	PRO	-	expression tag	UNP P49327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

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

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

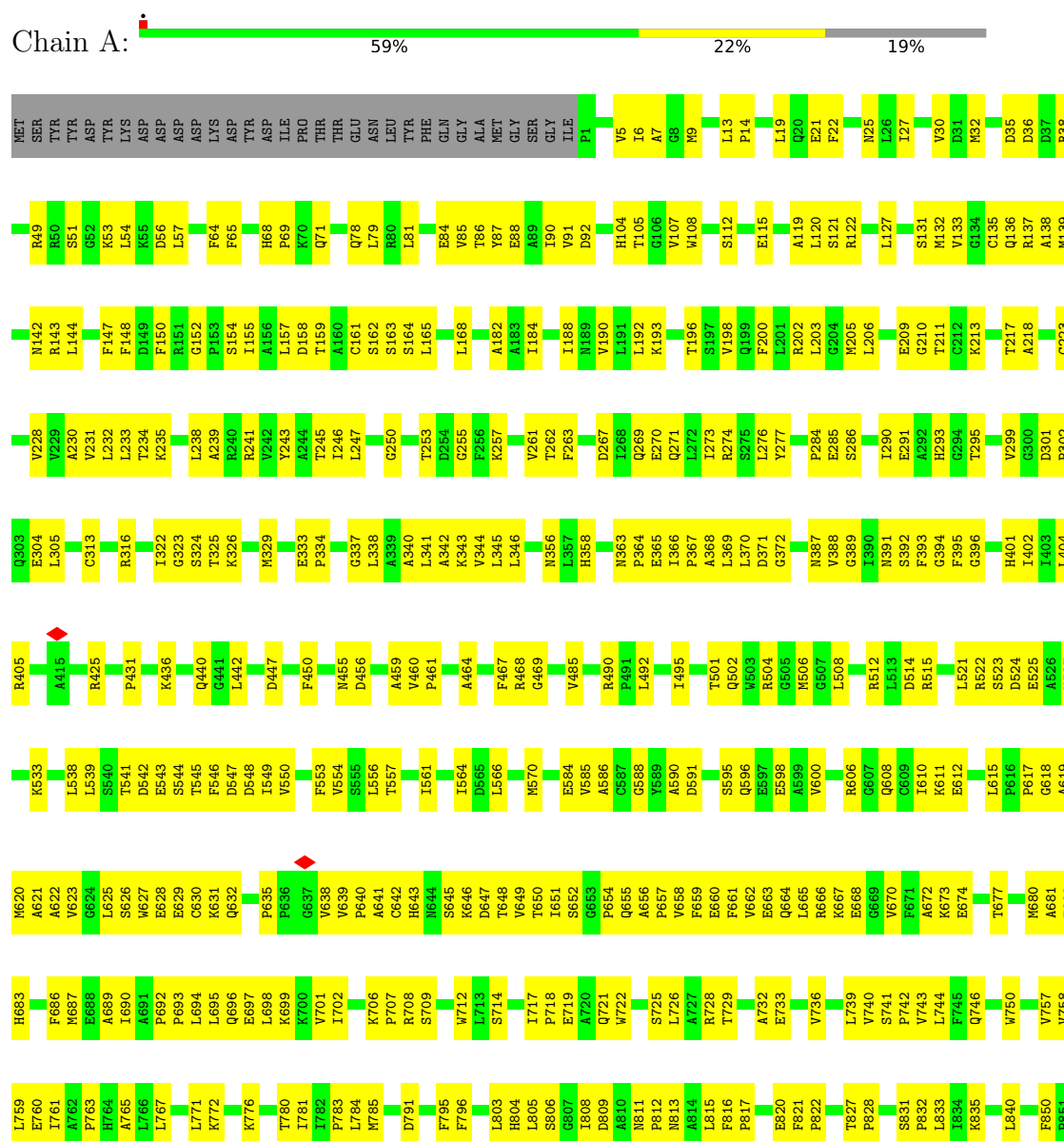


Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
2	A	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
2	B	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
2	B	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Fatty acid synthase



L1400	R1404	I1413	V1417	K1429	G1430	I1431	S1437	S1438	R1439	S1445	I1446	S1451	V1452	V1453	V1457	G1466	M1467	R1468	L1469	R1470	C1471	L1474	E1485	D1487	S1490	V1496	L1497	D1500	L1501	M1504	E1521	R1552	Q1555	C1558	Q1562	V1566																			
PRO	ARG	P1173	E1177	C1186	R1187	L1188	Q1189	L1190	M1191	G1192	M1193	L1194	Q1195	L1196	E1197	L1198	A1199	Q1200	V1201	L1202	A1203	E1205	R1206	P1207	K1208	L1209	P1210	L1214	L1215	L1218	L1228	V1242	V1245	L1246	H1249	H1251	L1252	L1256	L1265	Y1270	D1274	R1275													
Q1278	A1279	L1280	V1282	A1293	Q1294	V1297	D1298	P1299	A1300	D1301	S1305	A1306	L1312	L1313	V1314	C1315	N1316	C1317	S1327	M1331	M1332	V1333	G1339	H1345	L1348	R1349	G1354	D1355	I1356	Q1366	Y1367	G1368	Q1369	G1370	I1371	L1372	S1373	A1376	L1386	V1389	G1390	L1391	K1392	K1393											
H804	L805	S806	N813	A814	P822	A823	P824	S831	P832	L833	A841	W842	W852	GLY	SER	GLY	SER	PRO	SER	A859	T879	L880	T898	L899	V912	V913	I924	L933	E934	V935	E939	E948	N949	V958	P972	T976	P977	N978	P979	T980	E981	P982	Y991												
Q1006	E1014	L1021	F1029	T1032	V1052	I1055	T1068	L1069	Q1070	D1071	K1072	A1073	Q1074	V1079	Q1109	Q1110	V1111	E1125	G1126	C1127	L1128	L1134	C1141	V1145	T1150	THR	THR	GLN	GLN	GLY	LEU	LYS	MET	VAL	VAL	PRO	GLY	LEU	ASP	GLY	ALA	GLN	ILE												
R241	V242	Y243	A249	G250	T251	N252	D254	Q255	F256	K257	E258	Q259	G260	V261	T262	F263	P264	S265	G266	D267	T268	Q269	E270	Q271	L272	L273	R274	Y277	A283	P284	E285	E288	Y289	I290	G300	D301	P302	L305	R316	Q317	E318	P319	L320	I321	I322	G323	S324	T325	K326						
M329	G330	H331	P332	E333	P334	A335	L338	A339	A340	K343	V344	L345	S347	L348	G351	L352	I356	D371	G372	V388	G389	I390	N391	S392	F393	G394	F395	G396	N399	V400	E401	I402	P406	Q409	H417	L420	F421	R422	L423	L424	R425	A426	R429	T430	E435	P431									
V434	Q440	D447	L448	A449	F450	M453	D456	I457	V460	P461	A464	M465	P466	F467	R468	G469	Y470	E476	R477	V485	R490	W493	F494	I495	M499	G500	T501	Q502	W503	R504	G505	M506	G507	L508	M511	R512	L513	D514	R515	T520	L521	D524	E525	A526											
V527	L532	W534	L538	L539	S540	T541	S544	T545	F546	D547	I549	V550	H551	S552	S555	L556	T557	A558	I559	Q560	I561	I564	D565	L566	S568	C569	M570	G571	L572	R573	P574	D575	G576	I577	W578	G579	H580	S581	L582	G583	E584	C587	D591	G592	C593	L594	S595	E597							
V600	L601	W605	R606	G607	Q608	C609	I610	K611	E612	K673	A613	H614	L615	P616	P617	G618	A619	M620	A621	A622	V623	G624	L625	S626	W627	E628	E629	C630	K631	Q632	L633	C634	P635	P636	G637	V638	V639	P640	A641	H642	N644	S645	T648	V649	I651	S652	G653	P654	Q655	A656	P657	V658	F659	E660	F661
V662	E663	Q664	L665	R666	K667	E668	G669	V670	F671	A672	K673	E674	M680	A681	F682	M687	E688	A689	I690	A691	P692	P693	L694	L695	P696	P697	W701	I702	R703	E704	P705	K706	P707	R708	W712	L713	S714	I717	P718	E719	A720	Q721	W722	H723	L726	A727	R728	T729							
A732	E733	Y734	N735	V736	N737	N738	L739	W740	S741	P742	V743	L744	F745	Q746	E747	A748	L749	V752	P753	E754	H755	A756	V757	V758	L759	E760	I761	A762	P763	H764	A765	L766	L767	Q768	A769	V770	L771	K772	G773	R774	L775	K776	I781	I782	P783	K786	V787	D788	H789	R790	L793	L797	L803		

VAL	THR	VAL	SER	VAL	ARG	ALA	D2003	Q1595
LEU	THR	VAL	SER	GLN	GLN	VAL	D2006	D1596
LEU	GLY	PRO	GLY	PRO	ARG	GLU	R2007	S1597
ALA	CYS	GLY	GLY	GLY	SER	VAL	L2013	F1603
ARG	ALA	PRO	GLY	PRO	GLU	GLN	V2018	E1602
SER	GLU	THR	ARG	ARG	THR	THR	V2022	D1607
THR	THR	VAL	PHE	ALA	ARG	GLN	R1612	R1612
LYS	GLY	GLY	GLY	LEU	LYS	ASP	N2033	V1640
LEU	ALA	TYR	VAL	LEU	LEU	VAL	Y2034	V1650
SER	ILE	SER	SER	HIS	GLN	GLU	M2041	S1677
ARG	CYS	GLY	TYR	PRO	LEU	GLY	E2042	V1680
ALA	PHE	GLY	GLY	ILE	GLU	ALA	R2043	G1681
GLU	PHE	ALA	ALA	GLU	SER	VAL	E2051	Q1682
SER	VAL	CYS	VAL	CYS	SER	ALA	Q2059	Q1714
TYR	GLN	VAL	VAL	PHE	LYS	HIS	W2060	L1743
THR	GLN	ALA	THR	PHE	ALA	ILE	A2062	R1765
LYS	THR	GLY	THR	GLY	ASP	LEU	I2063	I1769
ALA	ASP	GLY	VAL	ALA	GLY	ILE	V2066	S1775
ALA	MET	VAL	ARG	PRO	VAL	ASN	GLY	H1792
LYS	MET	CYS	SER	LEU	THR	LEU	ILE	C1828
THR	GLY	GLN	SER	PRO	GLY	LEU	THR	E1837
HIS	LYS	GLN	GLY	LEU	ALA	ASP	THR	E1862
GLY	GLY	ASN	GLN	GLN	LEU	LEU	ASP	G1867
ALA	LEU	SER	CYS	GLN	GLY	THR	ASN	A1868
THR	GLY	THR	THR	GLN	THR	THR	ASP	X1869
GLY	ARG	PHE	LEU	ALA	GLN	SER	THR	I1889
ASP	VAL	PHE	ALA	ASP	LEU	LEU	ILE	F1896
LEU	ALA	GLY	PRO	LEU	ASN	MET	VAL	L1912
GLY	ALA	ASP	GLY	LEU	LEU	THR	G2082	V1968
ALA	ALA	SER	PRO	ARG	VAL	GLU	S2081	N1970
ASP	VAL	THR	THR	ILE	SER	GLY	P2085	L1971
TYR	ASP	THR	THR	SER	VAL	VAL	M2088	E1981
ASN	LEU	TYR	VAL	HIS	ARG	THR	C2091	S1997
LEU	ILE	VAL	VAL	LEU	THR	GLN	L2097	N2001
SER	LYS	LEU	ALA	ALA	PRO	LEU	F2098	I2002
VAL	SER	THR	THR	ALA	GLY	ARG	L2106	
CYS	HIS	THR	TYR	TYR	GLY	THR	E2113	
ASP	GLN	GLN	TYR	ILE	PRO	LEU	LYS	
GLY	GLY	SER	THR	ASP	THR	LEU	ALA	
LYS	LEU	ASP	THR	CYS	ARG	VAL	SER	
VAL	GLY	ARG	ALA	ILE	GLN	LEU	THR	
HIS	GLY	VAL	LYS	ARG	ASN	SER	ALA	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	114182	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	0.728	Depositor
Minimum map value	-0.169	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.182	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 [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.17	0/16198	0.30	2/22023 (0.0%)
1	B	0.19	0/16222	0.33	0/22055
All	All	0.18	0/32420	0.31	2/44078 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1786	LEU	N-CA-C	-6.68	104.00	111.28
1	A	1787	LYS	N-CA-C	-5.11	102.72	110.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	15833	9343	15809	537	0
1	B	15857	9380	15826	556	0
2	A	96	52	52	1	0
2	B	96	52	52	3	0
All	All	31882	18827	31739	1077	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 (1077) 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:165:LEU:HD12	1:A:392:SER:CB	1.74	1.17
1:A:165:LEU:HD12	1:A:392:SER:OG	1.52	1.07
1:A:803:LEU:HD11	1:A:808:ILE:HD12	1.41	1.00
1:A:628:GLU:HA	1:A:631:LYS:HE2	1.40	0.98
1:A:165:LEU:HG	1:A:337:GLY:HA3	1.45	0.97
1:B:1446:ILE:HG23	1:B:1474:LEU:HD12	1.46	0.97
1:A:165:LEU:HD12	1:A:392:SER:HB3	1.46	0.97
1:B:502:GLN:OE1	1:B:552:SER:HB2	1.65	0.96
1:B:620:MET:HG3	1:B:652:SER:HB3	1.45	0.96
1:B:511:MET:HE1	1:B:520:ILE:HG21	1.48	0.95
1:A:440:GLN:HG3	1:A:833:LEU:HD22	1.48	0.95
1:B:687:MET:HE2	1:B:739:LEU:HD11	1.50	0.92
1:B:290:ILE:HG23	1:B:322:ILE:HD12	1.52	0.91
1:A:640:PRO:HA	1:A:651:ILE:HG22	1.51	0.90
1:B:499:MET:HG2	1:B:582:LEU:HD22	1.54	0.90
1:B:782:ILE:HG22	1:B:782:ILE:O	1.71	0.89
1:B:333:GLU:HB2	1:B:334:PRO:HD3	1.55	0.89
1:B:749:LEU:HD22	1:B:775:LEU:HD21	1.53	0.88
1:A:620:MET:HB3	1:A:677:THR:HG21	1.55	0.88
1:B:654:PRO:HB2	1:B:657:PRO:HD2	1.56	0.87
1:B:581:SER:HA	1:B:738:ASN:HD21	1.38	0.86
1:A:164:SER:HB2	1:A:338:LEU:HD13	1.54	0.86
1:A:687:MET:HE2	1:A:739:LEU:HD11	1.57	0.86
1:B:78:GLN:HE21	1:B:188:ILE:HD12	1.38	0.86
1:B:499:MET:HE1	1:B:682:PHE:CD2	2.11	0.85
1:A:654:PRO:HB2	1:A:657:PRO:HD2	1.60	0.84
1:B:164:SER:HB3	1:B:338:LEU:HG	1.58	0.84
1:A:692:PRO:O	1:A:695:LEU:HG	1.78	0.84
1:B:325:THR:HB	1:B:343:LYS:HD3	1.59	0.83
1:A:396:GLY:HA3	1:B:142:ASN:HD22	1.43	0.83
1:A:1607:ASP:OD1	1:A:1608:ALA:N	2.13	0.82
1:B:78:GLN:NE2	1:B:188:ILE:HD12	1.95	0.82
1:B:717:ILE:HD12	1:B:727:ALA:HB2	1.62	0.82
1:A:1337:ARG:NH1	1:A:1338:GLU:O	2.13	0.82
1:A:54:LEU:HD12	1:A:57:LEU:HD21	1.63	0.81
1:B:1496:VAL:HG13	1:B:1504:ASN:ND2	1.96	0.81
1:B:1298:ASP:OD1	1:B:1299:PRO:HD2	1.79	0.81
1:A:51:SER:O	1:A:53:LYS:NZ	2.13	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:GLN:NE2	1:B:143:ARG:HH12	1.79	0.80
1:A:22:PHE:HD1	1:A:32:MET:HE1	1.46	0.80
1:B:477:ARG:HH12	1:B:790:ARG:HD2	1.46	0.79
1:B:752:VAL:O	1:B:776:LYS:NZ	2.14	0.79
1:B:581:SER:CB	1:B:683:HIS:HE2	1.95	0.79
1:B:1437:SER:OG	1:B:1468:ARG:NH1	2.16	0.79
1:B:695:LEU:HD11	1:B:699:LYS:HE2	1.65	0.79
1:B:1429:LYS:NZ	1:B:1981:GLU:O	2.16	0.79
1:B:556:LEU:HD23	1:B:582:LEU:HD23	1.64	0.79
1:A:165:LEU:CD1	1:A:392:SER:HB3	2.12	0.79
1:A:626:SER:HB3	1:A:629:GLU:HG2	1.63	0.79
1:A:217:THR:HG22	1:A:364:PRO:HD3	1.66	0.78
1:A:623:VAL:HG12	1:A:625:LEU:H	1.49	0.78
1:A:642:CYS:HA	1:A:743:VAL:HB	1.64	0.77
1:A:564:ILE:HD13	1:A:590:ALA:HB2	1.65	0.77
1:A:21:GLU:O	1:A:25:ASN:ND2	2.17	0.77
1:B:499:MET:CE	1:B:682:PHE:CD2	2.67	0.77
1:A:522:ARG:NH1	1:A:596:GLN:OE1	2.18	0.77
1:A:622:ALA:HA	1:A:650:THR:HA	1.67	0.77
1:A:656:ALA:HB3	1:A:657:PRO:HD3	1.66	0.77
1:B:654:PRO:HB2	1:B:657:PRO:CD	2.15	0.76
1:B:654:PRO:HG3	1:B:686:PHE:HZ	1.50	0.76
1:A:621:ALA:HB1	1:A:673:LYS:O	1.85	0.76
1:A:628:GLU:OE1	1:A:628:GLU:N	2.20	0.75
1:A:654:PRO:HG3	1:A:686:PHE:HZ	1.50	0.75
1:A:549:ILE:HD11	1:A:611:LYS:HG3	1.68	0.75
1:B:1145:VAL:HG21	1:B:1356:ILE:HG12	1.69	0.75
1:A:139:MET:HE2	1:A:142:ASN:HB2	1.67	0.75
1:B:621:ALA:HA	1:B:674:GLU:HA	1.69	0.75
1:A:139:MET:HE2	1:A:139:MET:HA	1.67	0.74
1:B:74:THR:HG21	1:B:128:VAL:HG21	1.70	0.74
1:A:694:LEU:HD23	1:A:698:LEU:HG	1.69	0.74
1:B:1242:VAL:HG22	1:B:1312:LEU:HB3	1.67	0.74
1:A:14:PRO:HD2	1:A:329:MET:HE3	1.69	0.74
1:A:293:HIS:N	1:A:304:GLU:OE2	2.18	0.74
1:A:783:PRO:HB2	1:A:795:PHE:HE2	1.53	0.73
1:B:136:GLN:HB3	1:B:139:MET:HG2	1.68	0.73
1:A:79:LEU:HD21	1:A:143:ARG:HG3	1.69	0.73
1:B:495:ILE:HD13	1:B:578:VAL:HB	1.69	0.73
1:B:548:ASP:OD1	1:B:550:VAL:N	2.22	0.73
1:B:1249:HIS:O	1:B:1251:HIS:ND1	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:ARG:NH1	1:B:464:ALA:O	2.22	0.72
1:B:633:ARG:NH2	1:B:668:GLU:OE2	2.18	0.72
1:A:759:LEU:HD22	1:A:784:LEU:HD11	1.70	0.72
1:B:499:MET:CE	1:B:682:PHE:HD2	2.03	0.72
1:A:623:VAL:HG13	1:A:665:LEU:HD13	1.71	0.72
1:A:718:PRO:HG3	1:A:744:LEU:HD11	1.72	0.72
1:B:1327:SER:O	1:B:1331:ASN:ND2	2.22	0.71
1:B:305:LEU:HD22	1:B:366:ILE:HD13	1.73	0.71
1:A:241:ARG:HD3	1:A:243:TYR:CZ	2.25	0.71
1:A:13:LEU:HD22	1:A:329:MET:HE1	1.72	0.71
1:A:660:GLU:O	1:A:663:GLU:HG2	1.90	0.71
1:A:1286:GLU:OE1	1:A:1286:GLU:N	2.23	0.71
1:B:468:ARG:HD2	1:B:485:VAL:HG21	1.73	0.71
1:A:570:MET:HE2	1:A:815:LEU:HD11	1.73	0.71
1:A:425:ARG:HH21	1:A:811:ASN:HD22	1.39	0.71
1:A:524:ASP:OD1	1:A:533:LYS:HA	1.91	0.71
1:A:741:SER:HB2	1:A:742:PRO:HD2	1.73	0.70
1:A:22:PHE:CD1	1:A:32:MET:HE1	2.27	0.70
1:A:78:GLN:HB3	1:A:188:ILE:HD12	1.73	0.70
1:B:329:MET:HE2	1:B:332:PRO:HD3	1.73	0.70
1:A:209:GLU:OE1	1:A:209:GLU:N	2.24	0.70
1:B:460:VAL:HG22	1:B:461:PRO:HD2	1.74	0.70
1:A:832:PRO:O	1:A:835:LYS:NZ	2.25	0.70
1:B:1274:ASP:OD1	1:B:1275:ARG:N	2.24	0.70
1:A:566:LEU:HD22	1:A:815:LEU:HD22	1.71	0.70
1:B:1552:ARG:O	1:B:1555:GLN:NE2	2.25	0.70
1:B:316:ARG:HH12	1:B:320:LEU:HD13	1.57	0.70
1:A:440:GLN:HG3	1:A:833:LEU:CD2	2.21	0.69
1:A:36:ASP:OD2	1:A:38:ARG:NE	2.26	0.69
1:B:569:CYS:SG	1:B:814:ALA:HB1	2.33	0.69
1:B:622:ALA:HA	1:B:650:THR:HA	1.74	0.69
1:B:1457:VAL:HG21	1:B:1471:CYS:HB3	1.75	0.69
1:B:654:PRO:HG3	1:B:686:PHE:CZ	2.27	0.69
1:A:1571:LEU:O	1:A:1843:MET:HE1	1.93	0.69
1:B:757:VAL:HG13	1:B:782:ILE:HD12	1.75	0.69
1:B:1349:ARG:NH2	1:B:1371:ILE:HG23	2.06	0.69
1:A:639:VAL:HB	1:A:640:PRO:HD2	1.75	0.69
1:A:1010:GLU:OE2	1:A:1019:ARG:NH2	2.26	0.69
1:B:79:LEU:HD21	1:B:143:ARG:HG3	1.75	0.69
1:B:2042:GLU:OE2	1:B:2059:GLN:NE2	2.25	0.69
1:A:538:LEU:HD23	1:A:546:PHE:HZ	1.59	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:776:LYS:H	1:A:776:LYS:HD2	1.56	0.68
1:B:524:ASP:OD1	1:B:534:VAL:HB	1.91	0.68
1:B:721:GLN:OE1	1:B:721:GLN:N	2.26	0.68
1:A:527:VAL:HG13	1:A:600:VAL:HG12	1.74	0.68
1:A:725:SER:HA	1:A:728:ARG:NH1	2.08	0.68
1:B:1300:ALA:O	1:B:1331:ASN:ND2	2.27	0.68
1:B:476:GLU:OE2	1:B:790:ARG:NH1	2.25	0.68
1:B:574:PRO:HG2	1:B:577:ILE:HD11	1.74	0.68
1:A:1827:LYS:NZ	1:A:1849:ILE:O	2.24	0.68
1:B:719:GLU:HA	1:B:722:TRP:CD1	2.28	0.68
1:A:697:GLU:O	1:A:701:VAL:HG23	1.93	0.68
1:B:261:VAL:HG13	1:B:262:THR:HG23	1.76	0.68
1:B:708:ARG:NH2	1:B:714:SER:HB2	2.09	0.68
1:B:2006:THR:CG2	1:B:2013:LEU:HD13	2.24	0.68
1:A:1457:VAL:HG11	1:A:1471:CYS:HB2	1.76	0.67
1:B:1177:GLU:N	1:B:1177:GLU:OE1	2.27	0.67
1:A:274:ARG:HA	1:A:277:TYR:CE2	2.30	0.67
1:B:274:ARG:HA	1:B:277:TYR:CE2	2.29	0.67
1:A:783:PRO:HB2	1:A:795:PHE:CE2	2.30	0.67
1:A:606:ARG:O	1:A:610:ILE:HG13	1.94	0.67
1:A:161:CYS:HB2	1:A:394:GLY:HA2	1.75	0.67
1:A:596:GLN:O	1:A:600:VAL:HG23	1.94	0.67
1:B:645:SER:HA	1:B:746:GLN:NE2	2.10	0.67
1:B:697:GLU:O	1:B:701:VAL:HG23	1.95	0.67
1:A:657:PRO:O	1:A:660:GLU:HG2	1.95	0.66
1:A:908:GLU:OE1	1:A:908:GLU:N	2.28	0.66
1:A:708:ARG:HG2	1:A:709:SER:N	2.11	0.66
1:A:831:SER:OG	1:A:832:PRO:HD3	1.95	0.66
1:A:165:LEU:CG	1:A:337:GLY:HA3	2.24	0.66
1:A:657:PRO:HA	1:A:660:GLU:HG2	1.75	0.66
1:B:47:LEU:HD21	1:B:198:VAL:CG2	2.25	0.66
1:A:138:ALA:CB	1:B:160:ALA:HB2	2.26	0.66
1:A:365:GLU:O	1:A:367:PRO:HD3	1.96	0.66
1:A:784:LEU:O	1:A:785:MET:HG3	1.96	0.66
1:A:763:PRO:HA	1:A:785:MET:HE2	1.77	0.66
1:A:635:PRO:HD3	1:A:661:PHE:CD1	2.30	0.66
1:A:285:GLU:OE1	1:A:285:GLU:N	2.27	0.66
1:A:619:ALA:HB3	1:A:655:GLN:HA	1.77	0.66
1:A:708:ARG:HG2	1:A:709:SER:H	1.60	0.66
1:A:706:LYS:O	1:A:729:THR:OG1	2.09	0.66
1:A:1942:SER:O	1:A:1943:THR:OG1	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:620:MET:CG	1:B:652:SER:HB3	2.21	0.66
1:B:655:GLN:O	1:B:658:VAL:HG12	1.96	0.66
1:A:460:VAL:HG13	1:A:461:PRO:HD2	1.78	0.66
1:A:542:ASP:OD2	1:A:544:SER:OG	2.13	0.65
1:A:64:PHE:HE1	1:A:464:ALA:HB1	1.61	0.65
1:A:665:LEU:HB3	1:A:670:VAL:CG2	2.27	0.65
1:B:1496:VAL:CG1	1:B:1504:ASN:HD22	2.09	0.65
1:B:625:LEU:CD2	1:B:670:VAL:HG11	2.26	0.65
1:A:14:PRO:O	1:A:32:MET:HE2	1.94	0.65
1:B:112:SER:C	1:B:137:ARG:HH12	2.04	0.65
1:B:635:PRO:HD2	1:B:638:VAL:HG11	1.78	0.65
1:A:165:LEU:CD1	1:A:392:SER:CB	2.64	0.65
1:A:1410:ASP:OD1	1:A:1411:SER:N	2.29	0.65
1:B:737:ASN:HA	1:B:740:VAL:HG22	1.77	0.65
1:A:621:ALA:HB2	1:A:674:GLU:HG2	1.78	0.65
1:B:639:VAL:HG13	1:B:640:PRO:HD2	1.78	0.65
1:B:65:PHE:HA	1:B:147:PHE:CE1	2.31	0.65
1:B:274:ARG:HA	1:B:277:TYR:CD2	2.31	0.65
1:B:737:ASN:HA	1:B:740:VAL:CG2	2.27	0.65
1:A:84:GLU:O	1:A:88:GLU:HG3	1.97	0.64
1:A:1176:GLN:N	1:A:1176:GLN:OE1	2.29	0.64
1:A:803:LEU:CD1	1:A:808:ILE:HD12	2.23	0.64
1:B:9:MET:HG2	1:B:19:LEU:HD11	1.79	0.64
1:B:581:SER:CA	1:B:738:ASN:HD21	2.07	0.64
1:B:591:ASP:OD2	1:B:712:TRP:HB2	1.97	0.64
1:B:440:GLN:HG3	1:B:833:LEU:HD22	1.79	0.64
1:B:548:ASP:OD1	1:B:550:VAL:HG12	1.96	0.64
1:B:1205:GLU:O	1:B:1209:LEU:N	2.30	0.64
1:A:523:SER:O	1:A:527:VAL:HG22	1.97	0.64
1:A:666:ARG:HH21	1:A:672:ALA:HB3	1.63	0.64
1:A:619:ALA:O	1:A:658:VAL:HG21	1.98	0.63
1:B:60:PHE:CD1	1:B:80:ARG:HB3	2.34	0.63
1:B:47:LEU:HD21	1:B:198:VAL:HG22	1.79	0.63
1:A:502:GLN:OE1	1:A:502:GLN:N	2.21	0.63
1:A:719:GLU:HA	1:A:722:TRP:CD1	2.33	0.63
1:B:782:ILE:O	1:B:782:ILE:CG2	2.44	0.63
1:A:267:ASP:O	1:A:271:GLN:HG3	1.99	0.63
1:B:113:GLY:N	1:B:137:ARG:HH12	1.97	0.63
1:B:597:GLU:O	1:B:601:LEU:HG	1.98	0.63
1:B:638:VAL:HG23	1:B:652:SER:O	1.99	0.63
1:A:645:SER:HA	1:A:746:GLN:HE21	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:SER:HB3	1:B:334:PRO:HG3	1.78	0.63
1:B:719:GLU:HA	1:B:722:TRP:CG	2.33	0.63
1:A:188:ILE:HG22	1:A:228:VAL:HG13	1.80	0.63
1:A:324:SER:H	1:A:356:ASN:HD21	1.47	0.63
1:A:468:ARG:HD3	1:A:804:HIS:CE1	2.33	0.63
1:A:664:GLN:NE2	1:A:668:GLU:OE2	2.32	0.63
1:B:625:LEU:HD21	1:B:670:VAL:HG11	1.80	0.63
1:B:1997:SER:O	1:B:2001:ASN:ND2	2.32	0.63
1:A:615:LEU:HB2	1:A:680:MET:HE1	1.80	0.63
1:B:622:ALA:N	1:B:673:LYS:O	2.29	0.63
1:B:25:ASN:HB2	1:B:32:MET:HE2	1.80	0.62
1:A:132:MET:HE2	1:B:200:PHE:CZ	2.34	0.62
1:A:161:CYS:HA	1:A:333:GLU:O	1.98	0.62
1:B:662:VAL:O	1:B:666:ARG:HG2	1.99	0.62
1:A:198:VAL:O	1:A:202:ARG:HG2	1.99	0.62
1:A:211:THR:HG22	1:A:213:LYS:HG3	1.81	0.62
1:A:305:LEU:HD12	1:A:366:ILE:HG12	1.80	0.62
1:B:768:GLN:OE1	1:B:781:ILE:HG21	1.99	0.62
1:A:290:ILE:HG23	1:A:322:ILE:HG13	1.80	0.62
1:B:168:LEU:CD2	1:B:233:LEU:HD21	2.29	0.62
1:A:431:PRO:HG3	1:A:467:PHE:CE2	2.34	0.62
1:B:241:ARG:HH21	1:B:453:MET:HE1	1.64	0.62
1:B:745:PHE:HE1	1:B:749:LEU:HD21	1.64	0.62
1:B:2088:MET:HE3	1:B:2091:CYS:HB2	1.81	0.62
1:A:217:THR:HG22	1:A:364:PRO:CD	2.29	0.62
1:A:276:LEU:HD12	1:A:401:HIS:HB3	1.80	0.62
1:B:581:SER:HB3	1:B:683:HIS:HE2	1.65	0.62
1:B:757:VAL:CG1	1:B:782:ILE:HD12	2.29	0.62
1:B:1496:VAL:HG13	1:B:1504:ASN:HD22	1.64	0.62
1:A:468:ARG:HD2	1:A:485:VAL:HG21	1.82	0.62
1:B:191:LEU:C	1:B:192:LEU:HD12	2.25	0.62
1:B:1250:GLY:O	1:B:1316:ASN:ND2	2.33	0.62
1:B:2006:THR:HG23	1:B:2013:LEU:HD13	1.81	0.62
1:B:1837:GLU:N	1:B:1837:GLU:OE1	2.29	0.62
1:B:704:GLU:OE1	1:B:704:GLU:N	2.33	0.61
1:B:25:ASN:CB	1:B:32:MET:HE2	2.31	0.61
1:B:114:SER:OG	1:B:117:SER:OG	2.18	0.61
1:B:639:VAL:CG1	1:B:640:PRO:HD2	2.30	0.61
1:A:1243:VAL:HG12	1:A:1271:THR:CG2	2.30	0.61
1:A:1616:LEU:HD13	1:A:1650:VAL:HG22	1.83	0.61
1:B:622:ALA:HB3	1:B:673:LYS:HG3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:726:LEU:HD11	1:B:733:GLU:HB3	1.82	0.61
1:B:766:LEU:HD23	1:B:766:LEU:O	2.00	0.61
1:B:1373:SER:O	1:B:1376:ALA:N	2.34	0.61
1:A:549:ILE:HD12	1:A:550:VAL:N	2.16	0.61
1:A:767:LEU:O	1:A:771:LEU:HD13	2.00	0.61
1:A:138:ALA:HB3	1:B:160:ALA:HB2	1.81	0.61
1:A:733:GLU:OE1	1:A:733:GLU:N	2.25	0.61
1:A:155:ILE:HG22	1:A:157:LEU:HD12	1.82	0.61
1:A:759:LEU:HD22	1:A:784:LEU:CD1	2.31	0.61
1:B:608:GLN:O	1:B:612:GLU:HG3	2.00	0.60
1:B:1521:GLU:OE1	1:B:1521:GLU:N	2.32	0.60
1:A:203:LEU:HD12	1:B:132:MET:CE	2.30	0.60
1:A:945:GLU:OE2	1:A:947:SER:HB2	2.00	0.60
1:B:501:THR:OG1	1:B:763:PRO:HG2	2.00	0.60
1:A:325:THR:HB	1:A:343:LYS:HD3	1.82	0.60
1:B:460:VAL:CG2	1:B:461:PRO:HD2	2.31	0.60
1:B:641:ALA:HB3	1:B:650:THR:O	2.00	0.60
1:B:2033:ASN:OD1	1:B:2034:TYR:N	2.33	0.60
1:B:168:LEU:HD23	1:B:233:LEU:HD21	1.83	0.60
1:B:765:ALA:HB1	1:B:768:GLN:HE21	1.66	0.60
1:A:460:VAL:O	1:A:468:ARG:NH2	2.34	0.60
1:B:627:TRP:NE1	1:B:631:LYS:HE2	2.17	0.60
1:A:626:SER:H	1:A:629:GLU:CG	2.14	0.60
1:B:267:ASP:O	1:B:271:GLN:HG3	2.01	0.60
1:B:289:TYR:OH	1:B:323:GLY:HA3	2.02	0.60
1:B:1195:GLN:O	1:B:1199:ALA:N	2.32	0.60
1:A:606:ARG:HE	1:A:739:LEU:HD13	1.67	0.60
1:A:645:SER:OG	1:A:648:THR:OG1	2.17	0.60
1:A:2042:GLU:OE2	1:A:2059:GLN:NE2	2.35	0.60
1:B:764:HIS:CE1	1:B:787:LYS:HB2	2.37	0.60
1:A:673:LYS:HD2	1:A:674:GLU:H	1.67	0.60
1:A:706:LYS:HB3	1:A:707:PRO:HD2	1.84	0.60
1:A:1275:ARG:NH2	1:A:1321:ALA:O	2.34	0.60
1:B:499:MET:HE1	1:B:682:PHE:HD2	1.62	0.60
1:A:556:LEU:CD1	1:A:763:PRO:HG3	2.32	0.59
1:A:557:THR:O	1:A:561:ILE:HG13	2.02	0.59
1:A:159:THR:O	1:A:163:SER:HB3	2.01	0.59
1:A:736:VAL:O	1:A:740:VAL:HG22	2.02	0.59
1:A:1617:VAL:HG12	1:A:1628:LEU:HD13	1.84	0.59
1:B:305:LEU:HD22	1:B:366:ILE:CD1	2.32	0.59
1:B:762:ALA:HB1	1:B:763:PRO:HD2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:THR:CG2	1:B:163:SER:HA	2.33	0.59
1:B:622:ALA:HB3	1:B:673:LYS:CG	2.33	0.59
1:A:539:LEU:HD23	1:A:539:LEU:O	2.02	0.59
1:B:506:MET:HE2	1:B:546:PHE:CZ	2.37	0.59
1:B:736:VAL:O	1:B:740:VAL:HG22	2.03	0.59
1:A:1909:VAL:HG12	1:A:1911:LYS:H	1.67	0.59
1:B:216:ASP:OD1	1:B:217:THR:N	2.36	0.59
1:A:687:MET:CE	1:A:690:ILE:HD12	2.33	0.59
1:A:695:LEU:HD12	1:A:696:GLN:N	2.17	0.59
1:B:495:ILE:CD1	1:B:578:VAL:HB	2.32	0.59
1:B:617:PRO:HB2	1:B:655:GLN:OE1	2.02	0.59
1:A:112:SER:C	1:A:137:ARG:HH12	2.11	0.59
1:A:305:LEU:CD1	1:A:366:ILE:HG12	2.33	0.59
1:B:689:ALA:O	1:B:692:PRO:HD2	2.03	0.59
1:A:291:GLU:HG2	1:A:340:ALA:HB1	1.83	0.59
1:A:1574:ARG:HD2	1:A:1588:ILE:HD12	1.84	0.59
1:A:87:TYR:O	1:A:91:VAL:HG22	2.03	0.58
1:B:264:PRO:HG3	1:B:300:GLY:HA2	1.85	0.58
1:B:440:GLN:HG3	1:B:833:LEU:CD2	2.33	0.58
1:B:674:GLU:N	1:B:674:GLU:OE1	2.36	0.58
1:B:767:LEU:O	1:B:771:LEU:HD13	2.03	0.58
1:A:646:LYS:HG3	1:A:647:ASP:OD1	2.02	0.58
1:B:703:ARG:HB2	1:B:704:GLU:OE1	2.03	0.58
1:A:276:LEU:CD1	1:A:401:HIS:HB3	2.32	0.58
1:A:1446:ILE:HG21	1:A:1486:VAL:HG21	1.85	0.58
1:B:290:ILE:HD12	1:B:389:GLY:O	2.03	0.58
1:B:717:ILE:CG2	1:B:721:GLN:HB2	2.33	0.58
1:B:1014:GLU:N	1:B:1014:GLU:OE1	2.36	0.58
1:A:64:PHE:CE1	1:A:464:ALA:HB1	2.38	0.58
1:A:506:MET:HG2	1:A:546:PHE:HE2	1.68	0.58
1:B:1680:VAL:HG23	2:B:2601:NDP:O1N	2.02	0.58
1:A:1411:SER:OG	1:A:1439:ARG:NH2	2.36	0.58
1:B:948:GLU:OE2	1:B:949:ASN:ND2	2.36	0.58
1:A:305:LEU:CD2	1:A:322:ILE:CD1	2.81	0.58
1:A:658:VAL:O	1:A:662:VAL:HG23	2.03	0.58
1:A:1125:GLU:N	1:A:1125:GLU:OE1	2.37	0.58
1:A:168:LEU:HD22	1:A:402:ILE:CD1	2.34	0.58
1:B:79:LEU:O	1:B:83:LEU:HD13	2.04	0.58
1:B:576:GLY:C	1:B:577:ILE:HD12	2.29	0.58
1:A:1970:ASN:C	1:A:1971:LEU:HD12	2.28	0.57
1:B:764:HIS:ND1	1:B:787:LYS:HB2	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:ALA:O	1:B:394:GLY:HA3	2.04	0.57
1:A:595:SER:HB3	1:A:598:GLU:HG3	1.86	0.57
1:A:1267:GLN:OE1	1:A:1267:GLN:N	2.36	0.57
1:B:290:ILE:HG23	1:B:322:ILE:CD1	2.32	0.57
1:B:351:GLY:C	1:B:352:LEU:HD12	2.29	0.57
1:B:1470:ARG:NE	1:B:1500:ASP:OD1	2.37	0.57
1:A:182:ALA:HB2	1:A:234:THR:HG22	1.87	0.57
1:A:184:ILE:HD11	1:A:232:LEU:HD13	1.86	0.57
1:A:492:LEU:HD22	1:A:808:ILE:HD13	1.87	0.57
1:B:347:SER:HB2	1:B:352:LEU:O	2.04	0.57
1:A:263:PHE:CE2	1:A:299:VAL:HG11	2.39	0.57
1:A:692:PRO:HD2	1:A:693:PRO:HD2	1.86	0.57
1:A:1488:PRO:HA	1:A:1493:LEU:HD23	1.86	0.57
1:B:456:ASP:OD1	1:B:813:ASN:ND2	2.37	0.57
1:B:534:VAL:O	1:B:538:LEU:HD13	2.05	0.57
1:B:615:LEU:HD12	1:B:615:LEU:O	2.04	0.57
1:B:1391:LEU:HD23	1:B:1392:LYS:N	2.20	0.57
1:A:1974:VAL:HG12	1:A:1994:PRO:HG3	1.86	0.57
1:B:1354:GLY:HA3	1:B:1371:ILE:HD11	1.85	0.57
1:A:6:ILE:HG23	1:A:231:VAL:CG1	2.35	0.57
1:A:654:PRO:HB2	1:A:657:PRO:CD	2.34	0.57
1:A:1860:GLU:N	1:A:1860:GLU:OE1	2.37	0.57
1:B:540:SER:OG	1:B:545:THR:HG21	2.05	0.57
1:A:527:VAL:CG1	1:A:600:VAL:HG12	2.35	0.57
1:B:460:VAL:HG11	1:B:465:MET:SD	2.45	0.57
1:B:972:PRO:HD2	1:B:1079:VAL:HG21	1.87	0.57
1:A:127:LEU:HD11	1:B:198:VAL:HG12	1.86	0.56
1:B:71:GLN:HE21	1:B:143:ARG:HH12	1.52	0.56
1:B:625:LEU:HB2	1:B:630:CYS:SG	2.45	0.56
1:B:793:LEU:O	1:B:797:LEU:HG	2.05	0.56
1:A:934:GLU:OE1	1:A:936:ARG:NH2	2.39	0.56
1:B:76:ASP:OD1	1:B:77:PRO:HD2	2.06	0.56
1:B:105:THR:O	1:B:150:PHE:HB3	2.06	0.56
1:B:596:GLN:O	1:B:600:VAL:HG23	2.06	0.56
1:B:627:TRP:HE1	1:B:631:LYS:HE2	1.70	0.56
1:B:704:GLU:HG2	1:B:704:GLU:O	2.04	0.56
1:B:732:ALA:O	1:B:736:VAL:HG23	2.05	0.56
1:B:1246:LEU:HD11	1:B:1299:PRO:HG3	1.86	0.56
1:A:492:LEU:HD13	1:A:808:ILE:CD1	2.35	0.56
1:A:584:GLU:HG3	1:A:712:TRP:HZ2	1.69	0.56
1:A:708:ARG:CZ	1:A:714:SER:HB2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:CYS:HA	1:A:316:ARG:HG2	1.87	0.56
1:B:159:THR:HG22	1:B:163:SER:HA	1.88	0.56
1:B:270:GLU:HG2	1:B:274:ARG:HH12	1.70	0.56
1:A:162:SER:OG	1:A:394:GLY:N	2.38	0.56
1:A:584:GLU:HG3	1:A:712:TRP:CZ2	2.41	0.56
1:A:1034:LEU:O	1:A:1037:SER:OG	2.16	0.56
1:B:112:SER:CB	1:B:334:PRO:HG3	2.35	0.56
1:B:555:SER:O	1:B:559:ILE:HG13	2.06	0.56
1:A:241:ARG:NH2	1:A:828:PRO:O	2.37	0.56
1:A:638:VAL:CG1	1:A:651:ILE:HD12	2.36	0.56
1:A:945:GLU:HG2	1:A:952:LEU:CD1	2.36	0.56
1:B:701:VAL:HG12	1:B:702:ILE:HD12	1.88	0.56
1:B:2018:VAL:HB	1:B:2041:MET:HE2	1.88	0.56
1:A:182:ALA:CB	1:A:234:THR:HG22	2.35	0.56
1:B:618:GLY:HA2	1:B:655:GLN:N	2.21	0.56
1:B:1141:CYS:O	1:B:1145:VAL:HG23	2.06	0.56
1:A:323:GLY:HA2	1:A:356:ASN:HD21	1.70	0.56
1:B:532:LEU:HD12	1:B:532:LEU:O	2.06	0.56
1:B:645:SER:HA	1:B:746:GLN:HE21	1.70	0.56
1:B:694:LEU:HD22	1:B:739:LEU:HD23	1.88	0.56
1:A:211:THR:CG2	1:A:213:LYS:HG3	2.36	0.55
1:B:277:TYR:CE1	1:B:284:PRO:HG3	2.41	0.55
1:B:502:GLN:OE1	1:B:552:SER:CB	2.48	0.55
1:B:557:THR:O	1:B:561:ILE:HG13	2.05	0.55
1:A:1278:GLN:OE1	1:A:1278:GLN:N	2.36	0.55
1:A:701:VAL:HG12	1:A:702:ILE:HD12	1.87	0.55
1:B:1242:VAL:HG13	1:B:1312:LEU:O	2.06	0.55
1:A:506:MET:HG3	1:A:506:MET:O	2.06	0.55
1:A:548:ASP:OD1	1:A:549:ILE:N	2.39	0.55
1:A:570:MET:HE3	1:A:815:LEU:HD21	1.88	0.55
1:A:620:MET:HB2	1:A:652:SER:OG	2.07	0.55
1:A:692:PRO:HA	1:A:695:LEU:CD2	2.36	0.55
1:B:690:ILE:HD12	1:B:690:ILE:H	1.71	0.55
1:A:253:THR:HG22	1:A:255:GLY:H	1.72	0.55
1:A:112:SER:CA	1:A:137:ARG:HH12	2.18	0.55
1:A:763:PRO:HA	1:A:785:MET:CE	2.37	0.55
1:B:508:LEU:CD2	1:B:539:LEU:HD23	2.36	0.55
1:B:621:ALA:C	1:B:650:THR:HG23	2.32	0.55
1:A:506:MET:HE2	1:A:546:PHE:CZ	2.41	0.55
1:A:542:ASP:O	1:A:545:THR:HG22	2.07	0.55
1:A:620:MET:HG3	1:A:651:ILE:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:663:GLU:O	1:B:667:LYS:HG3	2.06	0.55
1:A:654:PRO:HG3	1:A:686:PHE:CZ	2.38	0.55
1:B:659:PHE:O	1:B:663:GLU:HG3	2.07	0.55
1:B:164:SER:OG	1:B:335:ALA:HA	2.06	0.55
1:A:137:ARG:HD3	1:A:158:ASP:OD1	2.07	0.54
1:A:425:ARG:HG2	1:A:455:ASN:OD1	2.07	0.54
1:A:677:THR:HB	1:A:680:MET:O	2.07	0.54
1:A:1535:THR:HG23	1:A:1535:THR:O	2.07	0.54
1:B:252:ASN:ND2	1:B:268:ILE:HG22	2.22	0.54
1:B:504:ARG:NE	1:B:541:THR:O	2.28	0.54
1:B:527:VAL:HG12	1:B:527:VAL:O	2.07	0.54
1:B:1566:VAL:HG13	1:B:1603:PHE:HB2	1.88	0.54
1:B:1612:ARG:NH2	1:B:1640:TRP:O	2.40	0.54
1:A:305:LEU:CD2	1:A:322:ILE:HD13	2.37	0.54
1:A:1130:GLU:OE1	1:A:1130:GLU:N	2.38	0.54
1:A:25:ASN:O	1:A:30:VAL:HG12	2.07	0.54
1:A:661:PHE:O	1:A:665:LEU:HG	2.06	0.54
1:B:476:GLU:OE2	1:B:477:ARG:NH1	2.40	0.54
1:A:506:MET:HG2	1:A:546:PHE:CE2	2.42	0.54
1:B:477:ARG:NH1	1:B:790:ARG:HD2	2.20	0.54
1:B:493:TRP:CD2	1:B:576:GLY:HA3	2.42	0.54
1:A:570:MET:CE	1:A:815:LEU:HD11	2.37	0.54
1:B:606:ARG:O	1:B:610:ILE:HG13	2.07	0.54
1:A:36:ASP:OD1	1:A:53:LYS:HE3	2.06	0.54
1:A:889:THR:HB	1:A:1030:MET:HE3	1.89	0.54
1:B:717:ILE:HG23	1:B:718:PRO:HD2	1.90	0.54
1:B:749:LEU:HD22	1:B:775:LEU:CD2	2.32	0.54
1:A:620:MET:SD	1:A:652:SER:HB2	2.48	0.54
1:B:661:PHE:CE2	1:B:665:LEU:HD11	2.43	0.54
1:B:13:LEU:HD21	1:B:229:VAL:CG2	2.38	0.54
1:B:769:ALA:O	1:B:773:ARG:HG2	2.07	0.54
1:A:527:VAL:HG13	1:A:600:VAL:CG1	2.37	0.54
1:B:745:PHE:CE1	1:B:749:LEU:HD21	2.42	0.54
1:B:1071:ASP:OD1	1:B:1072:LYS:N	2.37	0.54
1:B:1889:ILE:HD11	1:B:1912:LEU:HD11	1.90	0.54
1:A:241:ARG:HD3	1:A:243:TYR:CE2	2.43	0.54
1:A:270:GLU:HG2	1:A:274:ARG:HH12	1.71	0.54
1:A:746:GLN:OE1	1:A:750:TRP:NE1	2.41	0.54
1:B:620:MET:HE1	1:B:682:PHE:HB2	1.90	0.54
1:B:1197:GLU:OE1	1:B:1197:GLU:N	2.39	0.54
1:A:781:ILE:N	1:A:781:ILE:HD12	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1457:VAL:HG23	1:A:1503:MET:HE1	1.90	0.53
1:A:1486:VAL:O	1:A:1493:LEU:HD22	2.08	0.53
1:B:1371:ILE:C	1:B:1372:LEU:HD12	2.33	0.53
1:A:469:GLY:HA2	1:A:805:LEU:HD21	1.91	0.53
1:A:544:SER:HA	1:A:547:ASP:HB2	1.91	0.53
1:A:621:ALA:CB	1:A:674:GLU:HA	2.38	0.53
1:A:627:TRP:CZ3	1:A:643:HIS:HB2	2.44	0.53
1:A:1274:ASP:OD1	1:A:1275:ARG:N	2.41	0.53
1:B:511:MET:HE1	1:B:520:ILE:CG2	2.30	0.53
1:A:68:HIS:CG	1:A:69:PRO:HD2	2.43	0.53
1:A:495:ILE:HD12	1:A:758:VAL:HG11	1.89	0.53
1:A:628:GLU:O	1:A:631:LYS:HG2	2.08	0.53
1:B:656:ALA:HB3	1:B:657:PRO:HD3	1.90	0.53
1:A:504:ARG:HD2	1:A:541:THR:O	2.08	0.53
1:B:224:ARG:NH1	1:B:333:GLU:OE2	2.42	0.53
1:B:629:GLU:O	1:B:633:ARG:HG2	2.08	0.53
1:B:1298:ASP:OD1	1:B:1299:PRO:CD	2.52	0.53
1:A:108:TRP:HD1	1:A:157:LEU:HD11	1.74	0.53
1:A:1349:ARG:HB2	1:A:1371:ILE:HG22	1.90	0.53
1:B:493:TRP:CE3	1:B:576:GLY:HA3	2.42	0.53
1:B:1214:LEU:HD12	1:B:1215:LEU:N	2.24	0.53
1:A:725:SER:HA	1:A:728:ARG:HH12	1.70	0.53
1:B:124:PRO:HA	1:B:127:LEU:HD23	1.90	0.53
1:B:2006:THR:HG21	1:B:2013:LEU:HD13	1.91	0.53
1:B:316:ARG:NH1	1:B:320:LEU:HD13	2.21	0.53
1:A:1725:ASP:OD1	1:A:1726:THR:N	2.39	0.52
1:A:641:ALA:HB3	1:A:650:THR:O	2.08	0.52
1:A:1020:LEU:HD22	1:A:1032:THR:HG22	1.91	0.52
1:B:9:MET:HG2	1:B:19:LEU:CD1	2.39	0.52
1:B:506:MET:HE2	1:B:546:PHE:CE2	2.44	0.52
1:A:68:HIS:HB3	1:A:71:GLN:OE1	2.10	0.52
1:A:261:VAL:HG23	1:A:262:THR:HG23	1.91	0.52
1:B:161:CYS:HB3	1:B:394:GLY:HA2	1.92	0.52
1:B:289:TYR:O	1:B:388:VAL:HG13	2.10	0.52
1:A:760:GLU:OE1	1:A:765:ALA:HB1	2.10	0.52
1:A:945:GLU:HG2	1:A:952:LEU:HD13	1.91	0.52
1:B:259:GLN:OE1	1:B:259:GLN:N	2.39	0.52
1:A:623:VAL:N	1:A:649:VAL:O	2.37	0.52
1:A:623:VAL:CG1	1:A:665:LEU:HD13	2.40	0.52
1:B:694:LEU:O	1:B:698:LEU:HG	2.10	0.52
1:B:1445:ALA:C	1:B:1446:ILE:HD13	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1445:ALA:O	1:B:1446:ILE:HD13	2.09	0.52
1:A:211:THR:HB	1:A:213:LYS:NZ	2.25	0.52
1:A:1344:LEU:HD21	1:A:1377:TRP:CH2	2.45	0.52
1:A:1570:SER:OG	1:A:1646:ALA:O	2.27	0.52
1:A:324:SER:H	1:A:356:ASN:ND2	2.06	0.52
1:A:717:ILE:HD11	1:A:726:LEU:HB3	1.91	0.52
1:A:1336:LEU:HD11	1:A:1340:GLY:HA3	1.91	0.52
1:A:1430:GLY:O	1:A:1433:ALA:N	2.42	0.52
1:A:290:ILE:CG2	1:A:322:ILE:HG13	2.40	0.52
1:A:617:PRO:HB2	1:A:655:GLN:CD	2.35	0.52
1:B:1190:LEU:O	1:B:1195:GLN:NE2	2.43	0.52
1:B:1366:GLN:O	1:B:1369:GLN:N	2.43	0.52
1:B:78:GLN:OE1	1:B:190:VAL:HG22	2.10	0.52
1:B:623:VAL:HG13	1:B:665:LEU:HD13	1.90	0.52
1:B:768:GLN:CD	1:B:781:ILE:HG21	2.35	0.52
1:B:768:GLN:NE2	1:B:783:PRO:HB3	2.25	0.52
1:A:368:ALA:HA	1:A:371:ASP:OD2	2.10	0.51
1:A:638:VAL:HG11	1:A:651:ILE:HD12	1.92	0.51
1:B:5:VAL:HB	1:B:242:VAL:HG13	1.92	0.51
1:B:692:PRO:HB2	1:B:693:PRO:CD	2.40	0.51
1:A:168:LEU:HD23	1:A:168:LEU:O	2.09	0.51
1:A:627:TRP:CZ3	1:A:640:PRO:HB2	2.45	0.51
1:B:269:GLN:O	1:B:273:ILE:HG13	2.10	0.51
1:A:120:LEU:HD12	1:A:135:CYS:SG	2.51	0.51
1:B:351:GLY:O	1:B:352:LEU:HD12	2.11	0.51
1:B:466:PRO:HG2	1:B:467:PHE:CD1	2.45	0.51
1:A:1212:ASP:OD1	1:A:1214:LEU:N	2.43	0.51
1:A:2034:TYR:O	1:A:2038:ASN:ND2	2.40	0.51
1:B:333:GLU:CB	1:B:334:PRO:HD3	2.35	0.51
1:B:627:TRP:CZ3	1:B:643:HIS:HB2	2.45	0.51
1:A:708:ARG:NH1	1:A:714:SER:HB2	2.26	0.51
1:A:1483:VAL:O	1:A:1483:VAL:HG13	2.11	0.51
1:B:301:ASP:HB2	1:B:302:PRO:HD3	1.93	0.51
1:A:205:MET:HE1	1:A:395:PHE:CD2	2.45	0.51
1:A:631:LYS:HG3	1:A:632:GLN:OE1	2.10	0.51
1:A:627:TRP:CE3	1:A:643:HIS:HB2	2.45	0.51
1:A:698:LEU:HB2	1:A:732:ALA:HB1	1.92	0.51
1:A:1145:VAL:HG21	1:A:1356:ILE:HG12	1.92	0.51
1:A:1913:VAL:C	1:A:1914:LEU:HD12	2.36	0.51
1:A:627:TRP:CH2	1:A:640:PRO:HB2	2.46	0.51
1:A:661:PHE:CE2	1:A:665:LEU:HD11	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:ARG:NH2	1:B:453:MET:HE1	2.26	0.51
1:B:521:LEU:O	1:B:525:GLU:HG2	2.11	0.51
1:A:168:LEU:HD22	1:A:402:ILE:HD11	1.91	0.51
1:A:772:LYS:NZ	1:A:781:ILE:HD13	2.26	0.51
1:A:772:LYS:NZ	1:A:781:ILE:HB	2.26	0.51
1:A:820:GLU:OE1	1:A:820:GLU:N	2.39	0.51
1:B:264:PRO:CG	1:B:300:GLY:HA2	2.41	0.51
1:B:265:SER:O	1:B:269:GLN:HG3	2.10	0.51
1:B:754:GLU:HG3	1:B:755:HIS:CD2	2.46	0.51
1:B:1206:ARG:NH1	1:B:1209:LEU:HD13	2.26	0.51
1:A:54:LEU:HD12	1:A:57:LEU:CD2	2.39	0.51
1:A:241:ARG:HH21	1:A:827:THR:HG22	1.76	0.51
1:A:620:MET:HE2	1:A:677:THR:HG22	1.93	0.51
1:A:692:PRO:CD	1:A:693:PRO:HD2	2.40	0.51
1:A:990:VAL:HG13	1:A:1039:LEU:HD12	1.93	0.51
1:A:1602:GLU:HB3	1:A:1650:VAL:HG23	1.92	0.51
1:B:60:PHE:CE2	1:B:62:ALA:HA	2.45	0.51
1:B:1487:ASP:O	1:B:1490:SER:OG	2.27	0.51
1:A:1453:VAL:CG2	1:A:1471:CYS:SG	2.99	0.50
1:B:108:TRP:HB3	1:B:167:ALA:HB1	1.92	0.50
1:A:1134:LEU:HD12	1:A:1214:LEU:HD23	1.92	0.50
1:A:1893:LEU:HD12	1:A:1916:SER:OG	2.10	0.50
1:B:1127:CYS:C	1:B:1128:LEU:HD12	2.35	0.50
1:A:241:ARG:NH2	1:A:827:THR:HG22	2.26	0.50
1:B:1349:ARG:NH2	1:B:1371:ILE:O	2.43	0.50
1:A:772:LYS:HZ2	1:A:781:ILE:HB	1.76	0.50
1:B:243:TYR:HB3	1:B:345:LEU:HD22	1.94	0.50
1:B:690:ILE:HD12	1:B:690:ILE:N	2.26	0.50
1:A:293:HIS:CD2	1:A:295:THR:HG23	2.47	0.50
1:A:693:PRO:O	1:A:697:GLU:HG2	2.11	0.50
1:A:14:PRO:CD	1:A:329:MET:HE3	2.38	0.50
1:A:512:ARG:HH22	1:A:791:ASP:CG	2.19	0.50
1:A:627:TRP:HA	1:A:630:CYS:SG	2.51	0.50
1:A:673:LYS:HE3	1:A:674:GLU:O	2.11	0.50
1:B:193:LYS:HG2	1:B:195:ASN:HD22	1.77	0.50
1:B:635:PRO:O	1:B:638:VAL:HG12	2.11	0.50
1:B:658:VAL:O	1:B:662:VAL:HG23	2.11	0.50
1:B:771:LEU:HB3	1:B:781:ILE:HD11	1.94	0.50
1:B:2003:ASP:OD1	1:B:2048:ARG:NH1	2.40	0.50
1:A:9:MET:HG2	1:A:19:LEU:HD11	1.93	0.50
1:A:200:PHE:HB3	1:A:206:LEU:HG	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:LEU:HB3	1:B:14:PRO:HD2	1.94	0.50
1:B:292:ALA:HB2	1:B:322:ILE:HD11	1.94	0.50
1:B:656:ALA:O	1:B:660:GLU:HG3	2.11	0.50
1:B:694:LEU:CD2	1:B:739:LEU:HD23	2.42	0.50
1:B:1896:PHE:CZ	1:B:2088:MET:HE1	2.47	0.50
1:A:776:LYS:HD2	1:A:776:LYS:N	2.24	0.50
1:A:184:ILE:CD1	1:A:232:LEU:HD13	2.42	0.50
1:A:269:GLN:O	1:A:273:ILE:HG13	2.11	0.50
1:A:1432:LEU:HD22	1:A:1980:LEU:HD23	1.94	0.50
1:A:1899:GLU:CB	1:A:2088:MET:HE2	2.42	0.50
1:B:431:PRO:HG3	1:B:467:PHE:CE2	2.46	0.50
1:A:56:ASP:OD1	1:A:57:LEU:N	2.45	0.49
1:A:521:LEU:O	1:A:525:GLU:HG2	2.11	0.49
1:A:654:PRO:O	1:A:658:VAL:HG23	2.12	0.49
1:A:1974:VAL:O	1:A:1974:VAL:HG13	2.11	0.49
1:B:426:ALA:HB3	1:B:434:VAL:HG13	1.94	0.49
1:B:431:PRO:HG3	1:B:467:PHE:CD2	2.46	0.49
1:A:9:MET:SD	1:A:345:LEU:HD12	2.52	0.49
1:A:1134:LEU:CD1	1:A:1214:LEU:HD23	2.42	0.49
1:A:1893:LEU:HD12	1:A:1916:SER:CB	2.42	0.49
1:B:115:GLU:OE1	1:B:192:LEU:HB2	2.13	0.49
1:B:692:PRO:HB2	1:B:693:PRO:HD3	1.95	0.49
1:B:740:VAL:HG23	1:B:741:SER:N	2.27	0.49
1:A:803:LEU:HD11	1:A:808:ILE:CD1	2.29	0.49
1:A:1327:SER:O	1:A:1331:ASN:ND2	2.40	0.49
1:A:1453:VAL:HG22	1:A:1471:CYS:SG	2.51	0.49
1:B:726:LEU:HD13	1:B:733:GLU:OE1	2.13	0.49
1:B:768:GLN:OE1	1:B:781:ILE:CG2	2.60	0.49
1:B:786:LYS:HZ2	1:B:789:HIS:HB2	1.76	0.49
1:B:1021:LEU:HD12	1:B:1074:GLN:O	2.12	0.49
1:A:550:VAL:O	1:A:554:VAL:HG23	2.12	0.49
1:A:702:ILE:HD12	1:A:702:ILE:N	2.28	0.49
1:A:1020:LEU:HD22	1:A:1032:THR:CG2	2.42	0.49
1:B:550:VAL:HG13	1:B:551:HIS:HD2	1.77	0.49
1:B:584:GLU:HA	1:B:587:CYS:HB2	1.94	0.49
1:B:670:VAL:HG12	1:B:671:PHE:N	2.27	0.49
1:B:694:LEU:HD11	1:B:698:LEU:HD11	1.94	0.49
1:B:1245:VAL:C	1:B:1246:LEU:HD12	2.38	0.49
1:B:1562:GLN:NE2	1:B:1607:ASP:OD1	2.45	0.49
1:B:469:GLY:HA2	1:B:805:LEU:HD21	1.93	0.49
1:B:547:ASP:OD1	1:B:548:ASP:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:MET:CE	1:A:739:LEU:HD11	2.36	0.49
1:A:689:ALA:O	1:A:692:PRO:HD2	2.13	0.49
1:B:105:THR:OG1	1:B:182:ALA:HB3	2.13	0.49
1:A:305:LEU:HD22	1:A:322:ILE:HD13	1.95	0.49
1:A:250:GLY:HA3	1:A:276:LEU:HD21	1.95	0.49
1:A:366:ILE:HD12	1:A:366:ILE:N	2.28	0.49
1:B:82:LEU:HD13	1:B:188:ILE:CG2	2.42	0.49
1:B:771:LEU:HB3	1:B:781:ILE:CD1	2.43	0.49
1:B:1596:ASP:O	1:B:1597:SER:OG	2.29	0.49
1:A:1312:LEU:C	1:A:1313:LEU:HD12	2.38	0.49
1:B:65:PHE:HA	1:B:147:PHE:HE1	1.75	0.49
1:B:564:ILE:HG12	1:B:761:ILE:HD13	1.95	0.49
1:B:635:PRO:HD3	1:B:661:PHE:CD1	2.48	0.49
1:B:706:LYS:O	1:B:729:THR:OG1	2.20	0.49
1:B:759:LEU:CD2	1:B:782:ILE:CG2	2.91	0.49
1:A:293:HIS:O	1:A:326:LYS:HD2	2.13	0.48
1:A:767:LEU:HB3	1:A:771:LEU:HD13	1.95	0.48
1:A:1670:THR:C	1:A:1671:LEU:HD12	2.38	0.48
1:A:340:ALA:O	1:A:344:VAL:HG23	2.13	0.48
1:B:166:MET:SD	1:B:251:THR:HG21	2.53	0.48
1:B:231:VAL:HG12	1:B:233:LEU:HD12	1.96	0.48
1:B:499:MET:SD	1:B:682:PHE:CD2	3.06	0.48
1:A:991:TYR:CZ	1:A:1006:GLN:HA	2.48	0.48
1:B:515:ARG:HB2	1:B:566:LEU:HD23	1.95	0.48
1:B:14:PRO:HG2	1:B:329:MET:HE3	1.95	0.48
1:B:391:ASN:HB2	1:B:393:PHE:CZ	2.47	0.48
1:B:508:LEU:HD21	1:B:539:LEU:HD23	1.95	0.48
1:B:754:GLU:HA	1:B:776:LYS:HE2	1.96	0.48
1:A:115:GLU:OE1	1:A:192:LEU:HB2	2.13	0.48
1:A:168:LEU:HD23	1:A:168:LEU:C	2.38	0.48
1:A:341:LEU:O	1:A:345:LEU:HG	2.13	0.48
1:B:64:PHE:HE1	1:B:464:ALA:HB1	1.79	0.48
1:B:515:ARG:HB2	1:B:566:LEU:CD2	2.43	0.48
1:B:1317:CYS:N	1:B:1345:HIS:O	2.47	0.48
1:A:1310:ALA:O	1:A:1336:LEU:HD12	2.13	0.48
1:A:1466:GLY:HA2	1:A:1469:LEU:HD23	1.96	0.48
1:B:619:ALA:O	1:B:658:VAL:HG21	2.13	0.48
1:A:235:LYS:CG	1:A:238:LEU:HD13	2.43	0.48
1:A:1790:THR:HG23	1:B:1792:HIS:CE1	2.49	0.48
1:B:158:ASP:O	1:B:159:THR:HG22	2.14	0.48
1:B:254:ASP:HB3	1:B:257:LYS:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:ASN:HA	1:B:400:VAL:O	2.14	0.48
1:B:644:ASN:HB2	1:B:648:THR:OG1	2.14	0.48
1:A:891:TYR:OH	1:A:923:THR:HG22	2.13	0.48
1:B:617:PRO:HB2	1:B:655:GLN:CD	2.39	0.48
1:B:621:ALA:O	1:B:651:ILE:N	2.46	0.48
1:A:290:ILE:HD12	1:A:389:GLY:HA3	1.96	0.48
1:A:549:ILE:CD1	1:A:611:LYS:HG3	2.40	0.48
1:B:74:THR:HG21	1:B:130:TYR:CE1	2.49	0.48
1:A:35:ASP:OD1	1:A:49:ARG:HB3	2.14	0.47
1:B:754:GLU:OE1	1:B:776:LYS:HE2	2.12	0.47
1:A:121:SER:HB3	1:B:199:GLN:NE2	2.29	0.47
1:A:1899:GLU:HB3	1:A:2088:MET:HE2	1.95	0.47
1:B:111:VAL:HG23	1:B:188:ILE:HG13	1.96	0.47
1:B:503:TRP:HB3	1:B:787:LYS:NZ	2.29	0.47
1:B:1677:SER:O	1:B:1682:GLN:NE2	2.44	0.47
1:A:57:LEU:CD2	1:A:81:LEU:HD11	2.44	0.47
1:A:119:ALA:O	1:A:122:ARG:NH1	2.47	0.47
1:B:51:SER:O	1:B:53:LYS:NZ	2.43	0.47
1:B:501:THR:OG1	1:B:764:HIS:HB3	2.14	0.47
1:B:764:HIS:CE1	1:B:787:LYS:CB	2.97	0.47
1:A:57:LEU:HD22	1:A:81:LEU:HD11	1.96	0.47
1:A:1246:LEU:HD11	1:A:1299:PRO:HG2	1.97	0.47
1:B:14:PRO:CD	1:B:329:MET:HE3	2.44	0.47
1:B:288:GLU:O	1:B:288:GLU:HG2	2.14	0.47
1:B:615:LEU:HD11	1:B:680:MET:CE	2.44	0.47
1:B:899:LEU:HD22	1:B:958:VAL:HG22	1.94	0.47
1:B:1125:GLU:N	1:B:1125:GLU:OE1	2.47	0.47
1:B:2042:GLU:OE1	1:B:2043:ARG:NH2	2.47	0.47
1:B:513:LEU:HD11	1:B:793:LEU:HD11	1.96	0.47
1:B:567:LEU:HA	1:B:570:MET:HE2	1.96	0.47
1:B:621:ALA:O	1:B:650:THR:HG23	2.14	0.47
1:A:131:SER:OG	1:B:199:GLN:NE2	2.47	0.47
1:A:213:LYS:HE2	1:A:218:ALA:O	2.14	0.47
1:A:277:TYR:CE1	1:A:284:PRO:HG3	2.50	0.47
1:A:442:LEU:HD23	1:A:442:LEU:C	2.39	0.47
1:A:1214:LEU:O	1:A:1396:TYR:OH	2.16	0.47
1:B:90:ILE:HA	1:B:232:LEU:HD22	1.97	0.47
1:B:235:LYS:HE3	1:B:238:LEU:CD1	2.45	0.47
1:B:880:LEU:HD12	1:B:880:LEU:N	2.30	0.47
1:A:717:ILE:CG2	1:A:721:GLN:HB2	2.44	0.47
1:B:113:GLY:HA2	1:B:137:ARG:HH22	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:ASP:O	1:B:163:SER:HB3	2.14	0.47
1:B:615:LEU:HD11	1:B:680:MET:HE1	1.96	0.47
1:B:1228:LEU:HD21	1:B:1256:ILE:HG23	1.97	0.47
1:A:1245:VAL:C	1:A:1246:LEU:HD12	2.39	0.47
1:B:333:GLU:OE1	1:B:333:GLU:N	2.44	0.47
1:B:759:LEU:HD21	1:B:803:LEU:HD13	1.97	0.47
1:A:155:ILE:N	1:A:155:ILE:HD12	2.30	0.47
1:A:508:LEU:HD11	1:A:538:LEU:O	2.15	0.47
1:A:1446:ILE:HD12	1:A:1447:ASN:N	2.29	0.47
1:B:291:GLU:HG2	1:B:340:ALA:HB1	1.97	0.47
1:B:577:ILE:HD12	1:B:577:ILE:N	2.30	0.47
1:A:642:CYS:SG	1:A:743:VAL:HG21	2.54	0.46
1:B:155:ILE:HG22	1:B:157:LEU:HD12	1.97	0.46
1:B:283:ALA:HB1	1:B:285:GLU:OE1	2.15	0.46
1:B:1205:GLU:OE1	1:B:1209:LEU:HD12	2.15	0.46
1:B:1497:LEU:HD12	1:B:1497:LEU:C	2.40	0.46
1:A:1346:THR:HG22	1:A:1347:LEU:N	2.30	0.46
1:A:1753:LEU:C	1:A:1753:LEU:HD23	2.39	0.46
1:B:5:VAL:HG22	1:B:234:THR:O	2.15	0.46
1:A:203:LEU:HD23	1:A:203:LEU:HA	1.79	0.46
1:A:570:MET:HE2	1:A:815:LEU:CD1	2.44	0.46
1:A:694:LEU:CD2	1:A:698:LEU:HG	2.44	0.46
1:A:1716:ASP:OD1	1:A:1717:SER:N	2.43	0.46
1:B:93:GLY:O	1:B:240:ARG:HB2	2.15	0.46
1:B:133:VAL:O	1:B:139:MET:HG3	2.16	0.46
1:B:453:MET:O	1:B:457:ILE:HG23	2.16	0.46
1:B:504:ARG:HH21	1:B:541:THR:HB	1.80	0.46
1:B:1111:VAL:O	1:B:1111:VAL:HG13	2.15	0.46
1:B:1333:VAL:HG12	1:B:1386:LEU:HD11	1.96	0.46
1:B:1366:GLN:O	1:B:1370:GLY:N	2.46	0.46
1:A:127:LEU:C	1:A:127:LEU:HD12	2.41	0.46
1:A:459:ALA:HB1	1:A:809:ASP:OD2	2.15	0.46
1:A:543:GLU:OE1	1:A:543:GLU:N	2.43	0.46
1:B:242:VAL:HG23	1:B:822:PRO:HB3	1.97	0.46
1:B:1485:GLU:OE1	1:B:1485:GLU:N	2.42	0.46
1:A:626:SER:CB	1:A:629:GLU:HG2	2.40	0.46
1:A:692:PRO:N	1:A:693:PRO:HD2	2.31	0.46
1:A:620:MET:HB2	1:A:652:SER:CB	2.45	0.46
1:A:663:GLU:O	1:A:667:LYS:HG2	2.16	0.46
1:B:627:TRP:CH2	1:B:640:PRO:HB2	2.51	0.46
1:B:717:ILE:HG22	1:B:721:GLN:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:ASP:OD2	1:A:709:SER:HB3	2.16	0.46
1:B:51:SER:HA	1:B:223:CYS:SG	2.56	0.46
1:B:87:TYR:CE1	1:B:97:PRO:HG2	2.50	0.46
1:B:249:ALA:CB	1:B:402:ILE:HG22	2.46	0.46
1:B:1970:ASN:C	1:B:1971:LEU:HD12	2.41	0.46
1:A:235:LYS:HG3	1:A:238:LEU:HD13	1.98	0.46
1:A:325:THR:CB	1:A:343:LYS:HD3	2.46	0.46
1:A:396:GLY:HA3	1:B:142:ASN:ND2	2.22	0.46
1:B:189:ASN:HB2	1:B:334:PRO:HD2	1.97	0.46
1:B:409:GLN:HB3	1:B:824:PRO:HA	1.97	0.46
1:B:620:MET:CB	1:B:652:SER:HB3	2.46	0.46
1:B:879:THR:C	1:B:880:LEU:HD12	2.40	0.46
1:B:1297:TRP:NE1	1:B:1301:ASP:O	2.35	0.46
1:A:301:ASP:HB2	1:A:302:PRO:HD3	1.98	0.46
1:A:506:MET:O	1:A:538:LEU:HD22	2.16	0.46
1:A:761:ILE:HD13	1:A:784:LEU:CD1	2.46	0.46
1:B:70:LYS:HE3	1:B:130:TYR:OH	2.16	0.46
1:B:110:GLY:HA3	1:B:163:SER:HB2	1.98	0.46
1:B:737:ASN:CA	1:B:740:VAL:HG22	2.44	0.46
1:B:747:GLU:OE1	1:B:747:GLU:N	2.36	0.46
1:B:1417:VAL:HG12	1:B:1417:VAL:O	2.15	0.46
1:A:139:MET:HE1	1:B:396:GLY:CA	2.46	0.45
1:A:370:LEU:HD12	1:A:370:LEU:N	2.31	0.45
1:A:620:MET:CG	1:A:652:SER:HB2	2.46	0.45
1:B:348:LEU:HD13	1:B:406:PRO:HB3	1.97	0.45
1:B:1413:ILE:HG21	1:B:1431:ILE:HD12	1.98	0.45
1:A:245:THR:O	1:A:404:LEU:HA	2.17	0.45
1:A:247:LEU:HD11	1:A:405:ARG:HB2	1.98	0.45
1:B:209:GLU:OE1	1:B:209:GLU:N	2.47	0.45
1:B:683:HIS:CD2	1:B:743:VAL:HG23	2.51	0.45
1:A:7:ALA:N	1:A:232:LEU:O	2.48	0.45
1:A:133:VAL:HG11	1:B:261:VAL:HG11	1.97	0.45
1:A:154:SER:C	1:A:155:ILE:HD12	2.42	0.45
1:A:761:ILE:HD13	1:A:784:LEU:HD13	1.98	0.45
1:A:1019:ARG:HD2	1:A:1075:VAL:HG21	1.96	0.45
1:B:155:ILE:HG22	1:B:156:ALA:N	2.32	0.45
1:B:579:GLY:HA3	1:B:587:CYS:SG	2.56	0.45
1:B:924:ILE:HD12	1:B:924:ILE:N	2.31	0.45
1:B:1265:LEU:HD21	1:B:2082:GLY:HA3	1.98	0.45
1:B:1354:GLY:CA	1:B:1371:ILE:CD1	2.93	0.45
1:B:105:THR:HG1	1:B:182:ALA:HB3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:ASP:O	1:B:305:LEU:HD13	2.17	0.45
1:B:511:MET:CE	1:B:520:ILE:HG13	2.46	0.45
1:A:993:GLU:OE2	1:A:1927:LYS:NZ	2.49	0.45
1:A:1519:LEU:HD12	1:A:1519:LEU:C	2.42	0.45
1:B:1214:LEU:HD12	1:B:1214:LEU:C	2.41	0.45
1:B:2097:LEU:O	1:B:2097:LEU:HD23	2.16	0.45
1:A:1337:ARG:O	1:A:1405:ARG:NE	2.43	0.45
1:B:513:LEU:HD11	1:B:793:LEU:CD1	2.47	0.45
1:B:1188:LEU:HD13	1:B:1197:GLU:HG2	1.97	0.45
1:B:661:PHE:O	1:B:665:LEU:HG	2.17	0.45
1:B:766:LEU:HD23	1:B:766:LEU:C	2.41	0.45
1:A:107:VAL:HG11	1:A:144:LEU:HD12	1.99	0.45
1:B:253:THR:HG22	1:B:255:GLY:H	1.82	0.45
1:B:316:ARG:HH21	1:B:318:GLU:HG3	1.81	0.45
1:B:447:ASP:OD2	1:B:450:PHE:HB2	2.17	0.45
1:B:620:MET:HA	1:B:652:SER:HA	1.99	0.45
1:B:1348:LEU:O	1:B:1371:ILE:HD11	2.17	0.45
1:B:1602:GLU:HB3	1:B:1650:VAL:HG23	1.98	0.45
1:A:1453:VAL:CG1	1:A:1471:CYS:SG	3.05	0.45
1:A:1897:GLY:HA2	1:A:1971:LEU:HD22	1.99	0.45
1:B:123:ASP:OD2	1:B:126:THR:OG1	2.35	0.45
1:B:422:ARG:NH1	1:B:448:LEU:HG	2.32	0.45
1:B:2088:MET:HE3	1:B:2088:MET:HA	1.99	0.45
1:A:468:ARG:CD	1:A:485:VAL:HG21	2.47	0.45
1:A:784:LEU:HD22	1:A:796:PHE:CE1	2.52	0.45
1:A:1909:VAL:HG11	1:A:1912:LEU:HD13	1.99	0.45
1:B:60:PHE:HB3	1:B:842:TRP:CD1	2.52	0.45
1:B:90:ILE:HG22	1:B:95:ILE:O	2.17	0.45
1:B:691:ALA:O	1:B:694:LEU:HB3	2.17	0.45
1:B:1896:PHE:CE2	1:B:2088:MET:HE1	2.52	0.45
1:A:213:LYS:HG2	1:A:358:HIS:HB3	1.98	0.44
1:A:371:ASP:OD1	1:A:372:GLY:N	2.50	0.44
1:A:1762:THR:HA	1:A:1787:LYS:HG3	1.99	0.44
1:A:6:ILE:HG12	1:A:233:LEU:CD2	2.47	0.44
1:A:92:ASP:O	1:A:241:ARG:NH1	2.49	0.44
1:A:211:THR:HG23	1:A:358:HIS:CD2	2.52	0.44
1:A:757:VAL:HG11	1:A:803:LEU:CD1	2.48	0.44
1:A:1453:VAL:HG13	1:A:1471:CYS:SG	2.58	0.44
1:A:85:VAL:HG12	1:A:230:ALA:HB3	2.00	0.44
1:A:211:THR:HB	1:A:213:LYS:HZ2	1.81	0.44
1:A:545:THR:HG23	1:A:546:PHE:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:ILE:HD12	1:B:95:ILE:N	2.32	0.44
1:B:574:PRO:CG	1:B:577:ILE:HD11	2.46	0.44
1:B:1451:SER:OG	1:B:1453:VAL:HG13	2.16	0.44
1:B:1769:ILE:HB	2:B:2601:NDP:H71N	1.82	0.44
1:A:655:GLN:O	1:A:659:PHE:HD2	2.00	0.44
1:A:694:LEU:HD23	1:A:694:LEU:O	2.17	0.44
1:A:1250:GLY:O	1:A:1316:ASN:ND2	2.50	0.44
1:A:1760:LEU:HD11	1:A:1766:PHE:HB2	1.98	0.44
1:A:1893:LEU:HD23	1:A:1898:LEU:HD21	1.98	0.44
1:B:64:PHE:CE1	1:B:464:ALA:HB1	2.52	0.44
1:B:708:ARG:HD2	1:B:734:TYR:CE2	2.53	0.44
1:A:79:LEU:HD11	1:A:143:ARG:HB2	1.98	0.44
1:A:584:GLU:O	1:A:588:GLY:N	2.43	0.44
1:A:619:ALA:CB	1:A:655:GLN:HA	2.46	0.44
1:B:1128:LEU:HD12	1:B:1128:LEU:N	2.32	0.44
1:B:2007:ARG:NH2	1:B:2051:GLU:OE1	2.51	0.44
1:A:553:PHE:CE2	1:A:610:ILE:HD12	2.53	0.44
1:A:666:ARG:NH2	1:A:672:ALA:O	2.50	0.44
1:A:1177:GLU:OE1	1:A:1178:LEU:N	2.50	0.44
1:A:1802:GLU:O	1:A:1803:SER:OG	2.29	0.44
1:A:2098:PHE:CD1	1:A:2106:LEU:HD13	2.53	0.44
1:B:593:CYS:O	1:B:594:LEU:HD23	2.17	0.44
1:B:605:TRP:CE3	1:B:605:TRP:HA	2.52	0.44
1:A:425:ARG:HD3	1:A:812:PRO:HD3	1.99	0.44
1:A:657:PRO:C	1:A:660:GLU:HG2	2.43	0.44
1:A:1887:TYR:HD1	1:A:1909:VAL:HG13	1.83	0.44
1:B:719:GLU:HA	1:B:722:TRP:CD2	2.53	0.44
1:A:158:ASP:O	1:B:138:ALA:HB2	2.17	0.44
1:A:217:THR:HG22	1:A:363:ASN:HA	2.00	0.44
1:A:344:VAL:CG1	1:A:388:VAL:HG11	2.48	0.44
1:A:344:VAL:HG11	1:A:388:VAL:HG11	2.00	0.44
1:B:190:VAL:HA	1:B:226:GLU:HG2	1.98	0.44
1:B:1391:LEU:HD23	1:B:1391:LEU:C	2.42	0.44
1:B:1391:LEU:HD21	1:B:1393:LYS:HB2	2.00	0.44
1:B:2063:ILE:HG12	2:B:2602:NDP:C7N	2.48	0.44
1:A:649:VAL:HG12	1:A:650:THR:N	2.32	0.43
1:B:371:ASP:OD1	1:B:372:GLY:N	2.45	0.43
1:B:393:PHE:CE1	1:B:399:ASN:HB3	2.53	0.43
1:B:661:PHE:CE2	1:B:665:LEU:HD21	2.53	0.43
1:B:1068:THR:HG22	1:B:1069:LEU:O	2.18	0.43
1:A:196:THR:HG22	1:A:200:PHE:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:620:MET:O	1:A:674:GLU:HG2	2.18	0.43
1:A:1228:LEU:HD11	1:A:1256:ILE:HD12	2.00	0.43
1:A:1446:ILE:HG22	1:A:1474:LEU:CD1	2.47	0.43
1:B:159:THR:HG22	1:B:163:SER:CA	2.48	0.43
1:B:506:MET:HE3	1:B:559:ILE:CD1	2.48	0.43
1:B:597:GLU:H	1:B:597:GLU:CD	2.24	0.43
1:B:1178:LEU:CD1	1:B:1214:LEU:HD11	2.48	0.43
1:A:556:LEU:HD11	1:A:763:PRO:HG3	1.98	0.43
1:A:620:MET:HG3	1:A:651:ILE:C	2.44	0.43
1:A:695:LEU:HD13	1:A:699:LYS:HZ1	1.83	0.43
1:A:1715:LEU:HD22	1:A:1720:PHE:CZ	2.53	0.43
1:A:1771:LYS:HE3	1:A:1795:LEU:HD22	2.00	0.43
1:B:326:LYS:HE3	1:B:331:HIS:CD2	2.54	0.43
1:B:583:GLY:O	1:B:584:GLU:C	2.61	0.43
1:B:1439:ARG:O	1:B:1468:ARG:NH1	2.51	0.43
1:A:217:THR:CG2	1:A:364:PRO:HD3	2.43	0.43
1:A:514:ASP:OD1	1:A:515:ARG:N	2.49	0.43
1:A:741:SER:HB2	1:A:742:PRO:CD	2.45	0.43
1:A:1446:ILE:HD12	1:A:1446:ILE:C	2.43	0.43
1:B:58:SER:O	1:B:841:ALA:HA	2.18	0.43
1:B:127:LEU:C	1:B:127:LEU:HD12	2.43	0.43
1:B:615:LEU:HD21	1:B:680:MET:HE1	2.00	0.43
1:A:105:THR:O	1:A:150:PHE:HB3	2.18	0.43
1:A:1651:VAL:HG23	1:A:1652:TYR:N	2.33	0.43
1:B:417:HIS:HA	1:B:420:LEU:HD13	1.99	0.43
1:B:527:VAL:HG11	1:B:532:LEU:HD11	2.00	0.43
1:B:582:LEU:HD12	1:B:582:LEU:HA	1.85	0.43
1:B:737:ASN:OD1	1:B:741:SER:HB3	2.18	0.43
1:A:6:ILE:HA	1:A:233:LEU:HD23	2.01	0.43
1:A:460:VAL:CG1	1:A:461:PRO:HD2	2.48	0.43
1:A:570:MET:CE	1:A:815:LEU:HD21	2.48	0.43
1:A:695:LEU:HD13	1:A:699:LYS:NZ	2.33	0.43
1:A:772:LYS:CE	1:A:781:ILE:HD13	2.49	0.43
1:B:490:ARG:HD3	1:B:806:SER:O	2.19	0.43
1:B:499:MET:HE2	1:B:683:HIS:HE1	1.84	0.43
1:B:760:GLU:OE1	1:B:760:GLU:HA	2.19	0.43
1:B:898:THR:OG1	1:B:935:VAL:HG11	2.19	0.43
1:A:257:LYS:HD2	1:A:263:PHE:O	2.19	0.43
1:A:525:GLU:OE1	1:A:525:GLU:HA	2.19	0.43
1:A:654:PRO:HD3	1:A:686:PHE:CE2	2.54	0.43
1:B:136:GLN:HG3	1:B:138:ALA:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:LYS:HE3	1:B:263:PHE:O	2.18	0.43
1:B:388:VAL:HG12	1:B:389:GLY:N	2.33	0.43
1:B:477:ARG:HH22	1:B:790:ARG:HD2	1.83	0.43
1:B:495:ILE:HA	1:B:578:VAL:O	2.18	0.43
1:A:168:LEU:HD22	1:A:402:ILE:HD13	1.99	0.43
1:A:549:ILE:CD1	1:A:550:VAL:HG23	2.49	0.43
1:A:618:GLY:HA3	1:A:681:ALA:N	2.33	0.43
1:A:615:LEU:HD12	1:A:680:MET:HE1	2.00	0.43
1:A:635:PRO:HD3	1:A:661:PHE:CE1	2.54	0.43
1:A:639:VAL:O	1:A:651:ILE:HB	2.19	0.43
1:A:1601:MET:O	1:A:1616:LEU:HD12	2.19	0.43
1:A:1973:VAL:HB	2:A:2602:NDP:H3D	2.01	0.43
1:B:291:GLU:OE2	1:B:325:THR:N	2.50	0.43
1:B:305:LEU:CD2	1:B:366:ILE:HD13	2.47	0.43
1:B:511:MET:HE1	1:B:520:ILE:HG13	2.01	0.43
1:B:768:GLN:HE22	1:B:781:ILE:HG22	1.83	0.43
1:A:366:ILE:HG22	1:A:369:LEU:H	1.84	0.42
1:B:235:LYS:HE3	1:B:237:SER:OG	2.18	0.42
1:B:654:PRO:C	1:B:657:PRO:HD2	2.44	0.42
1:B:159:THR:O	1:B:159:THR:HG23	2.19	0.42
1:B:702:ILE:HD12	1:B:702:ILE:N	2.34	0.42
1:A:9:MET:SD	1:A:342:ALA:HA	2.58	0.42
1:B:61:ASP:O	1:B:65:PHE:HD2	2.02	0.42
1:B:225:SER:OG	1:B:330:GLY:HA3	2.20	0.42
1:B:758:VAL:HG12	1:B:759:LEU:N	2.34	0.42
1:B:981:GLU:N	1:B:982:PRO:HD3	2.34	0.42
1:A:333:GLU:HB2	1:A:334:PRO:HD3	2.01	0.42
1:B:501:THR:HG23	1:B:501:THR:O	2.19	0.42
1:B:544:SER:OG	1:B:547:ASP:OD2	2.32	0.42
1:B:648:THR:HG23	1:B:773:ARG:HH11	1.84	0.42
1:B:720:ALA:HB3	1:B:721:GLN:OE1	2.20	0.42
1:B:1218:LEU:HD21	1:B:1400:LEU:HB2	2.01	0.42
1:B:1354:GLY:HA3	1:B:1371:ILE:CD1	2.48	0.42
1:A:136:GLN:OE1	1:A:136:GLN:HA	2.19	0.42
1:A:148:PHE:HB3	1:A:150:PHE:CZ	2.55	0.42
1:A:447:ASP:OD2	1:A:450:PHE:HB2	2.19	0.42
1:A:456:ASP:OD1	1:A:813:ASN:ND2	2.53	0.42
1:B:25:ASN:HB3	1:B:32:MET:HE2	2.01	0.42
1:B:86:THR:HG23	1:B:184:ILE:HG21	2.02	0.42
1:B:620:MET:HG2	1:B:650:THR:CG2	2.50	0.42
1:B:682:PHE:HB3	1:B:683:HIS:ND1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:695:LEU:O	1:B:699:LYS:HG2	2.20	0.42
1:B:758:VAL:O	1:B:759:LEU:HD23	2.19	0.42
1:B:1466:GLY:HA2	1:B:1469:LEU:HD23	2.02	0.42
1:A:139:MET:HE1	1:B:396:GLY:HA2	2.02	0.42
1:A:391:ASN:HB2	1:A:393:PHE:CE1	2.55	0.42
1:A:840:LEU:HD23	1:A:840:LEU:HA	1.90	0.42
1:A:1446:ILE:HG22	1:A:1474:LEU:HD12	2.02	0.42
1:B:717:ILE:CD1	1:B:727:ALA:HB2	2.40	0.42
1:B:1339:GLY:O	1:B:1404:ARG:NH1	2.53	0.42
1:B:1371:ILE:HG23	1:B:1371:ILE:O	2.19	0.42
1:B:1389:VAL:CG2	1:B:1501:LEU:HD11	2.49	0.42
1:B:1714:GLN:OE1	1:B:1714:GLN:N	2.48	0.42
1:A:719:GLU:HA	1:A:722:TRP:NE1	2.34	0.42
1:A:1640:TRP:CZ3	1:A:1648:VAL:HG21	2.55	0.42
1:B:78:GLN:HB3	1:B:188:ILE:HD12	2.02	0.42
1:B:115:GLU:OE1	1:B:193:LYS:N	2.52	0.42
1:B:991:TYR:CZ	1:B:1006:GLN:HA	2.54	0.42
1:A:501:THR:OG1	1:A:763:PRO:HG2	2.20	0.42
1:A:996:LEU:HD13	1:A:1899:GLU:OE2	2.20	0.42
1:A:235:LYS:HD2	1:A:238:LEU:HD13	2.01	0.42
1:A:780:THR:C	1:A:781:ILE:HD12	2.45	0.42
1:B:13:LEU:HB3	1:B:14:PRO:CD	2.49	0.42
1:B:159:THR:HG21	1:B:163:SER:HA	2.01	0.42
1:B:1199:ALA:O	1:B:1203:ALA:N	2.39	0.42
1:A:286:SER:OG	1:A:387:ASN:ND2	2.53	0.41
1:A:425:ARG:HH22	1:A:459:ALA:HB2	1.85	0.41
1:A:436:LYS:HE3	1:A:440:GLN:HE21	1.84	0.41
1:A:1069:LEU:HD11	1:A:1075:VAL:HG11	2.02	0.41
1:B:160:ALA:O	1:B:161:CYS:HB3	2.20	0.41
1:B:2062:ALA:HB3	1:B:2085:PRO:HA	2.02	0.41
1:A:112:SER:HA	1:A:137:ARG:NH1	2.35	0.41
1:A:210:GLY:O	1:A:223:CYS:HB3	2.20	0.41
1:A:1209:LEU:O	1:A:1215:LEU:HD12	2.19	0.41
1:A:1493:LEU:HA	1:A:1496:VAL:HG22	2.02	0.41
1:B:249:ALA:HB1	1:B:402:ILE:HG22	2.01	0.41
1:B:939:GLU:OE1	1:B:939:GLU:N	2.46	0.41
1:A:5:VAL:HG21	1:A:239:ALA:CB	2.51	0.41
1:A:654:PRO:HD3	1:A:686:PHE:HE2	1.85	0.41
1:A:946:VAL:O	1:A:953:VAL:HG12	2.19	0.41
1:A:1391:LEU:HD23	1:A:1391:LEU:C	2.45	0.41
1:A:1888:ILE:CD1	1:A:1956:ILE:HD13	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:706:LYS:HB3	1:B:707:PRO:HD2	2.01	0.41
1:B:1270:TYR:HB3	1:B:1292:VAL:HG12	2.01	0.41
1:A:627:TRP:O	1:A:631:LYS:HG2	2.20	0.41
1:A:783:PRO:O	1:A:784:LEU:HB2	2.21	0.41
1:B:572:LEU:HD11	1:B:803:LEU:CD2	2.49	0.41
1:B:626:SER:HB2	1:B:629:GLU:CD	2.45	0.41
1:B:635:PRO:HD2	1:B:638:VAL:CG1	2.48	0.41
1:B:831:SER:HB3	1:B:832:PRO:HD3	2.02	0.41
1:B:1280:LEU:HD13	1:B:1294:GLN:HG2	2.01	0.41
1:A:27:ILE:HD12	1:A:27:ILE:HA	1.91	0.41
1:A:78:GLN:HG2	1:A:190:VAL:HG13	2.02	0.41
1:A:706:LYS:HB3	1:A:707:PRO:CD	2.48	0.41
1:B:420:LEU:N	1:B:420:LEU:HD12	2.36	0.41
1:B:424:LEU:O	1:B:470:TYR:HA	2.20	0.41
1:B:740:VAL:HG23	1:B:741:SER:H	1.85	0.41
1:B:1052:VAL:HG11	1:B:1055:ILE:HD11	2.02	0.41
1:B:2022:VAL:HG13	1:B:2060:TRP:O	2.21	0.41
1:A:6:ILE:HG23	1:A:231:VAL:HG13	2.02	0.41
1:A:86:THR:O	1:A:90:ILE:HG13	2.20	0.41
1:A:157:LEU:HD12	1:A:157:LEU:N	2.36	0.41
1:A:274:ARG:HA	1:A:277:TYR:CD2	2.54	0.41
1:A:816:PHE:HB3	1:A:817:PRO:HD2	2.03	0.41
1:A:1066:LEU:HD23	1:A:1076:ALA:HB2	2.02	0.41
1:A:1115:GLU:HG2	1:A:1518:LEU:HD23	2.02	0.41
1:B:508:LEU:HD22	1:B:539:LEU:HD23	2.02	0.41
1:B:620:MET:HG2	1:B:650:THR:HG22	2.01	0.41
1:A:65:PHE:HA	1:A:147:PHE:CE1	2.56	0.41
1:A:104:HIS:O	1:A:152:GLY:HA3	2.20	0.41
1:A:196:THR:HG22	1:A:200:PHE:HE2	1.85	0.41
1:A:585:VAL:HG23	1:A:586:ALA:N	2.35	0.41
1:A:608:GLN:HG2	1:A:612:GLU:OE2	2.21	0.41
1:A:1148:LEU:HD12	1:A:1148:LEU:N	2.36	0.41
1:A:897:LYS:HG2	1:A:907:VAL:HG21	2.03	0.41
1:A:1677:SER:HA	1:A:1708:LEU:HD11	2.03	0.41
1:A:1942:SER:OG	1:A:1958:GLU:OE2	2.34	0.41
1:B:81:LEU:O	1:B:85:VAL:HG23	2.20	0.41
1:B:333:GLU:HB2	1:B:334:PRO:CD	2.38	0.41
1:B:391:ASN:HB2	1:B:393:PHE:CE1	2.56	0.41
1:B:1029:PHE:O	1:B:1032:THR:OG1	2.33	0.41
1:B:2098:PHE:CD1	1:B:2106:LEU:HD13	2.55	0.41
1:A:68:HIS:ND1	1:A:69:PRO:HD2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:LEU:HD12	1:A:157:LEU:H	1.86	0.41
1:A:193:LYS:HD3	1:A:850:PHE:CD2	2.55	0.41
1:A:549:ILE:CG1	1:A:611:LYS:HG3	2.51	0.41
1:A:1140:LEU:HD13	1:A:1174:SER:OG	2.21	0.41
1:A:1904:LEU:HB3	1:A:1909:VAL:HG21	2.03	0.41
1:A:1922:THR:HG22	1:A:1923:GLY:N	2.36	0.41
1:B:9:MET:HE2	1:B:9:MET:HB3	1.86	0.41
1:B:191:LEU:HD22	1:B:224:ARG:NH2	2.35	0.41
1:B:215:PHE:CE1	1:B:305:LEU:HD11	2.56	0.41
1:B:252:ASN:HD21	1:B:268:ILE:HG22	1.86	0.41
1:B:623:VAL:CG1	1:B:665:LEU:HD13	2.51	0.41
1:B:687:MET:HA	1:B:690:ILE:HD13	2.02	0.41
1:B:692:PRO:N	1:B:693:PRO:HD2	2.35	0.41
1:B:726:LEU:HD11	1:B:733:GLU:CB	2.51	0.41
1:B:912:VAL:HG22	1:B:913:VAL:N	2.36	0.41
1:B:1968:VAL:HG11	1:B:2002:LEU:HD22	2.03	0.41
1:A:538:LEU:HD23	1:A:546:PHE:CZ	2.48	0.41
1:A:2018:VAL:HG11	1:A:2041:MET:HB3	2.03	0.41
1:B:191:LEU:HD22	1:B:224:ARG:HH21	1.86	0.41
1:B:485:VAL:HG22	1:B:805:LEU:O	2.21	0.41
1:B:615:LEU:HD12	1:B:615:LEU:C	2.46	0.41
1:A:92:ASP:OD1	1:A:241:ARG:NH1	2.54	0.40
1:A:342:ALA:O	1:A:346:LEU:HG	2.21	0.40
1:A:821:PHE:HB3	1:A:822:PRO:HA	2.03	0.40
1:B:78:GLN:NE2	1:B:188:ILE:CD1	2.77	0.40
1:B:114:SER:HG	1:B:117:SER:HG	1.51	0.40
1:B:242:VAL:CG2	1:B:822:PRO:HB3	2.50	0.40
1:A:127:LEU:HD12	1:A:127:LEU:O	2.20	0.40
1:A:490:ARG:HD3	1:A:806:SER:O	2.22	0.40
1:A:1971:LEU:HD12	1:A:1971:LEU:N	2.35	0.40
1:B:159:THR:OG1	1:B:166:MET:HE3	2.20	0.40
1:B:645:SER:OG	1:B:770:VAL:HG13	2.22	0.40
1:B:933:LEU:HD12	1:B:933:LEU:N	2.35	0.40
1:A:302:PRO:HG2	1:A:365:GLU:OE1	2.21	0.40
1:A:666:ARG:HE	1:A:672:ALA:HB3	1.85	0.40
1:A:682:PHE:HB3	1:A:683:HIS:HD2	1.86	0.40
1:A:698:LEU:CB	1:A:732:ALA:HB1	2.50	0.40
1:A:1077:ASP:OD1	1:A:1078:VAL:N	2.54	0.40
1:B:1372:LEU:HB3	1:B:1376:ALA:HB3	2.03	0.40
1:A:5:VAL:HG21	1:A:239:ALA:HB2	2.04	0.40
1:A:138:ALA:HB1	1:B:160:ALA:HB2	2.00	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:THR:HG21	1:A:340:ALA:HA	2.03	0.40
1:A:1219:LEU:HD13	1:A:1255:ARG:HH21	1.85	0.40
1:A:1261:SER:N	1:A:1262:PRO:CD	2.85	0.40
1:B:548:ASP:CG	1:B:550:VAL:HG12	2.46	0.40
1:B:1209:LEU:N	1:B:1210:PRO:HD2	2.36	0.40
1:A:168:LEU:HD21	1:A:246:ILE:HD13	2.04	0.40
1:A:247:LEU:CD1	1:A:405:ARG:HB2	2.52	0.40
1:A:1786:LEU:HD11	1:B:1775:SER:HA	2.03	0.40
1:A:1896:PHE:CD1	1:A:2063:ILE:HG13	2.56	0.40
1:B:110:GLY:CA	1:B:163:SER:HB2	2.52	0.40
1:B:759:LEU:CD2	1:B:782:ILE:HG22	2.51	0.40
1:B:1128:LEU:HD23	1:B:1134:LEU:HD22	2.03	0.40
1:B:1252:LEU:HD23	1:B:1314:VAL:HB	2.02	0.40
1:B:1743:LEU:HD23	1:B:1765:ARG:HB2	2.03	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%)	2006 (97%)	54 (3%)	0	100	100
1	B	2063/2553 (81%)	2009 (97%)	54 (3%)	0	100	100
All	All	4123/5106 (81%)	4015 (97%)	108 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1705/2117 (80%)	1705 (100%)	0	100	100
1	B	1708/2117 (81%)	1706 (100%)	2 (0%)	88	90
All	All	3413/4234 (81%)	3411 (100%)	2 (0%)	87	90

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	580	HIS
1	B	1828	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	104	HIS
1	A	142	ASN
1	A	173	GLN
1	A	293	HIS
1	A	356	ASN
1	A	358	HIS
1	A	379	GLN
1	A	387	ASN
1	A	399	ASN
1	A	444	HIS
1	A	446	GLN
1	A	551	HIS
1	A	614	HIS
1	A	751	HIS
1	A	804	HIS
1	A	987	GLN
1	A	1044	HIS
1	A	1139	GLN
1	A	1191	ASN
1	A	1290	HIS
1	A	1296	GLN
1	A	1504	ASN
1	A	1562	GLN
1	A	1572	ASN

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Mol	Chain	Res	Type
1	A	1595	GLN
1	A	1731	HIS
1	A	1763	HIS
1	A	1815	GLN
1	A	1835	GLN
1	B	71	GLN
1	B	142	ASN
1	B	170	ASN
1	B	173	GLN
1	B	195	ASN
1	B	199	GLN
1	B	306	ASN
1	B	331	HIS
1	B	358	HIS
1	B	375	GLN
1	B	440	GLN
1	B	446	GLN
1	B	551	HIS
1	B	644	ASN
1	B	737	ASN
1	B	738	ASN
1	B	746	GLN
1	B	755	HIS
1	B	768	GLN
1	B	789	HIS
1	B	804	HIS
1	B	813	ASN
1	B	949	ASN
1	B	1006	GLN
1	B	1195	GLN
1	B	1278	GLN
1	B	1288	GLN
1	B	1516	HIS
1	B	1731	HIS
1	B	1845	GLN
1	B	1848	HIS
1	B	1855	GLN
1	B	1884	HIS

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	A	2601	-	51,52,52	0.48	0	71,80,80	0.62	0
2	NDP	B	2602	-	51,52,52	0.49	0	71,80,80	0.72	1 (1%)
2	NDP	A	2602	-	51,52,52	0.50	0	71,80,80	0.64	1 (1%)
2	NDP	B	2601	-	51,52,52	0.51	0	71,80,80	0.68	1 (1%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NDP	A	2601	-	-	12/34/77/77	0/5/5/5
2	NDP	B	2602	-	-	6/34/77/77	0/5/5/5
2	NDP	A	2602	-	-	11/34/77/77	0/5/5/5
2	NDP	B	2601	-	-	13/34/77/77	0/5/5/5

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2602	NDP	P2B-O2B-C2B	-3.77	113.37	123.43
2	B	2601	NDP	P2B-O2B-C2B	-3.74	113.44	123.43
2	A	2602	NDP	P2B-O2B-C2B	-3.23	114.81	123.43

There are no chirality outliers.

All (42) torsion outliers are listed below:

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

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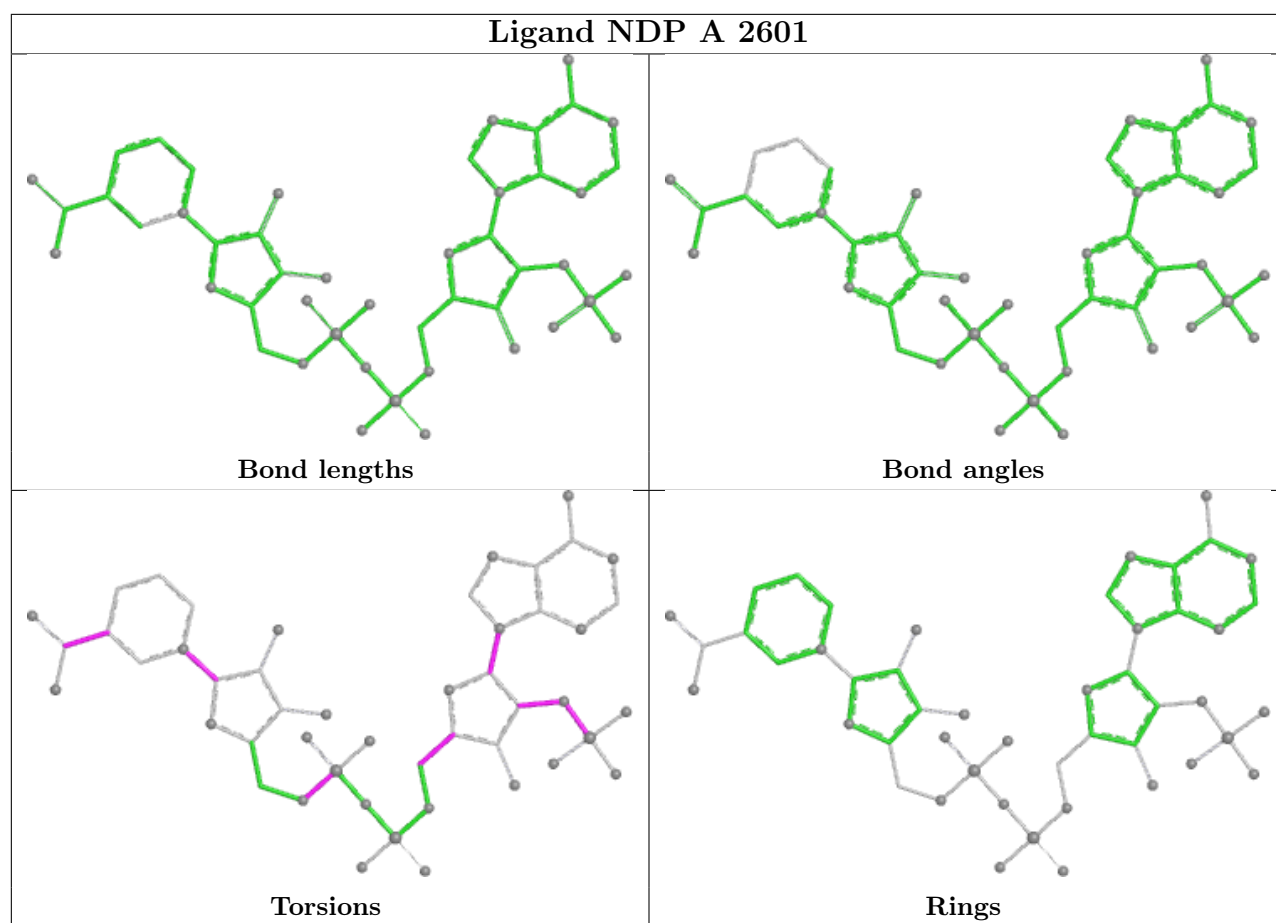
Mol	Chain	Res	Type	Atoms
2	A	2601	NDP	C2B-O2B-P2B-O1X
2	B	2602	NDP	C2D-C1D-N1N-C6N
2	B	2601	NDP	PA-O3-PN-O2N
2	A	2602	NDP	C2B-O2B-P2B-O3X
2	A	2601	NDP	C2B-C1B-N9A-C8A
2	A	2602	NDP	C2B-C1B-N9A-C8A
2	A	2602	NDP	PA-O3-PN-O2N

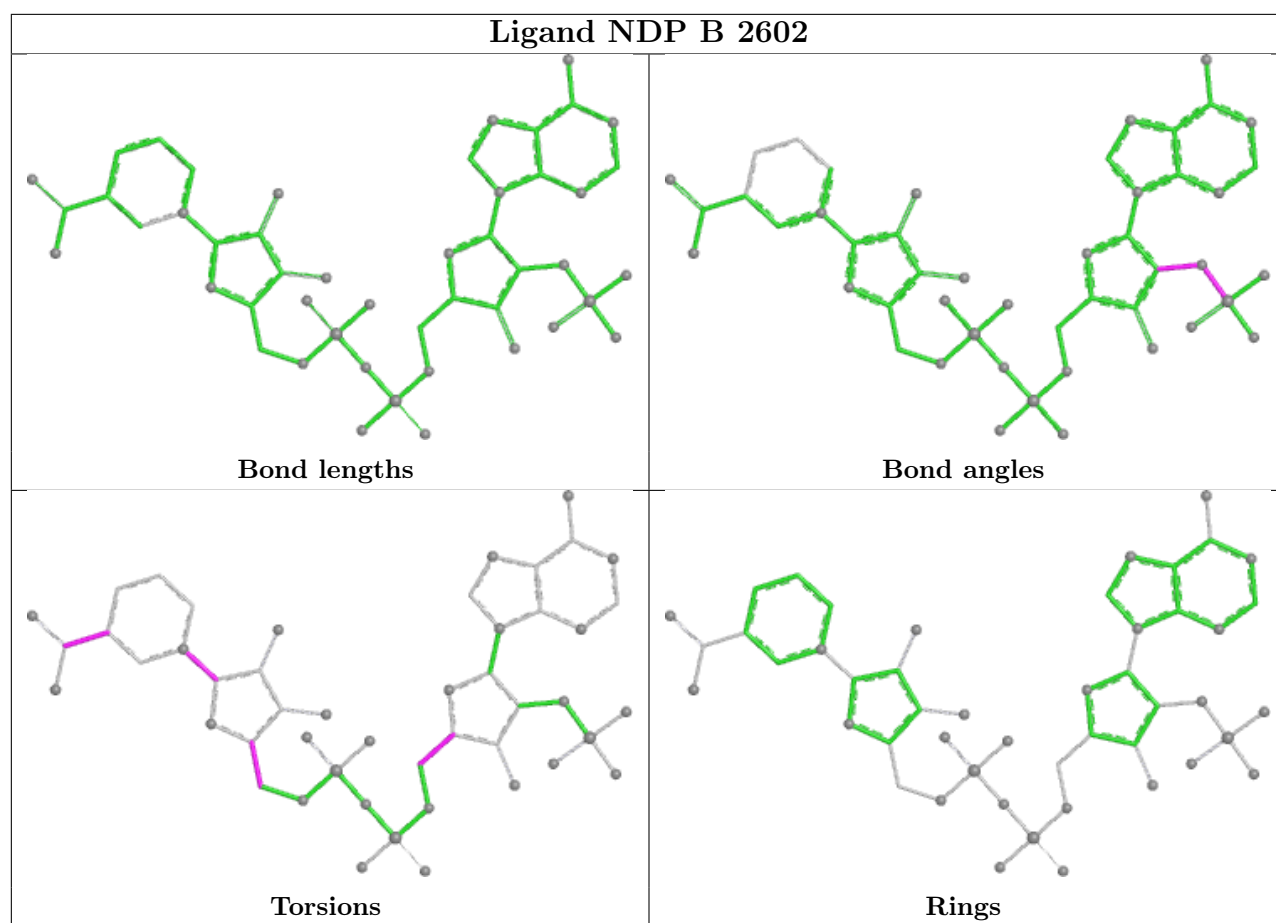
There are no ring outliers.

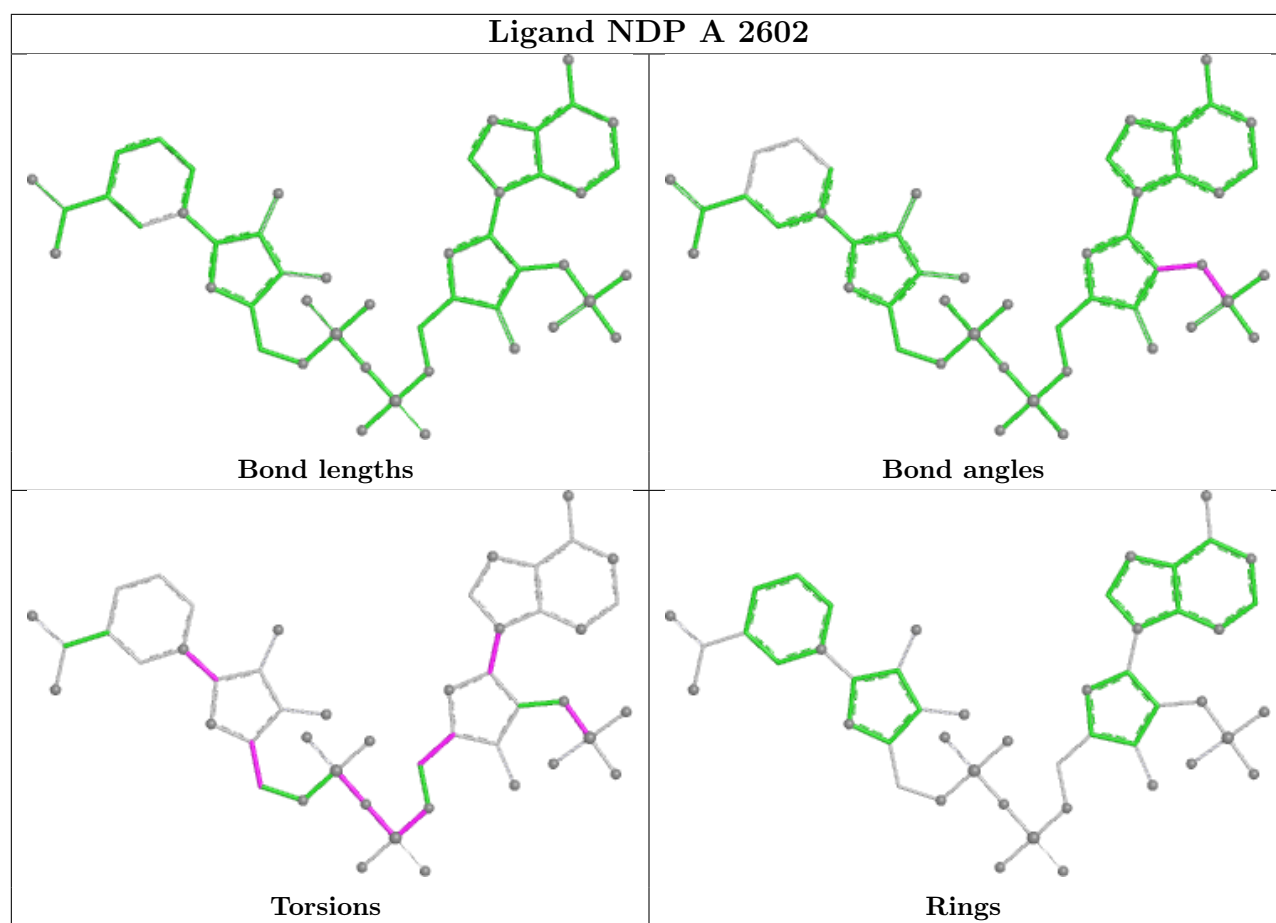
3 monomers are involved in 4 short contacts:

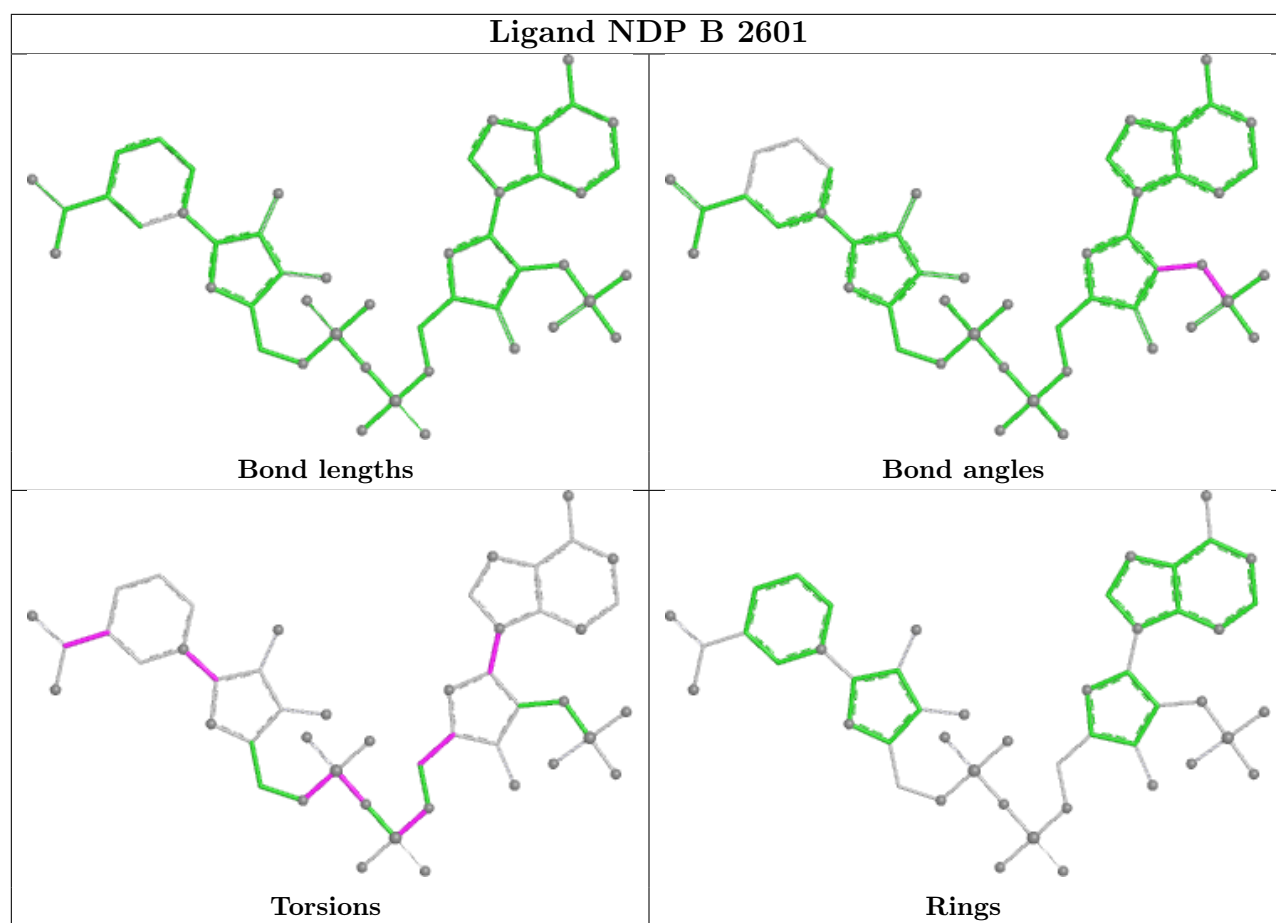
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2602	NDP	1	0
2	A	2602	NDP	1	0
2	B	2601	NDP	2	0

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.

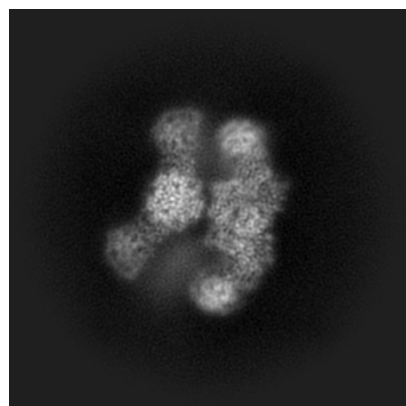
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43350. These allow visual inspection of the internal detail of the map and identification of artifacts.

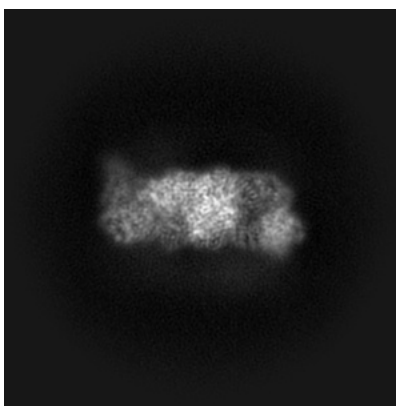
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

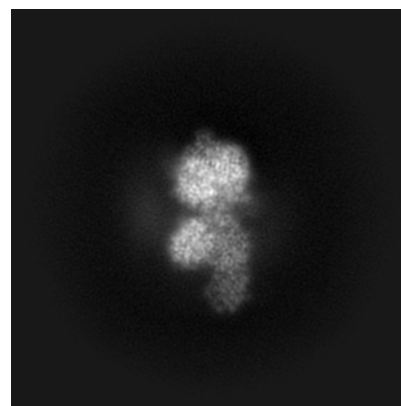
6.1.1 Primary map



X

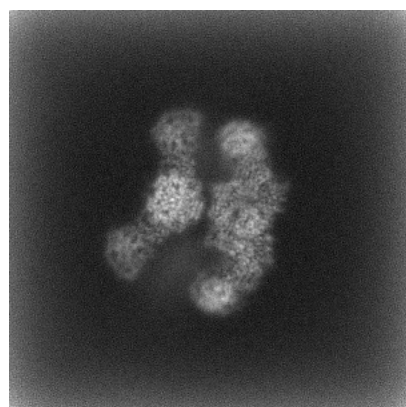


Y

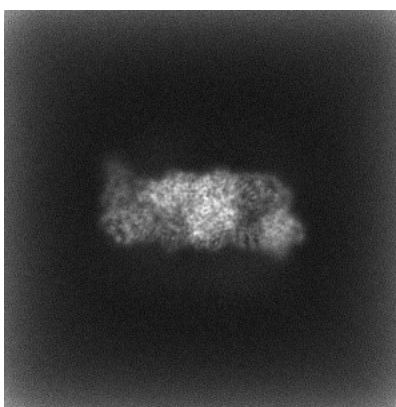


Z

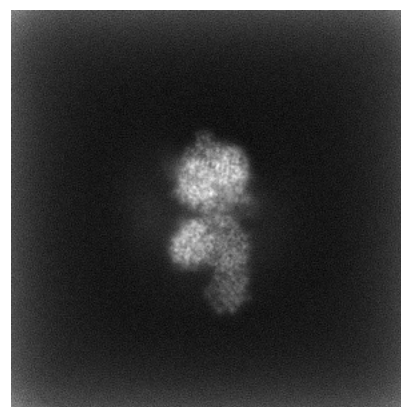
6.1.2 Raw map



X



Y

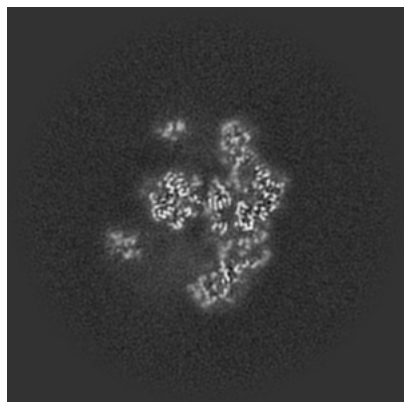


Z

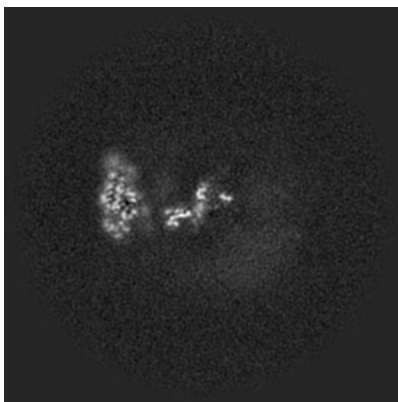
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

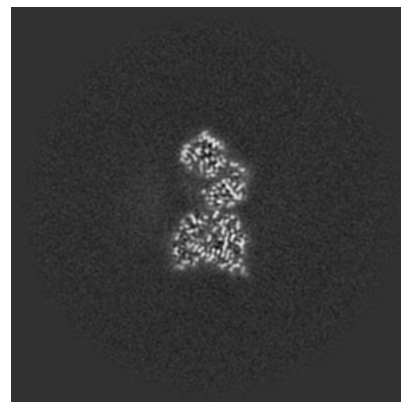
6.2.1 Primary map



X Index: 180

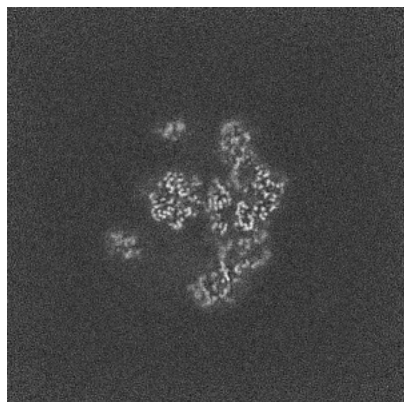


Y Index: 180



Z Index: 180

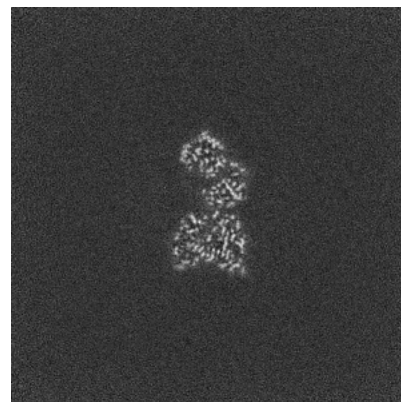
6.2.2 Raw map



X Index: 180



Y Index: 180

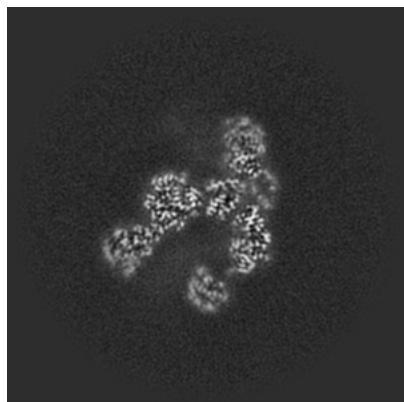


Z Index: 180

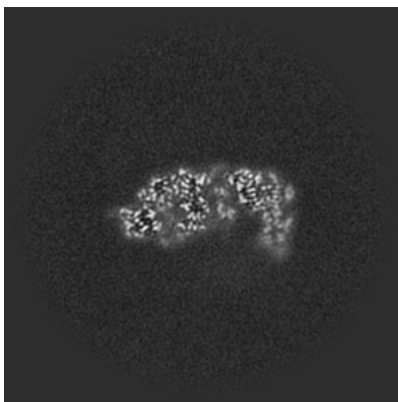
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

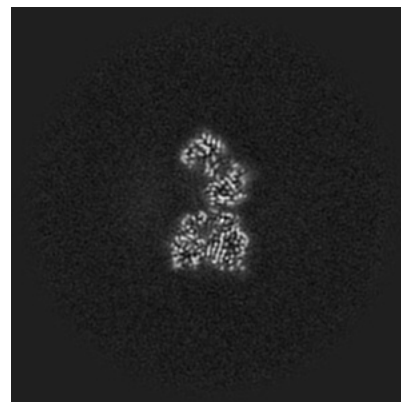
6.3.1 Primary map



X Index: 190

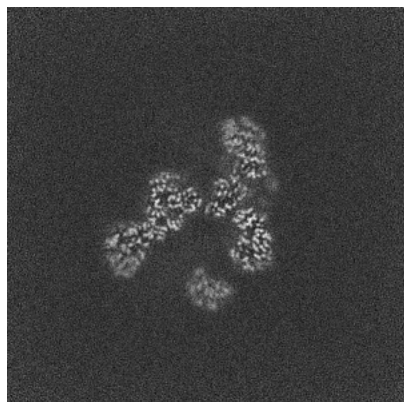


Y Index: 214

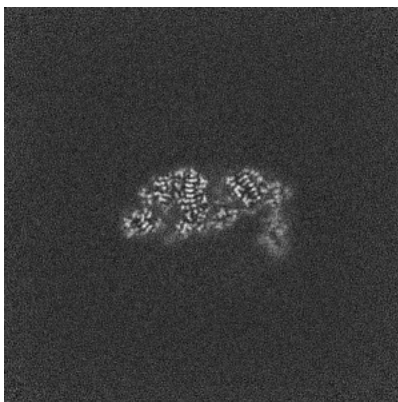


Z Index: 182

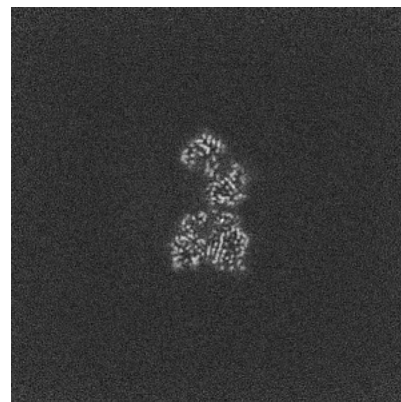
6.3.2 Raw map



X Index: 194



Y Index: 218

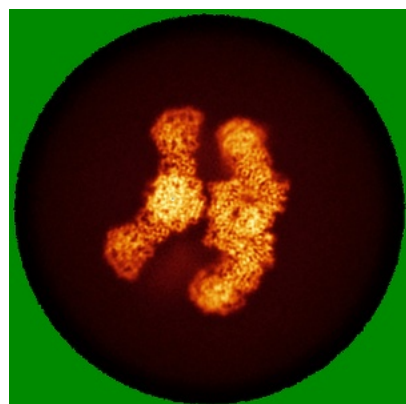


Z Index: 182

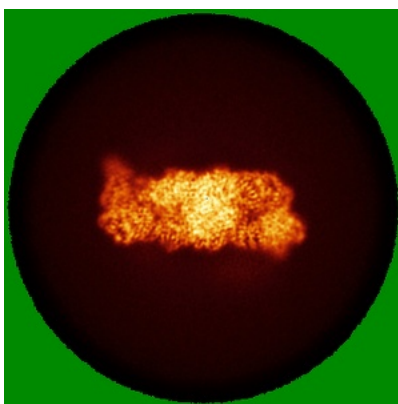
The images above show the largest variance slices of the map in three orthogonal directions.

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

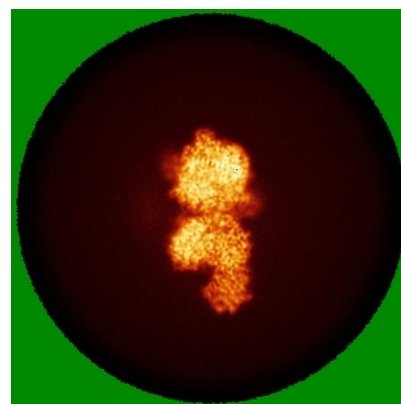
6.4.1 Primary map



X

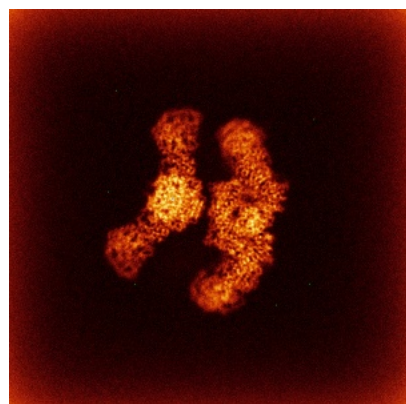


Y

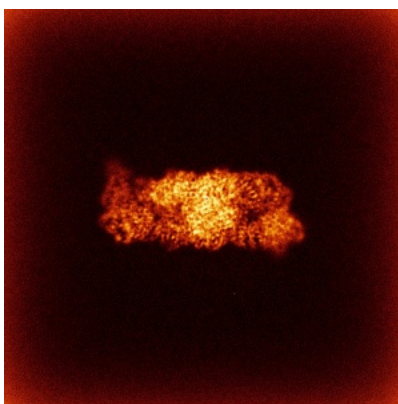


Z

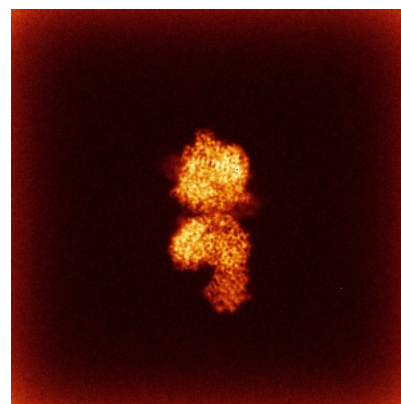
6.4.2 Raw map



X



Y

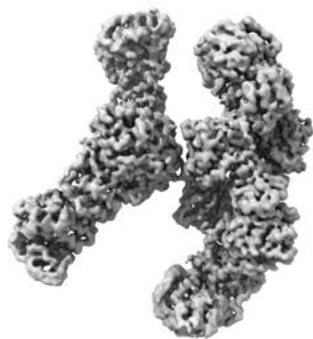


Z

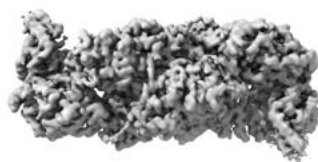
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

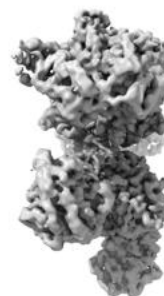
6.5.1 Primary map



X



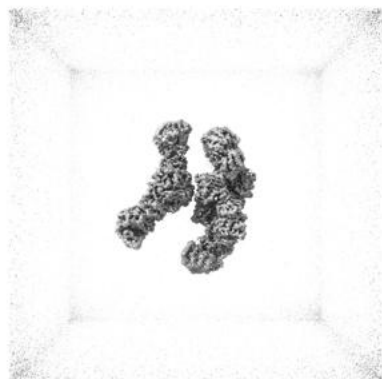
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.182. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

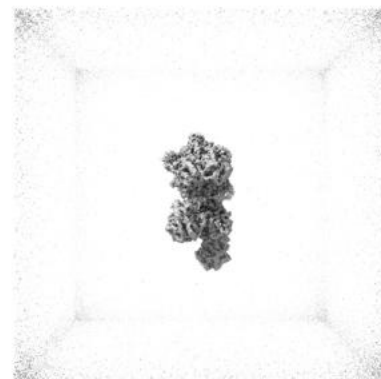
6.5.2 Raw map



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.

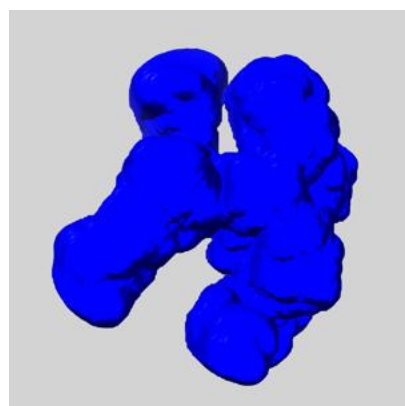
6.6 Mask visualisation [i](#)

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

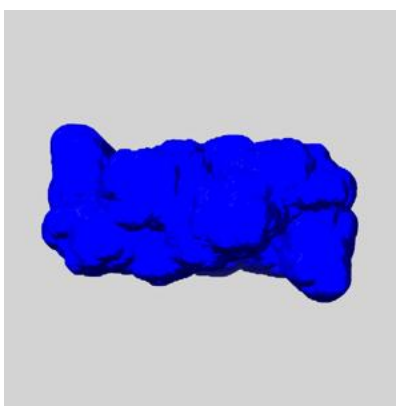
A mask typically either:

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

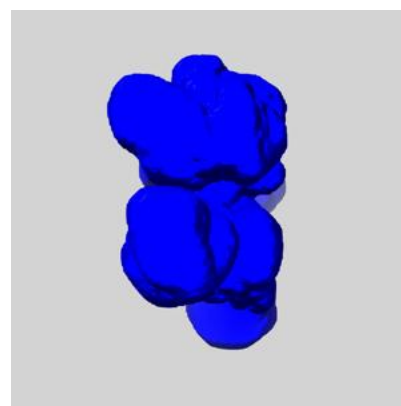
6.6.1 emd_43350_msk_1.map [i](#)



X



Y

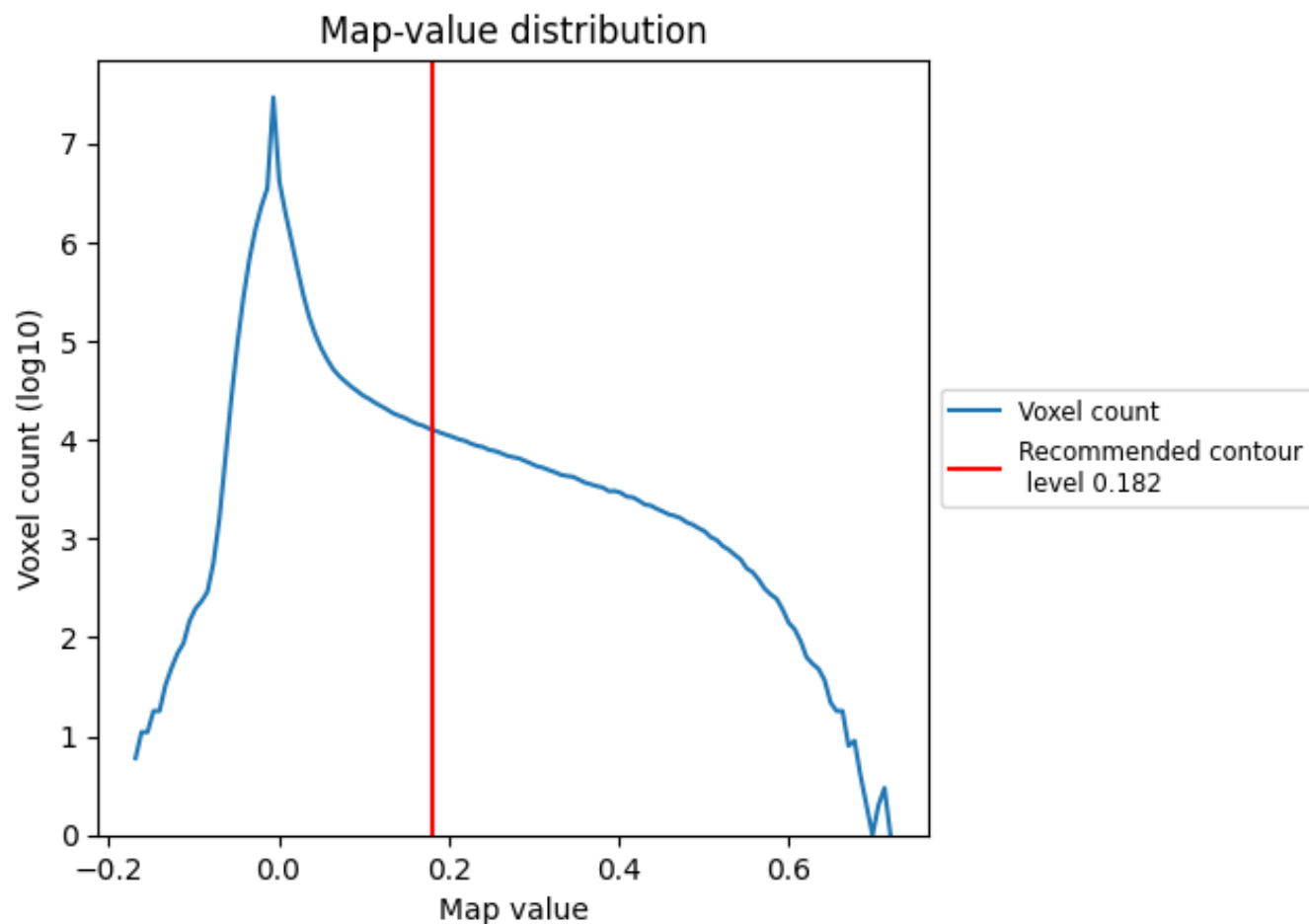


Z

7 Map analysis [i](#)

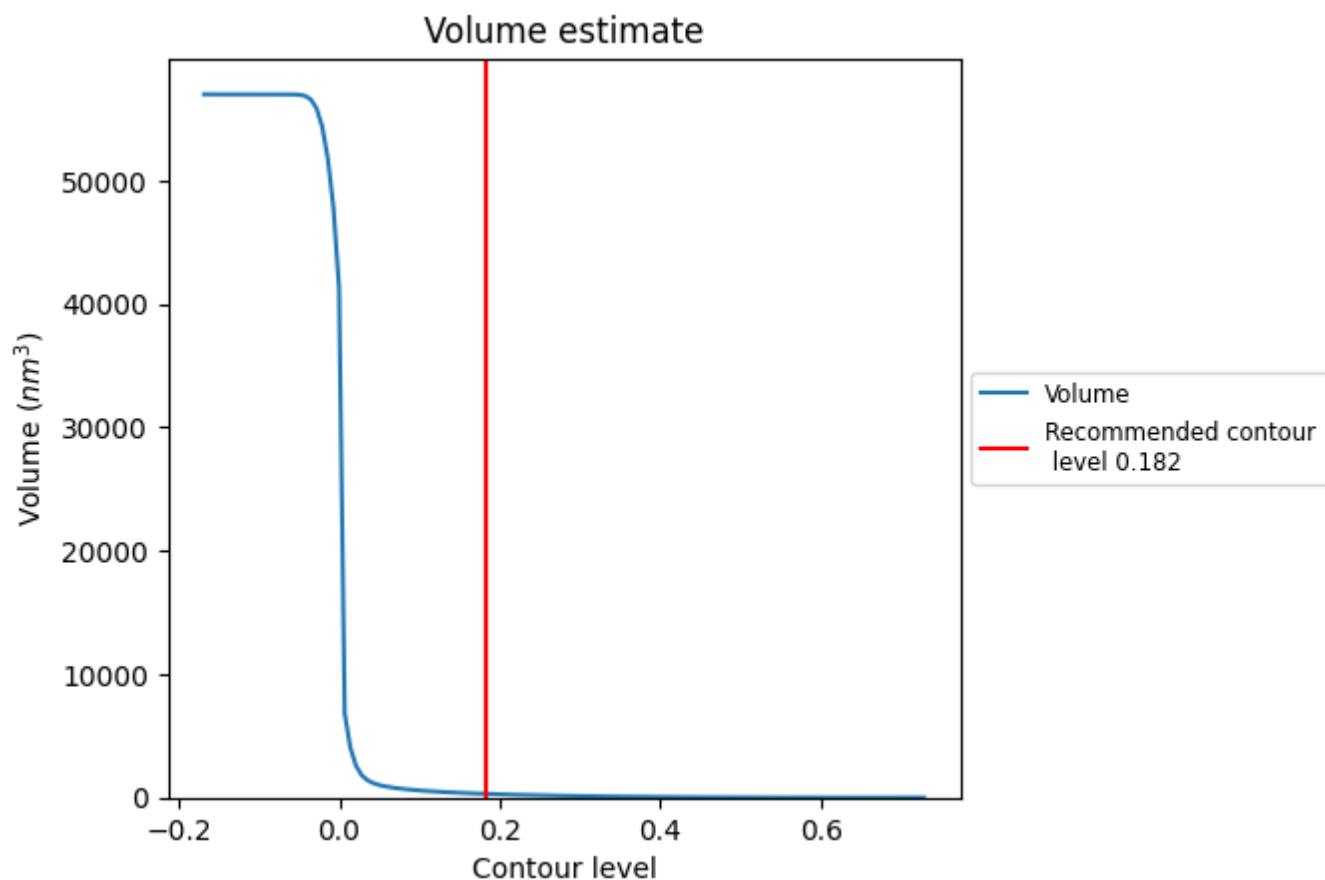
This section contains the results of statistical analysis of the map.

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.

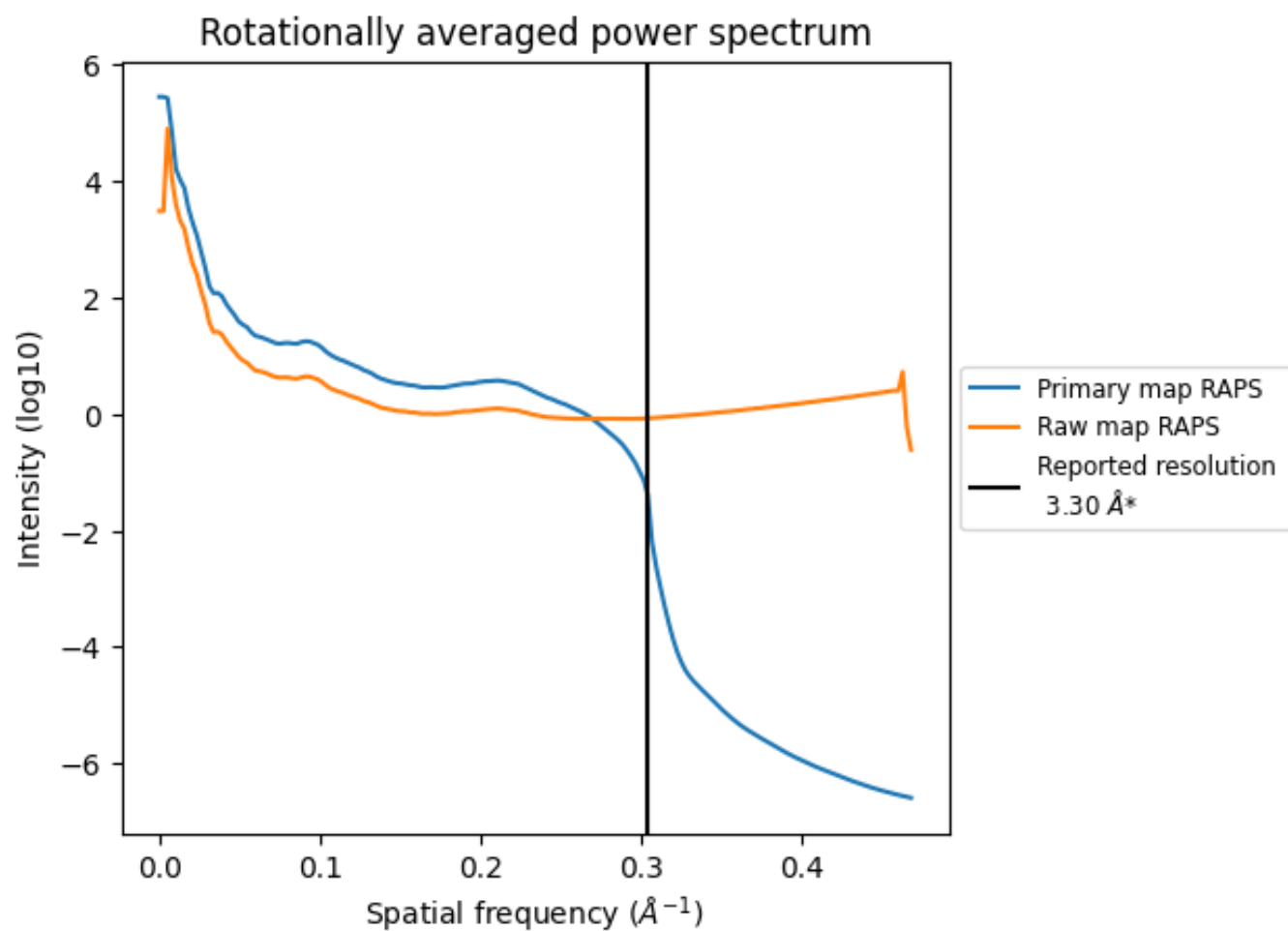
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 301 nm³; this corresponds to an approximate mass of 272 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 ⓘ

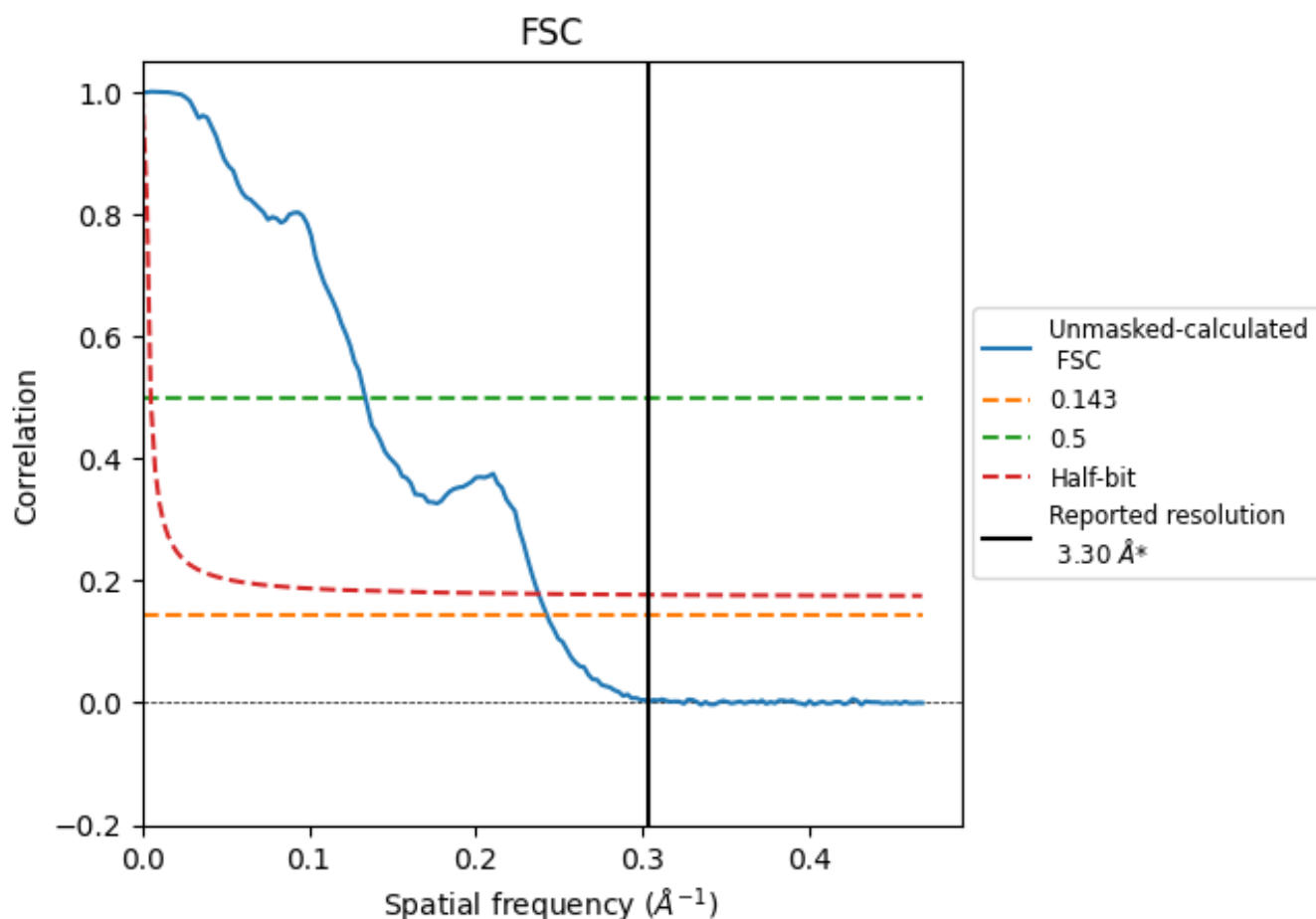


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

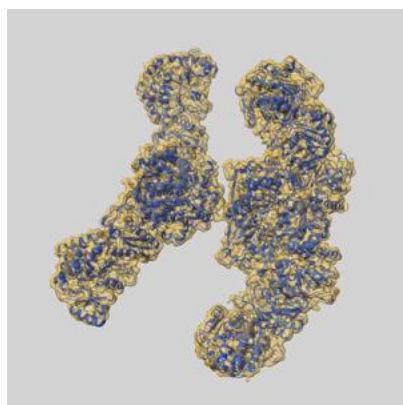
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.12	7.48	4.21

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

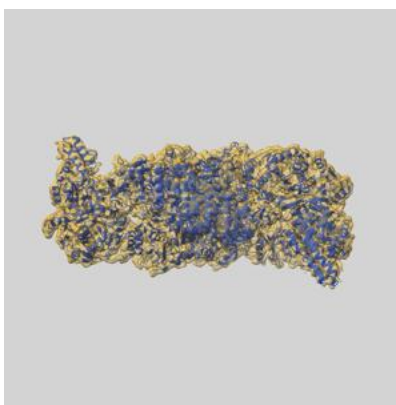
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-43350 and PDB model 8VM0. Per-residue inclusion information can be found in section 3 on page 7.

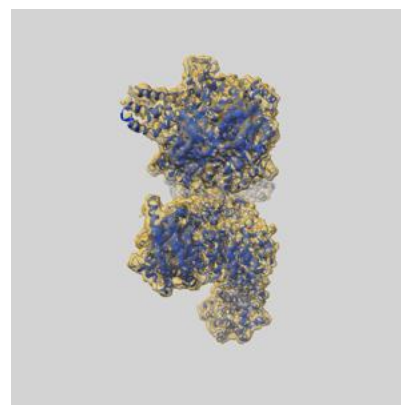
9.1 Map-model overlay [i](#)



X



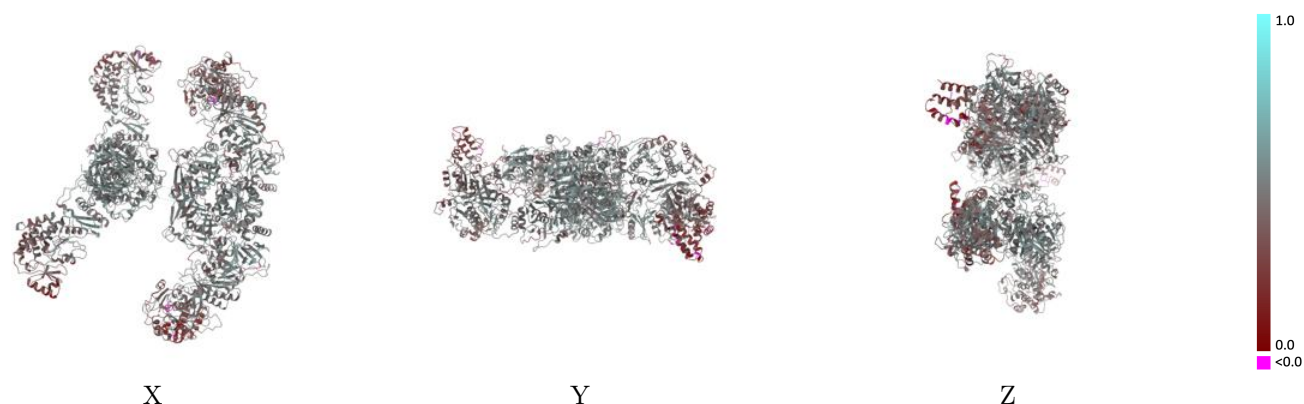
Y



Z

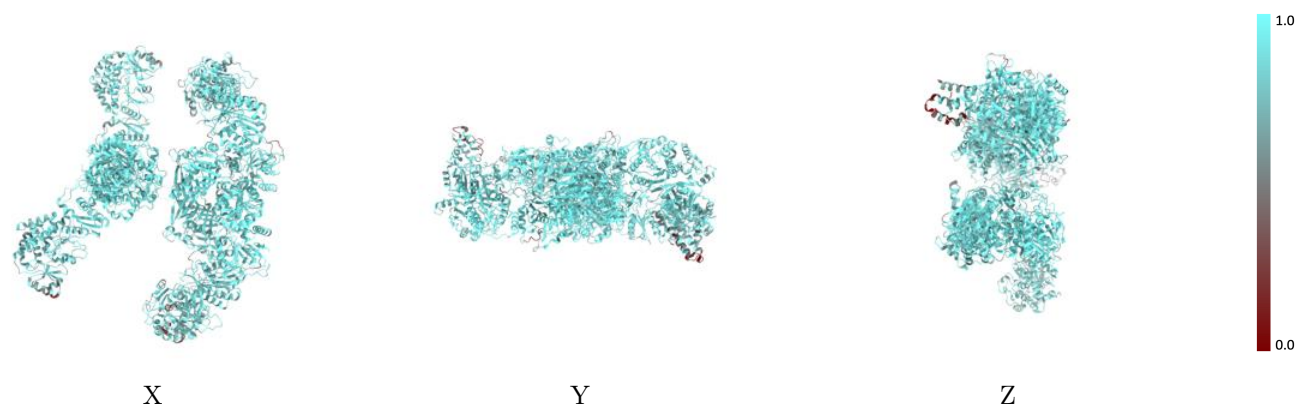
The images above show the 3D surface view of the map at the recommended contour level 0.182 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



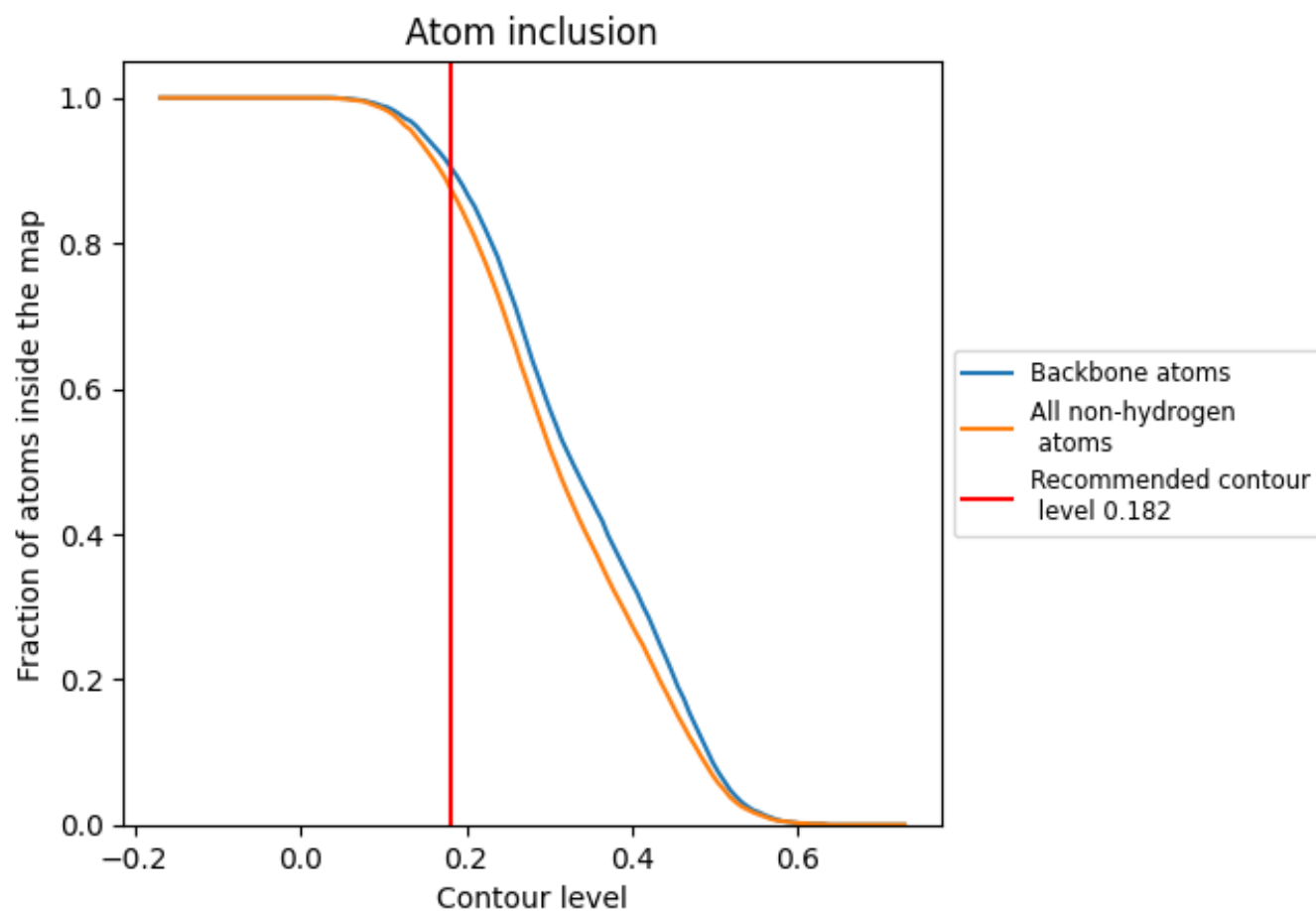
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.182).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 87% 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 (0.182) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8730	0.4530
A	0.8790	0.4560
B	0.8660	0.4510

