



Full wwPDB EM Validation Report ⓘ

May 8, 2025 – 02:37 PM EDT

PDB ID : 8VM6 / pdb_00008vm6
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

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

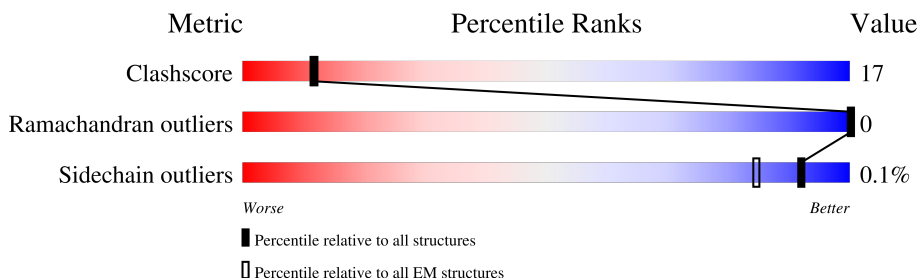
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2553	
1	B	2553	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 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

Continued on next page...

Continued from previous page...

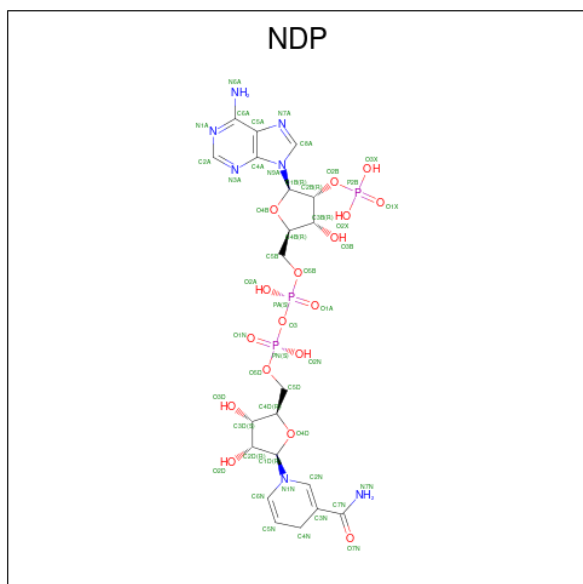
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	ALA	-	expression tag	UNP P49327
A	-4	MET	-	expression tag	UNP P49327
A	-3	GLY	-	expression tag	UNP P49327
A	-2	SER	-	expression tag	UNP P49327
A	-1	GLY	-	expression tag	UNP P49327
A	0	ILE	-	expression tag	UNP P49327
A	1	PRO	-	expression tag	UNP P49327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

Continued on next page...

Continued from previous page...

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).

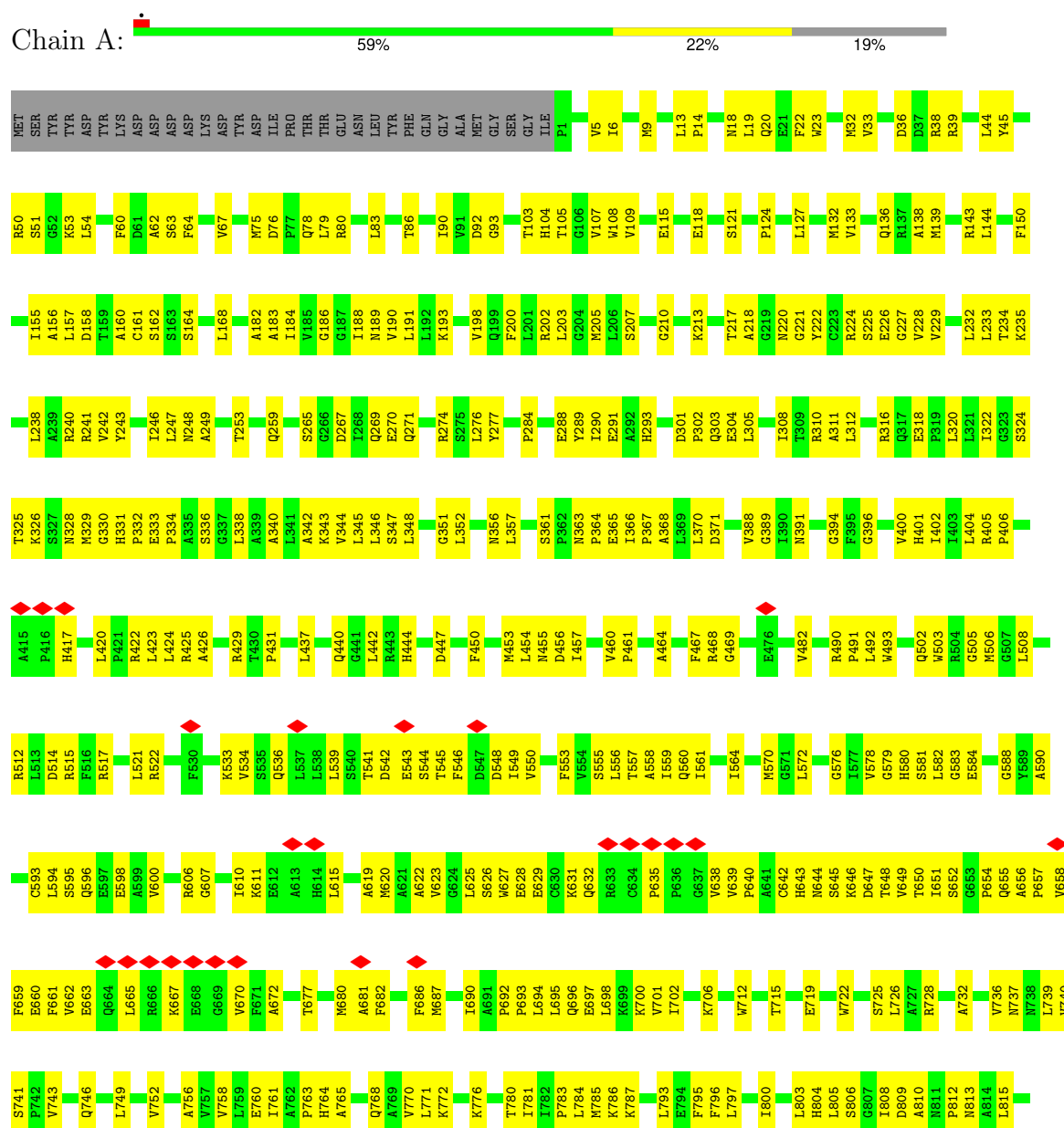


Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
2	A	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
2	B	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
2	B	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	

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



V1292	A1293	Q1294	D1298	P1299	L1313	C1317	A1318	V1319	S1327	M1331	M1332	V1333	L1336	L1343	L1344	H1345	I1356	V1357	T1361	E1364	Q1366	Y1367	G1370	I1371	L1372	M1377	L1386	V1389	G1390	L1391	L1400	D1410	V1417	K1429	E1435	D1436	A1445	I1446																			
ILE	PRO	ARG	ASP	P1173	E1177	L1178	R1187	L1190	M1191	G1192	M1193	L1194	Q1195	E1197	L1198	A1199	Q1200	V1201	L1202	A1203	Q1204	E1205	P1207	K1208	L1209	P1210	P1213	L1214	L1215	S1216	G1217	L1228	D1229	T1230	M1234	L1246	I1256	Y1270	D1274	R1275	L1280	E1286	Q1289														
G1018	N1025	S1028	D1031	Q1035	K1043	L1046	V1052	I1055	D1071	K1072	V1078	V1079	V1080	T1087	A1102	Q1104	P1112	I1113	E1125	E1130	C1141	V1145	T1150	THR	VAL	THR	GLN	GLN	GLY	LEU	LYS	MET	VAL	PRO	GLY	LEU	ASP	GLY	ALA	GLN																	
N811	P812	N813	A814	L815	F816	P817	F821	I830	S831	P832	L833	E848	D849	H852	GLY	SER	GLY	SER	PRO	SER	A859	T879	L880	D881	I894	V912	Q913	V935	E939	V946	T976	P977	N978	P979	Y991	R995	L996	G998	Y999	Q1006	G1007	E1014															
S741	P742	V743	L744	F745	Q746	E747	A748	L749	W750	E754	H755	A756	V757	L758	E760	I761	A762	P763	A765	L766	L767	Q768	A769	V770	L771	K772	R773	G774	L775	S778	C779	T780	I781	I782	K786	D787	H788	R789	D791	L793	E794	F795	I800	G801	R802	L803	H804	L805	I808								
G679	M680	A681	F682	H683	S684	Y685	F686	L687	E688	A689	E690	A691	P692	P693	L694	L695	Q696	E697	L698	K699	K700	V701	I702	R703	E704	P705	K706	F707	R708	R711	W712	L713	S714	T715	S716	I717	P718	E719	A720	Q721	W722	H723	S724	A727	R728	T729	S730	S731	A732	E733	Y734	N735	V736	N737	W738	L739	V740
L348	G351	L352	W353	A354	L357	I366	L374	Q375	V376	V377	V383	V388	Q389	I390	G394	F395	G396	V400	H401	L402	I403	P406	P414	A415	P416	H417	A418	T419	L420	P421	L424	R425	A426	R429	T430	P431	E432	L437	L438	A439	A440	F450	M453	L454													
L120	S121	R122	D123	P124	E125	T126	L127	V128	M132	V133	A138	M139	N142	R143	L144	S145	F148	D149	F150	R151	G152	A156	L157	D158	T159	A160	C161	S162	S163	S164	L165	M166	A167	L168	I175	A183	L184	V185	G186	G187	L188	T189	V190	G191	S192	D193	P194	S195	T196	S197	V198	Q199					
F200	L201	R202	L203	G204	M205	L206	S207	P208	E209	C212	F215	D216	T217	G221	Y222	C223	R224	S225	E226	V229	A230	V231	L232	L233	T234	K235	L238	A239	R240	R241	L247	M248	A249	G250	T251	N252	T253	D254	G255	F256	K257	P264	S265	G266	D267	L268	Q269	K270	Q271	R274	S275						
L276	Y277	Q278	S279	V282	E285	S286	F287	E288	Y289	I290	E291	A292	H293	G294	G300	D301	P302	Q303	E304	L305	T309	R310	A311	L312	C313	R316	Q317	E318	L321	I322	G323	S324	T325	K326	S327	N328	M329	G330	H331	P332	E333	P334	L338	A339	A340	L341	A342	K343	V344	L345	S347						



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 (Å)	384.84, 384.84, 384.84	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.069, 1.069, 1.069	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.20	0/16198	0.30	3/22023 (0.0%)
1	B	0.21	0/16222	0.31	3/22055 (0.0%)
All	All	0.20	0/32420	0.30	6/44078 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1649	PRO	N-CA-C	7.81	124.63	113.47
1	B	587	CYS	N-CA-C	-6.23	104.49	111.28
1	A	1649	PRO	CB-CA-C	-6.21	103.18	113.06
1	B	580	HIS	N-CA-C	-5.78	103.30	110.41
1	B	582	LEU	N-CA-C	-5.45	105.34	111.28
1	A	1648	VAL	CB-CA-C	-5.40	108.62	114.35

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	559	0
1	B	15857	9371	15826	568	0
2	A	96	52	52	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	96	52	52	0	0
All	All	31882	18818	31739	1103	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 (1103) 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:620:MET:HE1	1:B:682:PHE:HB2	1.35	1.05
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	0.80
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
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:570:MET:HE1	1:B:800:ILE:HD12	1.65	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:A:139:MET:HE2	1:A:139:MET:HA	1.71	0.73
1:B:1562:GLN:NE2	1:B:1607:ASP:OD1	2.21	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:B:25:ASN:HB2	1:B:32:MET:HE2	1.72	0.71
1:A:763:PRO:HA	1:A:785:MET:HE2	1.72	0.71
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:139:MET:HE1	1:B:396:GLY:HA3	1.73	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:A:453:MET:HE2	1:A:830:ILE:HD12	1.71	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:343:LYS:HZ3	1:B:354:ALA:HB3	1.56	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:132:MET:HE2	1:B:200:PHE:CZ	2.28	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: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:570:MET:HE1	1:B:800:ILE:CD1	2.24	0.67
1:A:22:PHE:HD1	1:A:32:MET:HE1	1.59	0.67
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: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:A:203:LEU:HD13	1:A:205:MET:HE3	1.75	0.67
1:A:687:MET:HE2	1:A:739:LEU:HD21	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:203:LEU:HD13	1:B:205:MET:HE3	1.74	0.66
1:B:293:HIS:N	1:B:304:GLU:OE2	2.15	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:620:MET:HE2	1:A:650:THR:HG21	1.78	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:13:LEU:HD22	1:A:329:MET:HE1	1.78	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
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:329:MET:HE2	1:B:332:PRO:HD3	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:THR:HG23	1:A:361:SER:O	2.00	0.62
1:A:570:MET:HE1	1:A:800:ILE:HG13	1.81	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:351:GLY:C	1:B:352:LEU:HD12	2.24	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:191:LEU:H	1:B:226:GLU:CD	2.08	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
1:A:444:HIS:NE2	1:A:828:PRO:HG2	2.14	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:A:1942:SER:O	1:A:1943:THR:OG1	2.15	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:SER:OG	1:A:394:GLY:N	2.34	0.60
1:A:687:MET:HE2	1:A:739:LEU:HD11	1.83	0.60
1:B:127:LEU:HD12	1:B:127:LEU:O	2.02	0.60
1:A:14:PRO:O	1:A:32:MET:HE2	2.00	0.60
1:A:33:VAL:HG13	1:A:51:SER:C	2.26	0.60
1:A:189:ASN:HB2	1:A:334:PRO:CG	2.31	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:289:TYR:OH	1:A:291:GLU:OE1	2.20	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:A:687:MET:HE1	1:A:690:ILE:HD12	1.83	0.59
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
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:A:200:PHE:CD1	1:B:132:MET:HE1	2.37	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1970:ASN:C	1:A:1971:LEU:HD12	2.28	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:14:PRO:CD	1:A:329:MET:HE3	2.34	0.58
1:A:737:ASN:HA	1:A:740:VAL:HG22	1.86	0.58
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2088:MET:HE3	1:B:2091:CYS:HB2	1.86	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:311:ALA:C	1:B:312:LEU:HD23	2.28	0.57
1:B:1031:ASP:OD2	1:B:1035:GLN:NE2	2.37	0.57
1:A:351:GLY:C	1:A:352:LEU:HD12	2.30	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:203:LEU:HD12	1:B:132:MET:HE3	1.86	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:A:889:THR:HB	1:A:1030:MET:HE3	1.87	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:A:316:ARG:NH1	1:A:320:LEU:HB2	2.20	0.56
1:A:505:GLY:C	1:A:508:LEU:HD13	2.30	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
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:687:MET:HE2	1:B:739:LEU:HD11	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:542:ASP:OD1	1:A:544:SER:OG	2.15	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: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:322:ILE:HG13	1:B:323:GLY:N	2.20	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: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
1:B:420:LEU:HD21	1:B:512:ARG:HB3	1.88	0.55
1:B:1371:ILE:C	1:B:1372:LEU:HD12	2.32	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1535:THR:HG23	1:A:1535:THR:O	2.07	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:A:610:ILE:CG2	1:A:680:MET:HE2	2.38	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:644:ASN:CG	1:A:770:VAL:HG11	2.33	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:A:22:PHE:CD1	1:A:32:MET:HE1	2.42	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:B:289:TYR:OH	1:B:291:GLU:OE1	2.18	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
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:B:16:SER:HA	1:B:21:GLU:CD	2.34	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:B:577:ILE:HD13	1:B:591:ASP:OD1	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:763:PRO:HA	1:A:785:MET:CE	2.38	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:A:610:ILE:HG23	1:A:680:MET:HE2	1.91	0.52
1:A:654:PRO:C	1:A:657:PRO:HD2	2.34	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: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: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
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:B:1391:LEU:C	1:B:1391:LEU:HD23	2.35	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:1913:VAL:C	1:A:1914:LEU:HD12	2.35	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: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:A:1670:THR:C	1:A:1671:LEU:HD12	2.35	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:1753:LEU:C	1:A:1753:LEU:HD23	2.36	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:B:1896:PHE:CZ	1:B:2088:MET:HE1	2.46	0.50
1:A:662:VAL:HG13	1:A:672:ALA:HB1	1.92	0.50
1:B:879:THR:C	1:B:880:LEU:HD12	2.36	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:A:293:HIS:ND1	1:A:326:LYS:HE2	2.27	0.50
1:A:442:LEU:HD23	1:A:442:LEU:C	2.35	0.50
1:B:766:LEU:HD23	1:B:766:LEU:C	2.37	0.50
1:A:155:ILE:N	1:A:155:ILE:HD12	2.26	0.50
1:A:506:MET:HE2	1:A:546:PHE:CE2	2.47	0.50
1:B:44:LEU:HG	1:B:45:TYR:CD2	2.46	0.50
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:651:ILE:C	1:B:651:ILE:HD12	2.37	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:138:ALA:HB2	1:B:158:ASP:CG	2.37	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:541:THR:HG22	1:A:541:THR:O	2.11	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: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:1214:LEU:HD12	1:B:1214:LEU:C	2.38	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
1:B:1046:LEU:HD12	1:B:1046:LEU:C	2.38	0.49
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:772:LYS:HZ3	1:A:781:ILE:HB	1.75	0.49
1:A:772:LYS:HZ2	1:A:781:ILE:HB	1.77	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:A:1245:VAL:C	1:A:1246:LEU:HD12	2.38	0.48
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: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:453:MET:HE2	1:B:830:ILE:CD1	2.43	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:B:2018:VAL:HB	1:B:2041:MET:HE2	1.94	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:203:LEU:CD1	1:B:205:MET:HE3	2.41	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:1250:GLY:O	1:A:1316:ASN:ND2	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:HE3	1:A:559:ILE:CD1	2.45	0.47
1:B:745:PHE:CD2	1:B:749:LEU:HD11	2.49	0.47
1:B:848:GLU:H	1:B:848:GLU:CD	2.21	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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:527:VAL:HG12	1:B:527:VAL:O	2.15	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:453:MET:HE2	1:B:830:ILE:HD12	1.96	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:570:MET:HE3	1:A:815:LEU:HD11	1.97	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:B:595:SER:HG	1:B:598:GLU:HG3	1.80	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:706:LYS:O	1:B:729:THR:OG1	2.31	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:B:2097:LEU:HD23	1:B:2097:LEU:C	2.40	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:1571:LEU:O	1:A:1843:MET:HE1	2.15	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:B:881:ASP:CG	1:B:1046:LEU:HD21	2.41	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:628:GLU:H	1:B:628:GLU:CD	2.23	0.45
1:A:238:LEU:HD12	1:A:238:LEU:N	2.32	0.45
1:A:290:ILE:HD12	1:A:389:GLY:C	2.41	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: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:B:532:LEU:C	1:B:532:LEU:HD12	2.41	0.45
1:B:615:LEU:HD12	1:B:615:LEU:C	2.41	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1457:VAL:HG23	1:A:1503:MET:HE1	1.99	0.45
1:A:1617:VAL:HG12	1:A:1628:LEU:HD13	1.99	0.45
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:139:MET:HE2	1:A:139:MET:CA	2.42	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
1:A:155:ILE:HG13	1:B:166:MET:HE3	1.99	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: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: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:B:655:GLN:C	1:B:658:VAL:HG12	2.42	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:THR:HG21	1:B:145:SER:CB	2.47	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
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:168:LEU:HD23	1:A:168:LEU:C	2.43	0.43
1:A:1317:CYS:SG	1:A:1322:LEU:HD12	2.57	0.43
1:B:254:ASP:CG	1:B:265:SER:HB3	2.43	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: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:1583:LEU:HD11	1:A:1587:ALA:CB	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:MET:HE2	1:B:9:MET:HB3	1.94	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
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:333:GLU:HB2	1:A:334:PRO:CD	2.49	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:645:SER:HG	1:B:648:THR:H	1.57	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:1205:GLU:CD	1:B:1209:LEU:HD12	2.43	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:A:502:GLN:HG3	1:A:506:MET:HE1	2.00	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:780:THR:C	1:A:781:ILE:HD12	2.44	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:1899:GLU:HB3	1:A:2088:MET:HE2	2.00	0.42
1:A:1922:THR:HG22	1:A:1923:GLY:N	2.33	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:127:LEU:HD12	1:A:127:LEU:C	2.44	0.42
1:A:160:ALA:O	1:A:161:CYS:HB2	2.19	0.42
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:B:1445:ALA:C	1:B:1446:ILE:HD13	2.44	0.42
1:A:60:PHE:CE2	1:A:62:ALA:HA	2.54	0.42
1:A:692:PRO:C	1:A:695:LEU:HG	2.44	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:1196:LEU:C	1:B:1196:LEU:HD23	2.44	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:923:THR:O	1:A:923:THR:HG23	2.19	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:587:CYS:O	1:B:588:GLY:C	2.63	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:A:760:GLU:CD	1:A:765:ALA:HA	2.43	0.42
1:B:621:ALA:CB	1:B:674:GLU:HA	2.50	0.42
1:B:830:ILE:O	1:B:830:ILE:HG22	2.20	0.42
1:B:1970:ASN:C	1:B:1971:LEU:HD12	2.44	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:MET:HE2	1:A:830:ILE:CD1	2.45	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: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: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:702:ILE:HD12	1:A:702:ILE:N	2.35	0.42
1:A:1446:ILE:HD12	1:A:1446:ILE:C	2.45	0.42
1:B:311:ALA:O	1:B:312:LEU:HD23	2.19	0.42
1:B:576:GLY:C	1:B:577:ILE:HD12	2.45	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:105:THR:HG23	1:A:182:ALA:C	2.45	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:67:VAL:HG21	1:A:75:MET:HE1	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:712:TRP:CD1	1:A:712:TRP:C	2.97	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:B:721:GLN:HB3	1:B:724:SER:HG	1.86	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:166:MET:HE1	1:B:251:THR:HG21	2.03	0.41
1:B:620:MET:CE	1:B:682:PHE:HB2	2.26	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:52:GLY:C	1:B:53:LYS:HG3	2.46	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
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:804:HIS:CD2	1:B:804:HIS:C	2.99	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:1132:ALA:O	1:A:1133:ALA:C	2.63	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:1018:GLY:O	1:B:1078:VAL:HG12	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1333:VAL:HG12	1:B:1386:LEU:HD11	2.01	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:570:MET:HE3	1:A:815:LEU:HD21	2.03	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:1344:LEU:C	1:B:1344:LEU:HD23	2.45	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: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:277:TYR:CD1	1:A:277:TYR:C	2.99	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
1:B:139:MET:HE3	1:B:143:ARG:CD	2.52	0.40
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: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:534:VAL:HG12	1:B:538:LEU:HD13	2.02	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:787:LYS:HG2	1:B:788:ASP:CG	2.47	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 [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%)	2001 (97%)	59 (3%)	0	100	100
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 [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%)	92	97
All	All	3413/4234 (81%)	3411 (100%)	2 (0%)	92	97

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

Mol	Chain	Res	Type
1	B	104	HIS
1	B	580	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	328	ASN
1	A	350	HIS
1	A	356	ASN
1	A	358	HIS
1	A	379	GLN
1	A	387	ASN
1	A	399	ASN
1	A	596	GLN
1	A	614	HIS
1	A	755	HIS
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	1682	GLN
1	A	2101	GLN
1	B	78	GLN
1	B	173	GLN
1	B	199	GLN
1	B	220	ASN
1	B	350	HIS
1	B	356	ASN
1	B	358	HIS
1	B	360	HIS
1	B	375	GLN
1	B	387	ASN
1	B	768	GLN
1	B	804	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	813	ASN
1	B	920	HIS
1	B	1006	GLN
1	B	1025	ASN
1	B	1056	HIS
1	B	1074	GLN
1	B	1204	GLN
1	B	1278	GLN
1	B	1482	HIS
1	B	1595	GLN
1	B	1722	ASN
1	B	1845	GLN
1	B	1848	HIS
1	B	1855	GLN
1	B	1983	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NDP	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%)
2	NDP	B	2602	-	47,52,52	0.66	0	61,80,80	0.84	2 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NDP	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
2	NDP	B	2602	-	-	11/30/77/77	0/5/5/5

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	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

Continued on next page...

Continued from previous page...

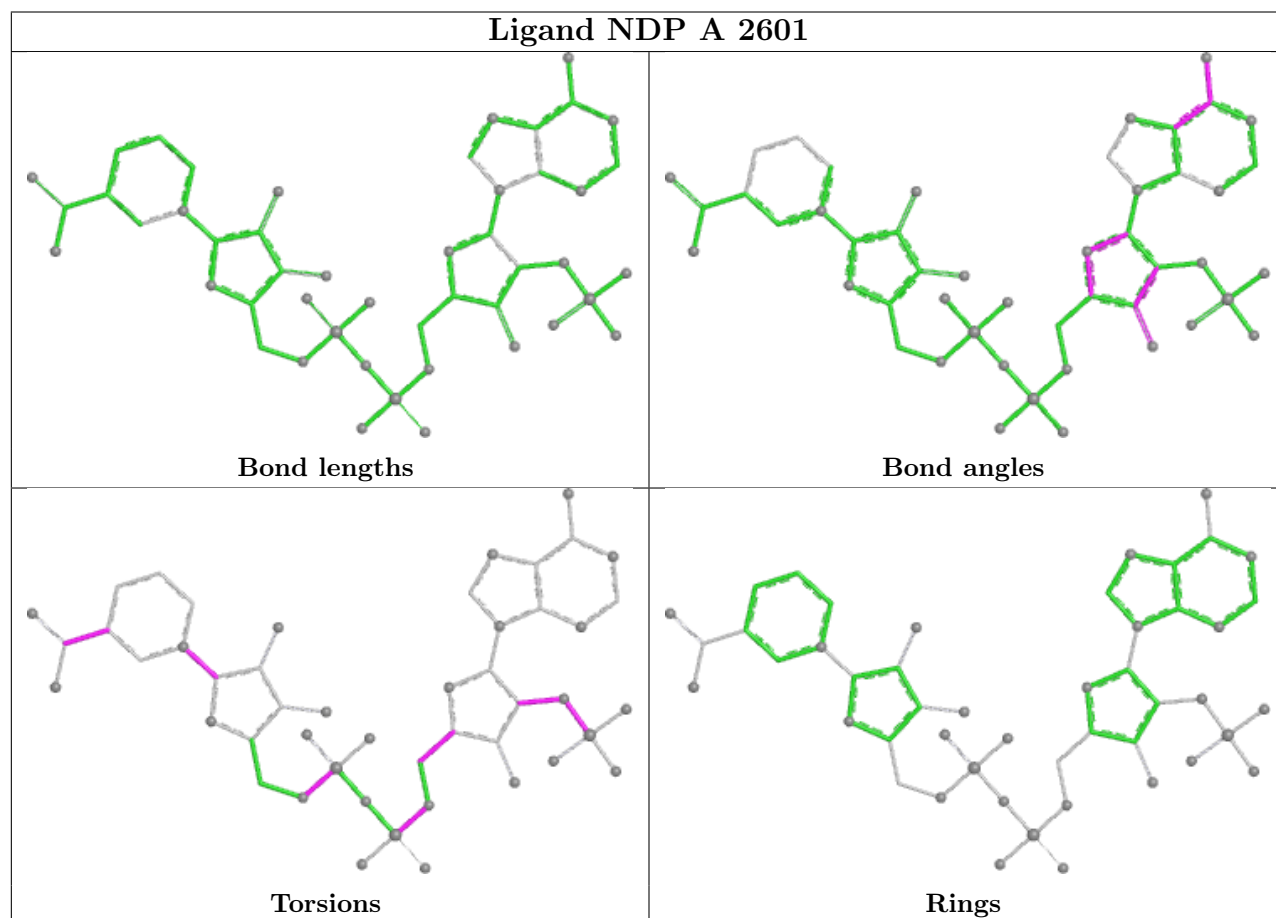
Mol	Chain	Res	Type	Atoms
2	B	2601	NDP	C2N-C3N-C7N-N7N
2	B	2602	NDP	C5B-O5B-PA-O2A
2	B	2602	NDP	C2N-C3N-C7N-N7N
2	A	2601	NDP	O4D-C1D-N1N-C2N
2	B	2601	NDP	O4B-C4B-C5B-O5B
2	A	2601	NDP	C3B-C2B-O2B-P2B
2	B	2601	NDP	C3B-C4B-C5B-O5B
2	B	2602	NDP	C4B-C5B-O5B-PA
2	A	2601	NDP	C1B-C2B-O2B-P2B
2	B	2602	NDP	O4B-C4B-C5B-O5B
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
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

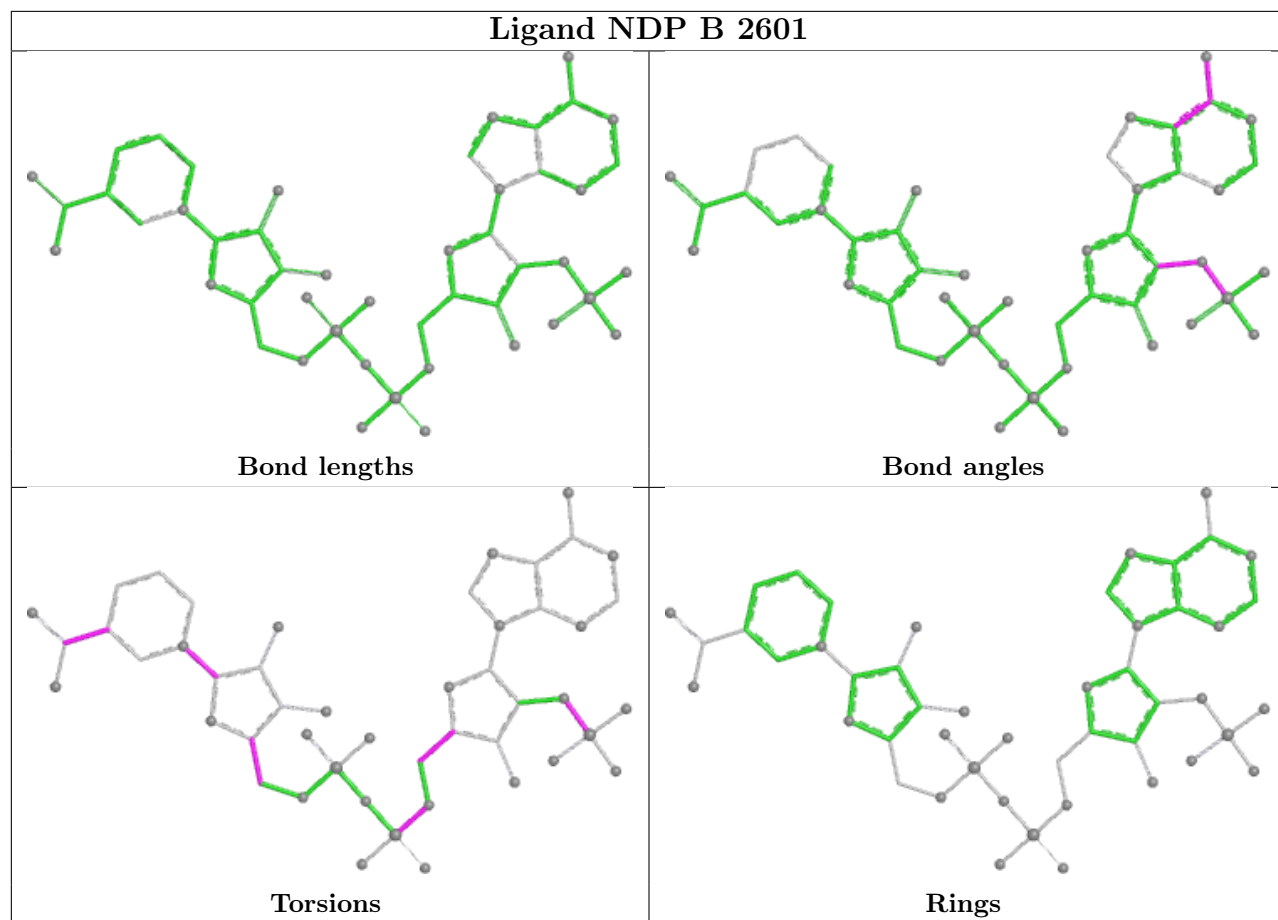
There are no ring outliers.

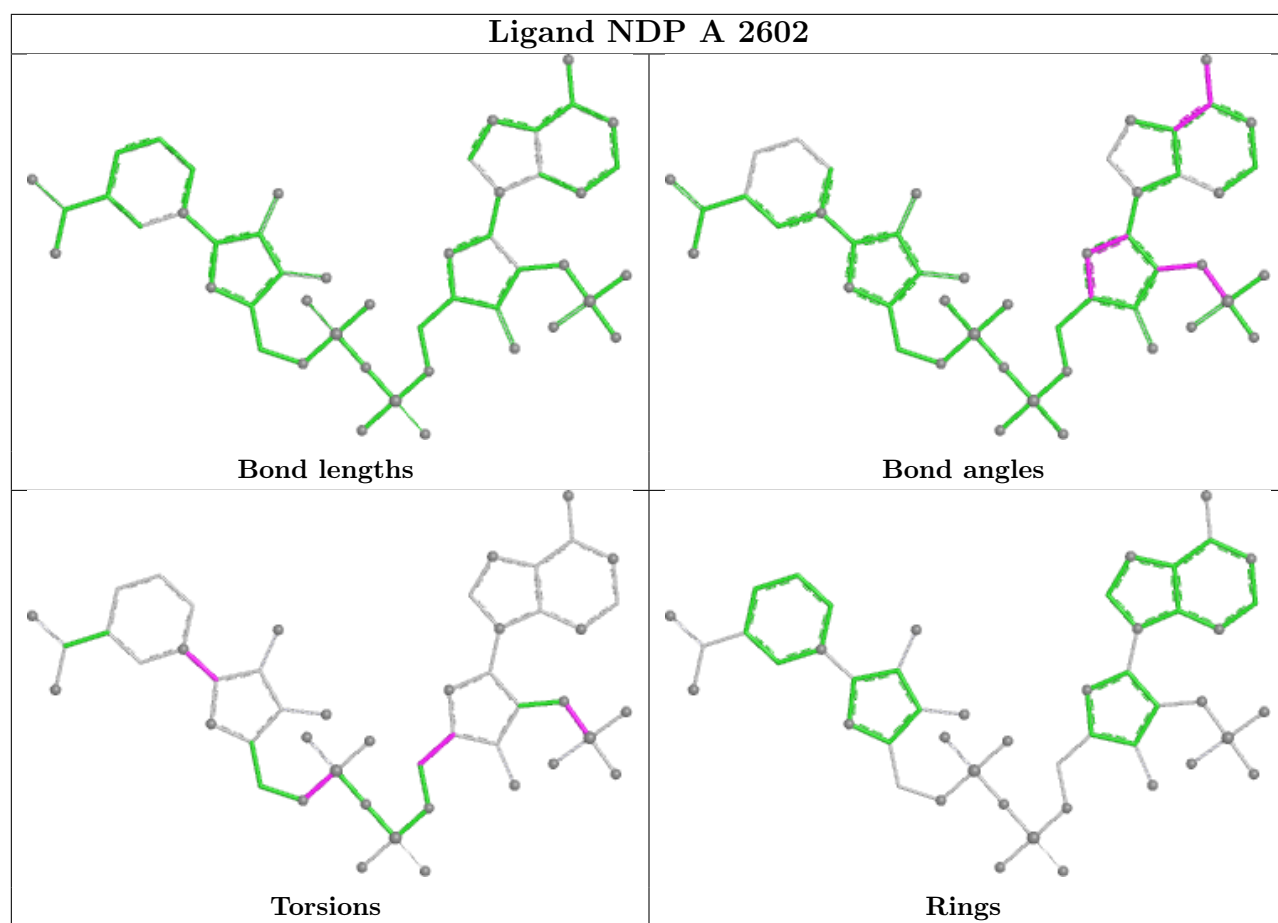
No monomer is involved in short contacts.

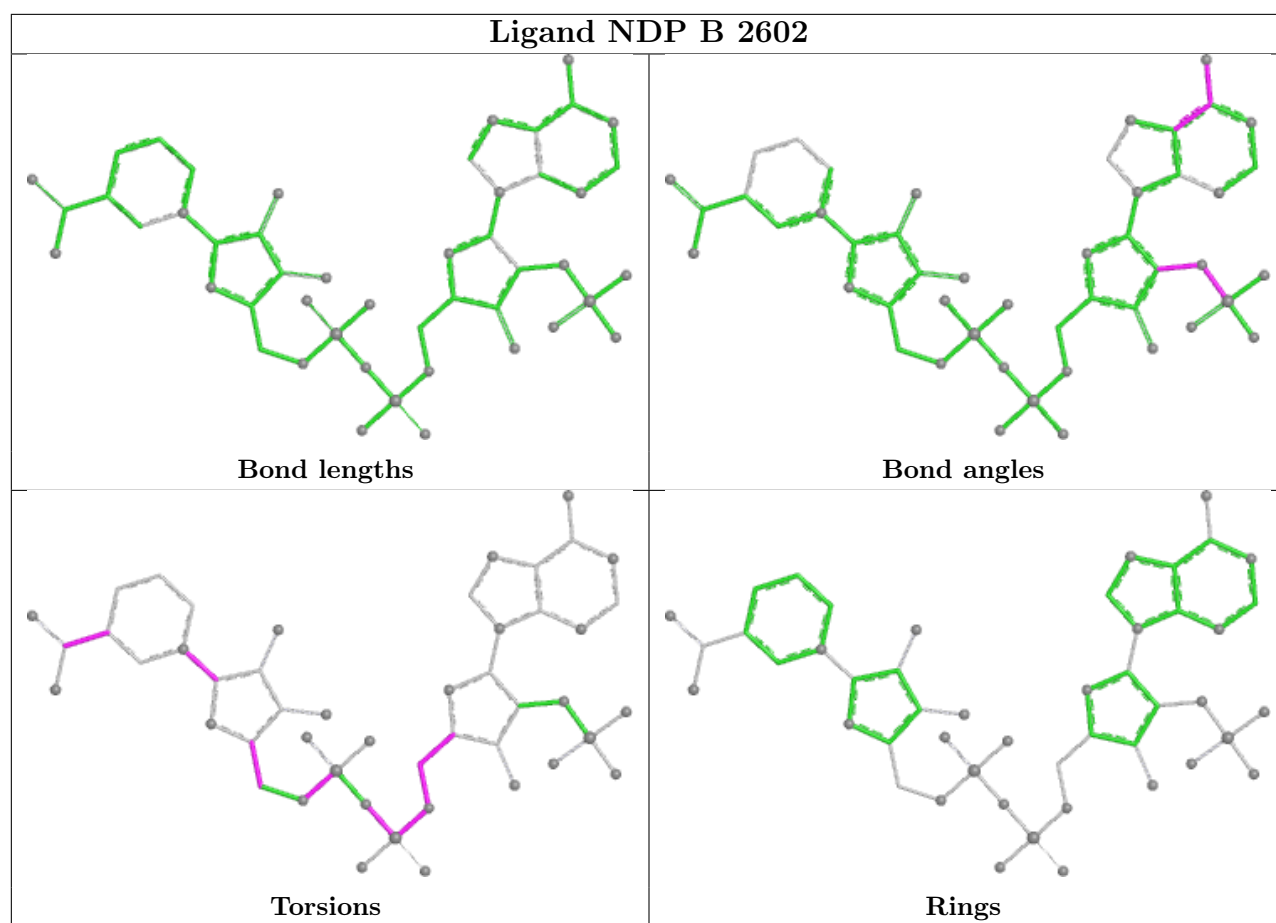
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

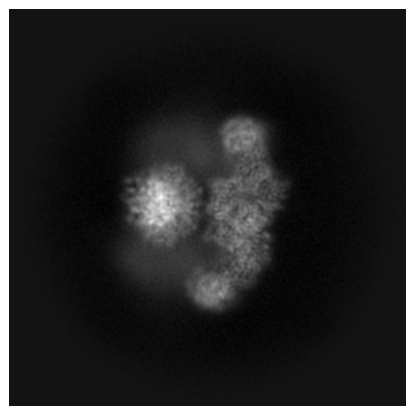
6 Map visualisation [i](#)

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.

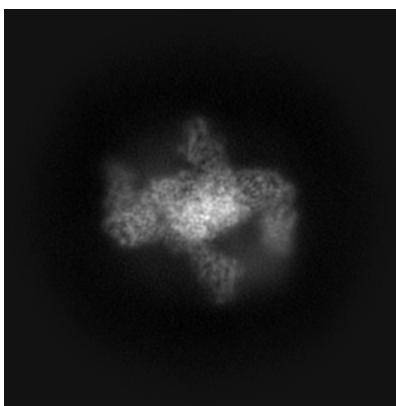
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

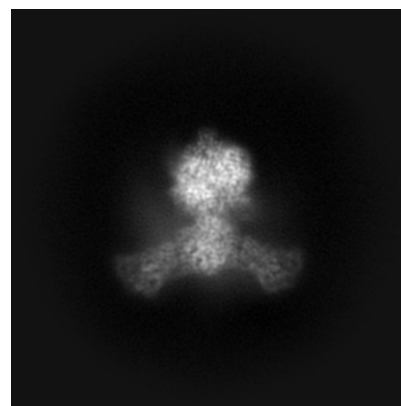
6.1.1 Primary map



X

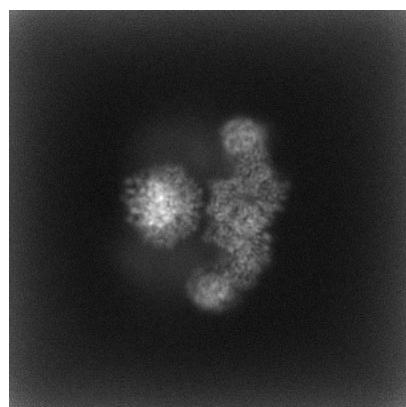


Y

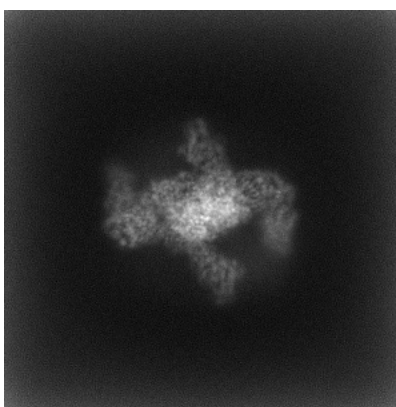


Z

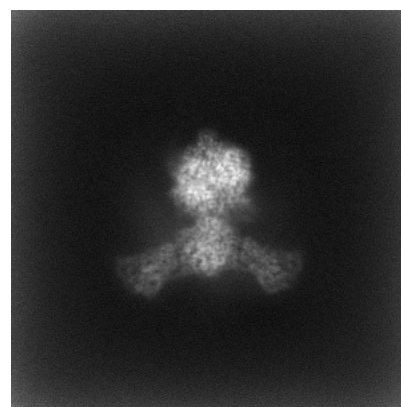
6.1.2 Raw map



X



Y

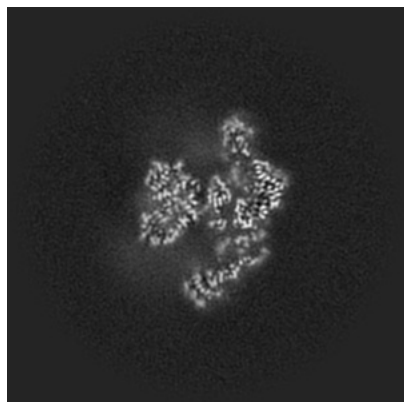


Z

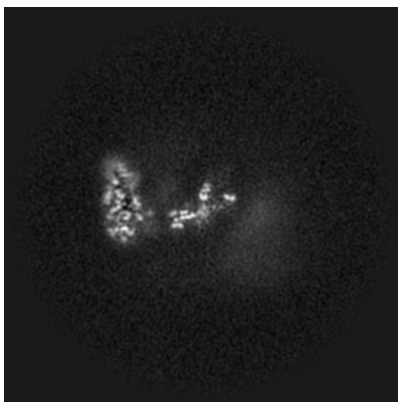
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

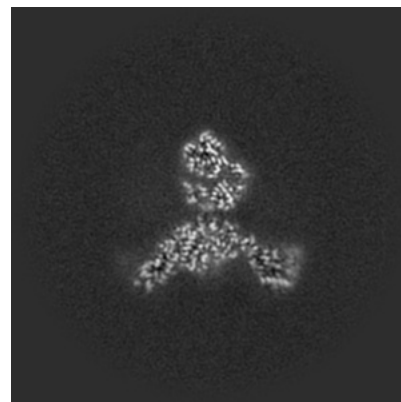
6.2.1 Primary map



X Index: 180

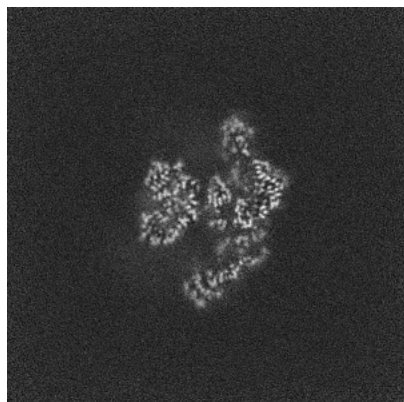


Y Index: 180



Z Index: 180

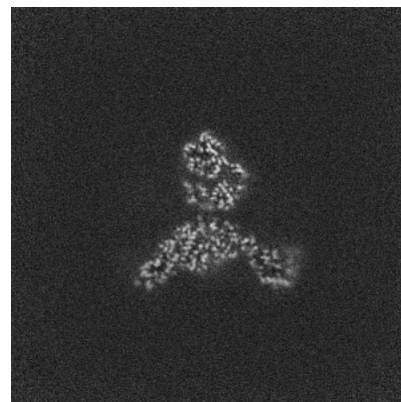
6.2.2 Raw map



X Index: 180



Y Index: 180

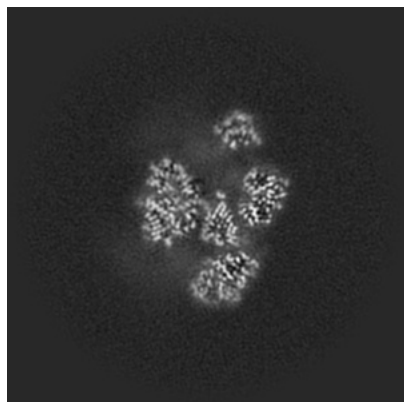


Z Index: 180

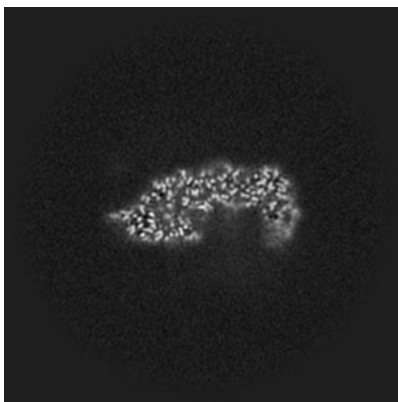
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

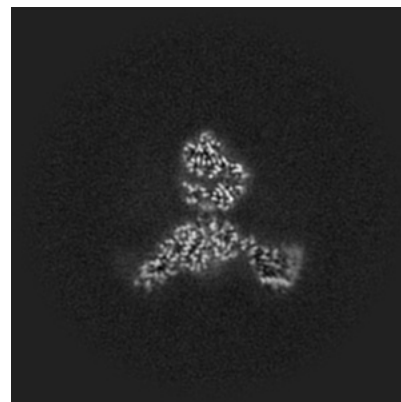
6.3.1 Primary map



X Index: 173

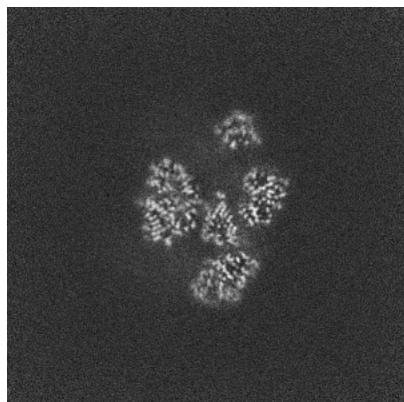


Y Index: 207

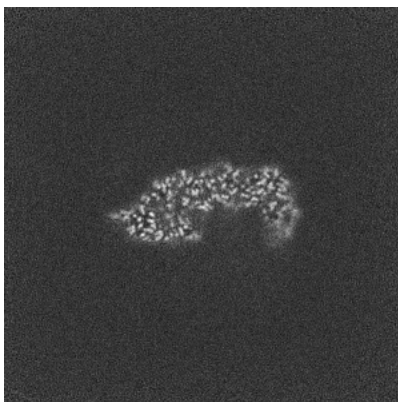


Z Index: 179

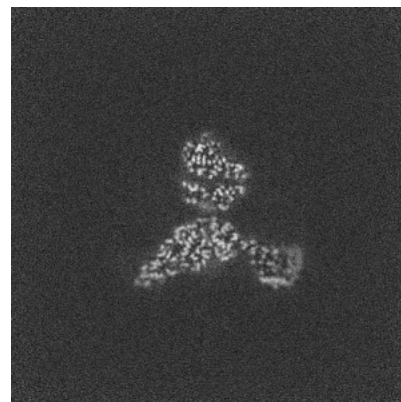
6.3.2 Raw map



X Index: 173



Y Index: 207

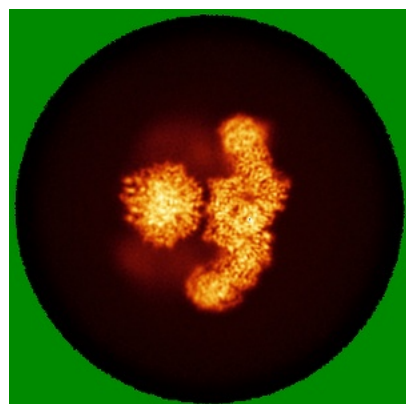


Z Index: 178

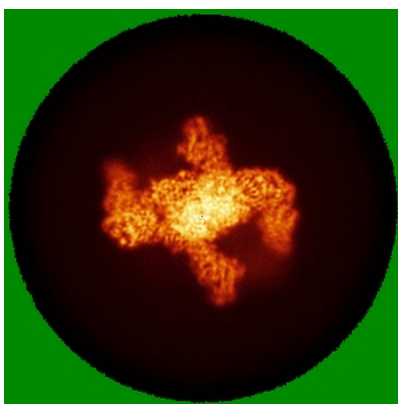
The images above show the largest variance slices of the map in three orthogonal directions.

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

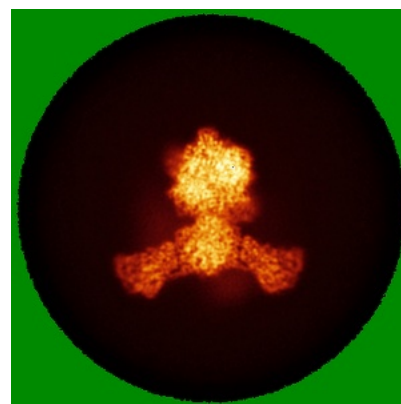
6.4.1 Primary map



X

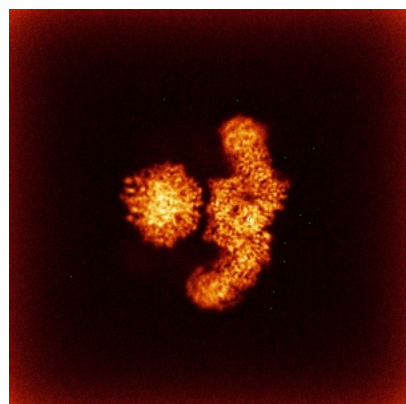


Y

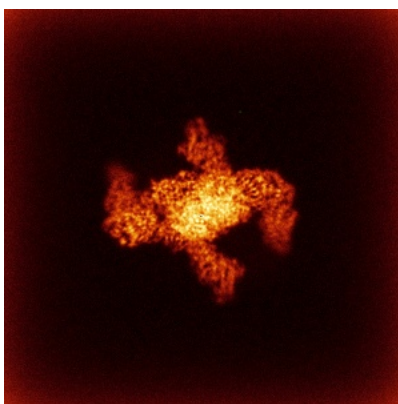


Z

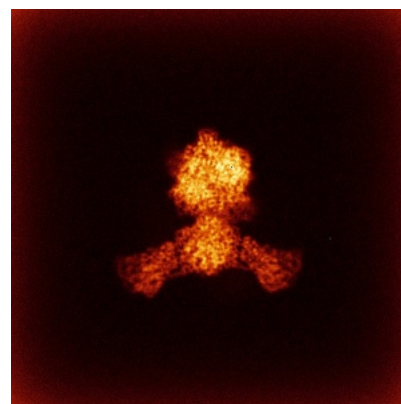
6.4.2 Raw map



X



Y

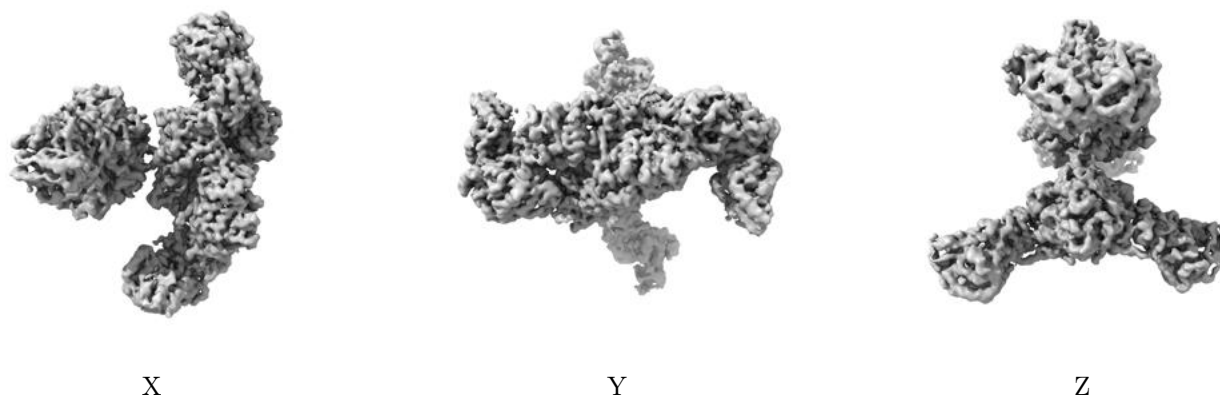


Z

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.

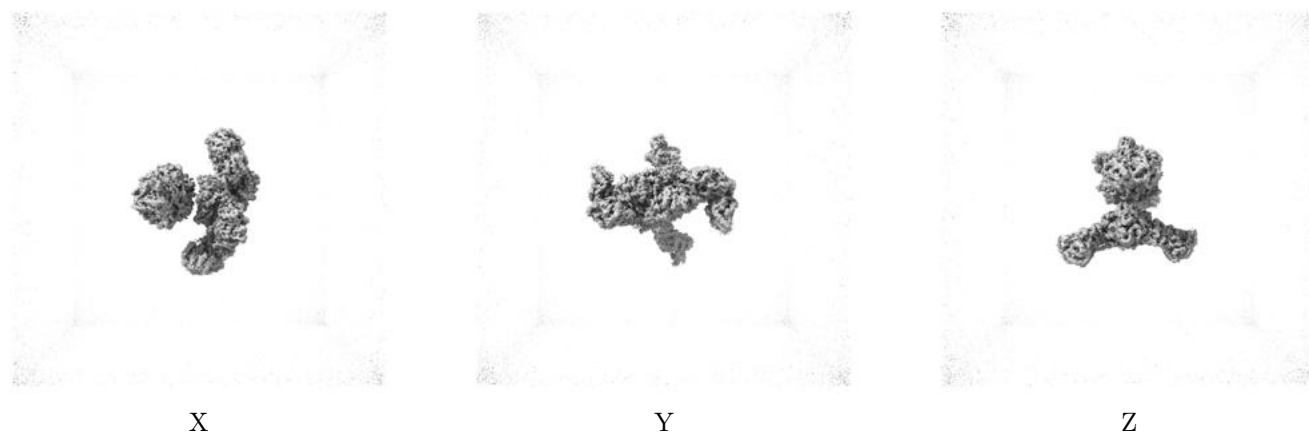
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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



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.

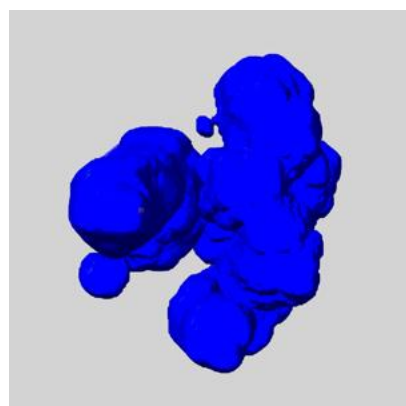
6.6 Mask visualisation [i](#)

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

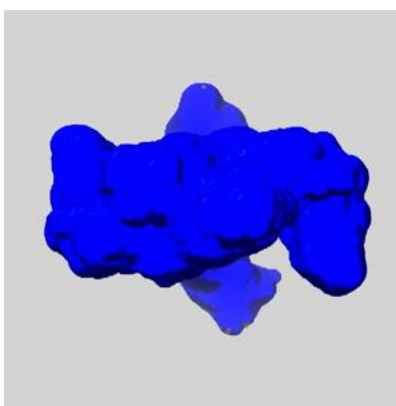
A mask typically either:

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

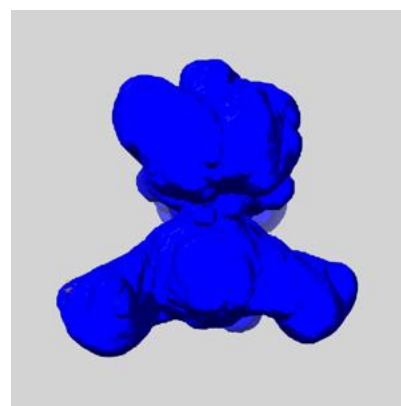
6.6.1 emd_43353_msk_1.map [i](#)



X



Y

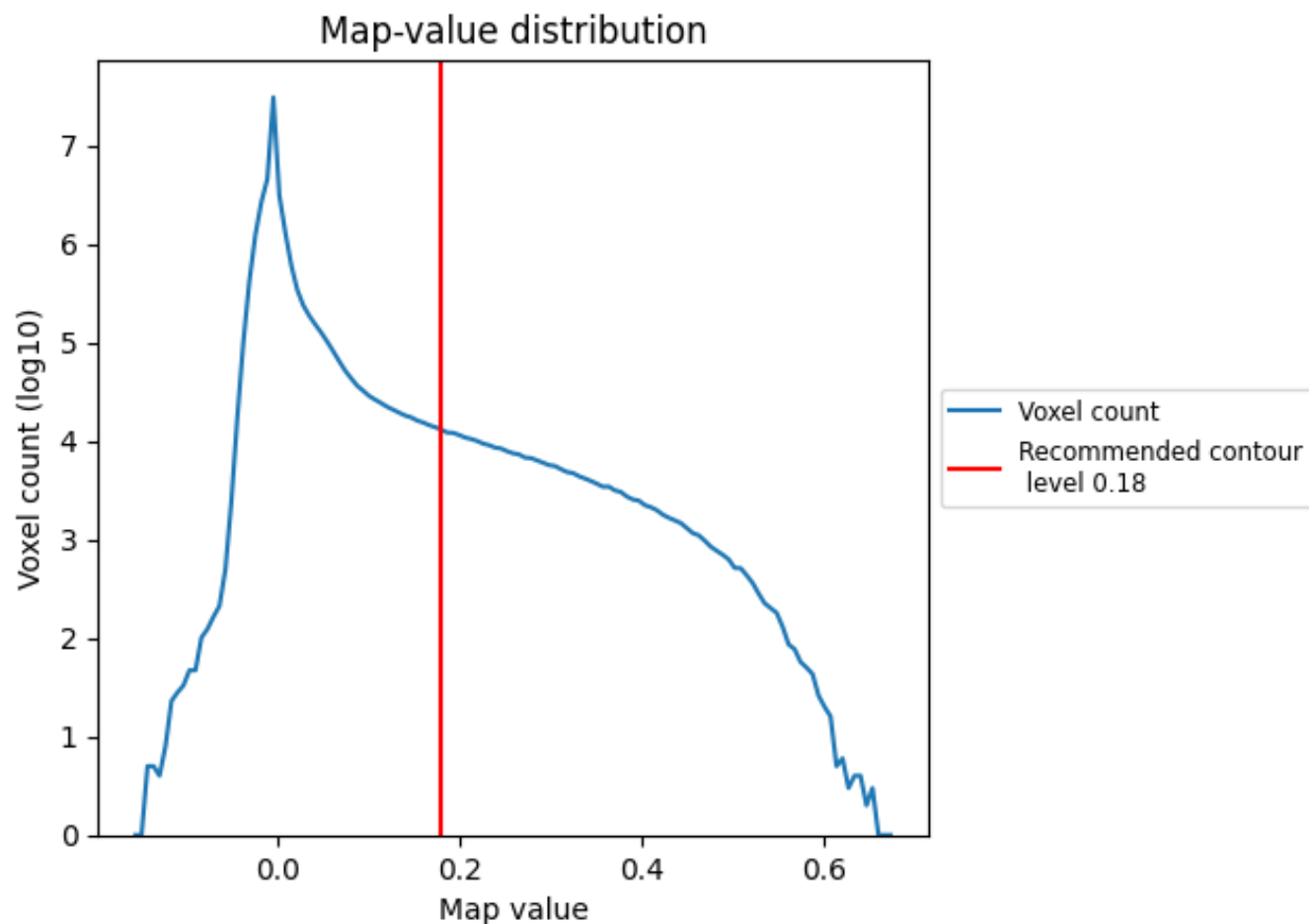


Z

7 Map analysis [i](#)

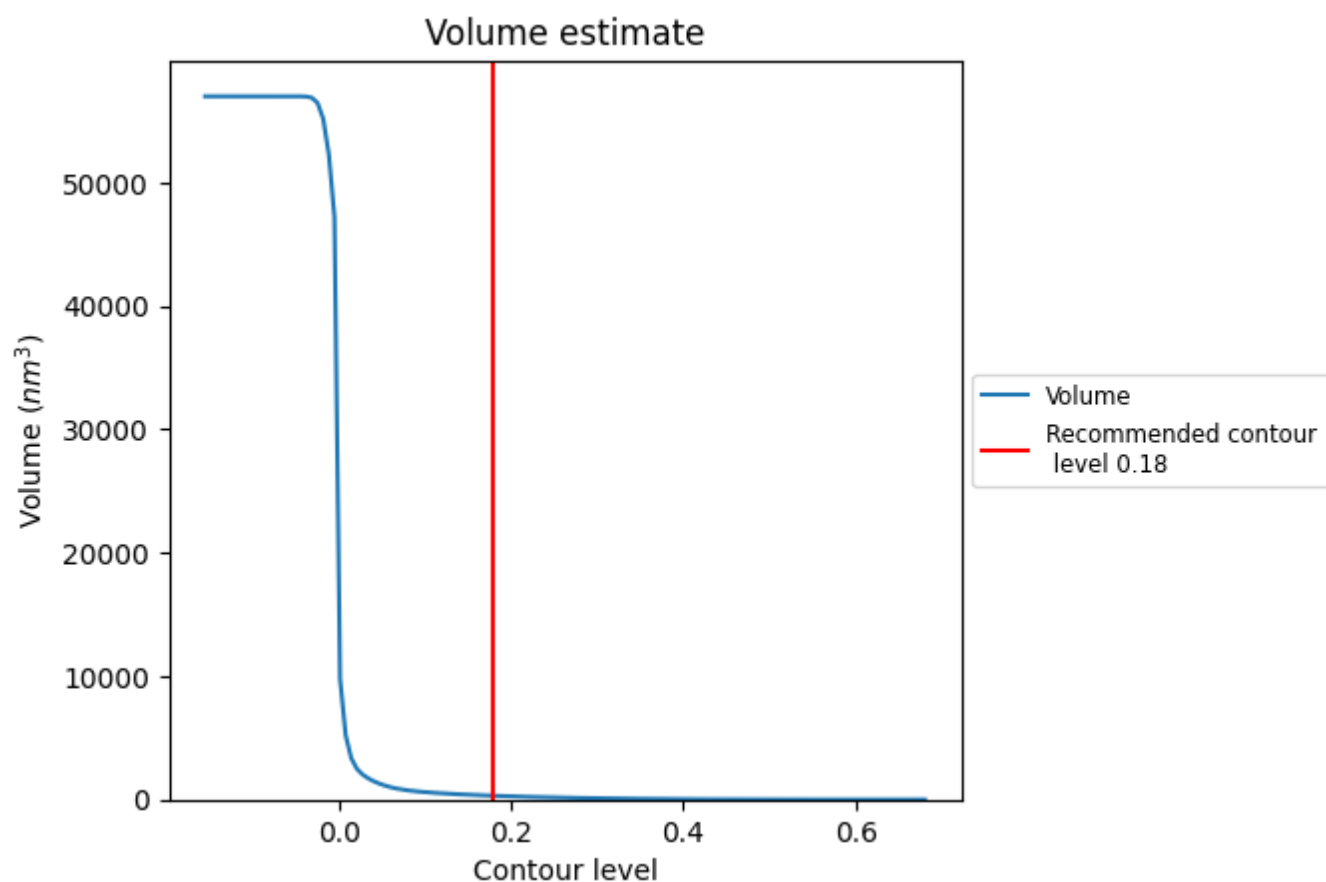
This section contains the results of statistical analysis of the map.

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.

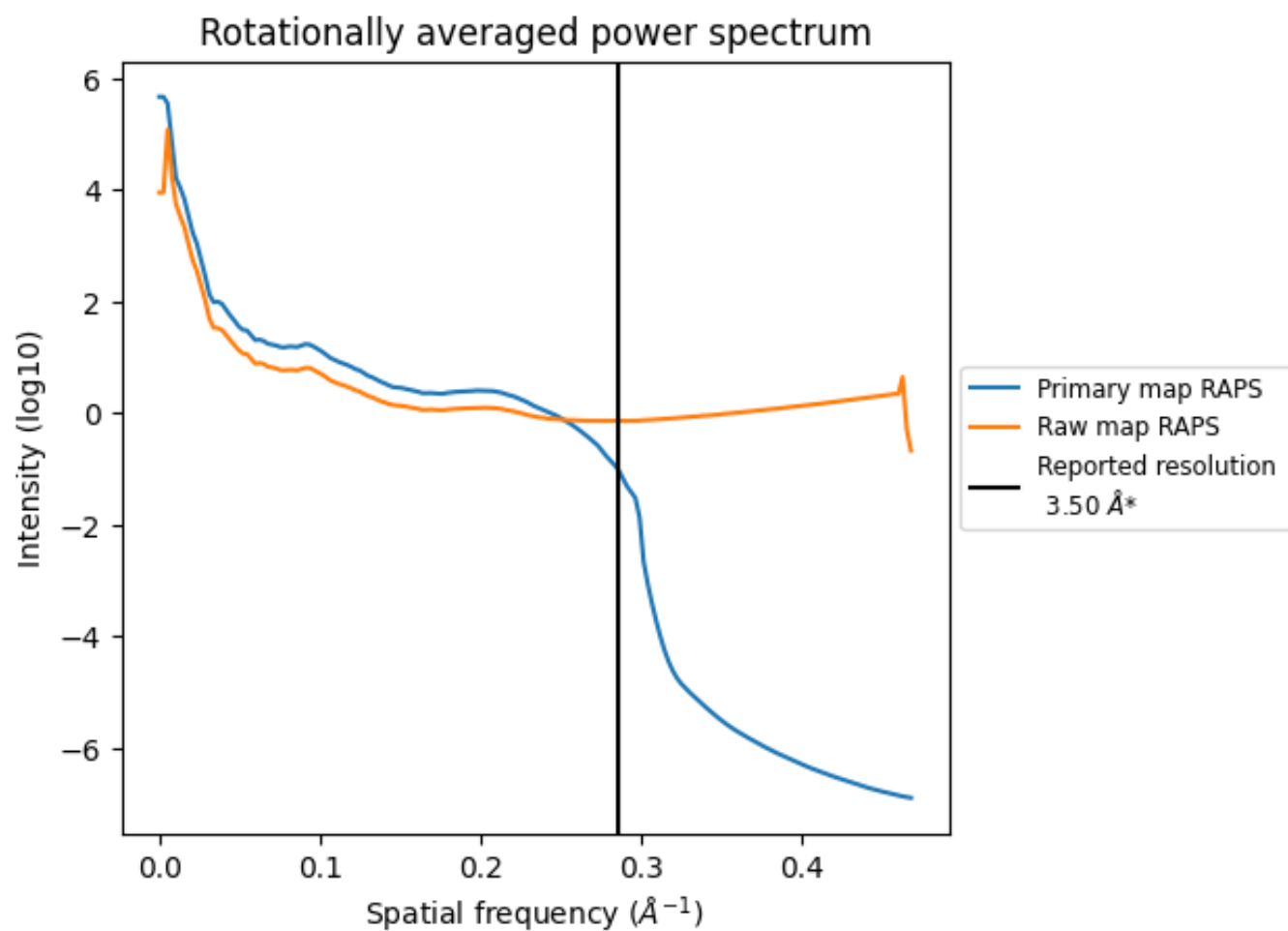
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 307 nm³; 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 ⓘ

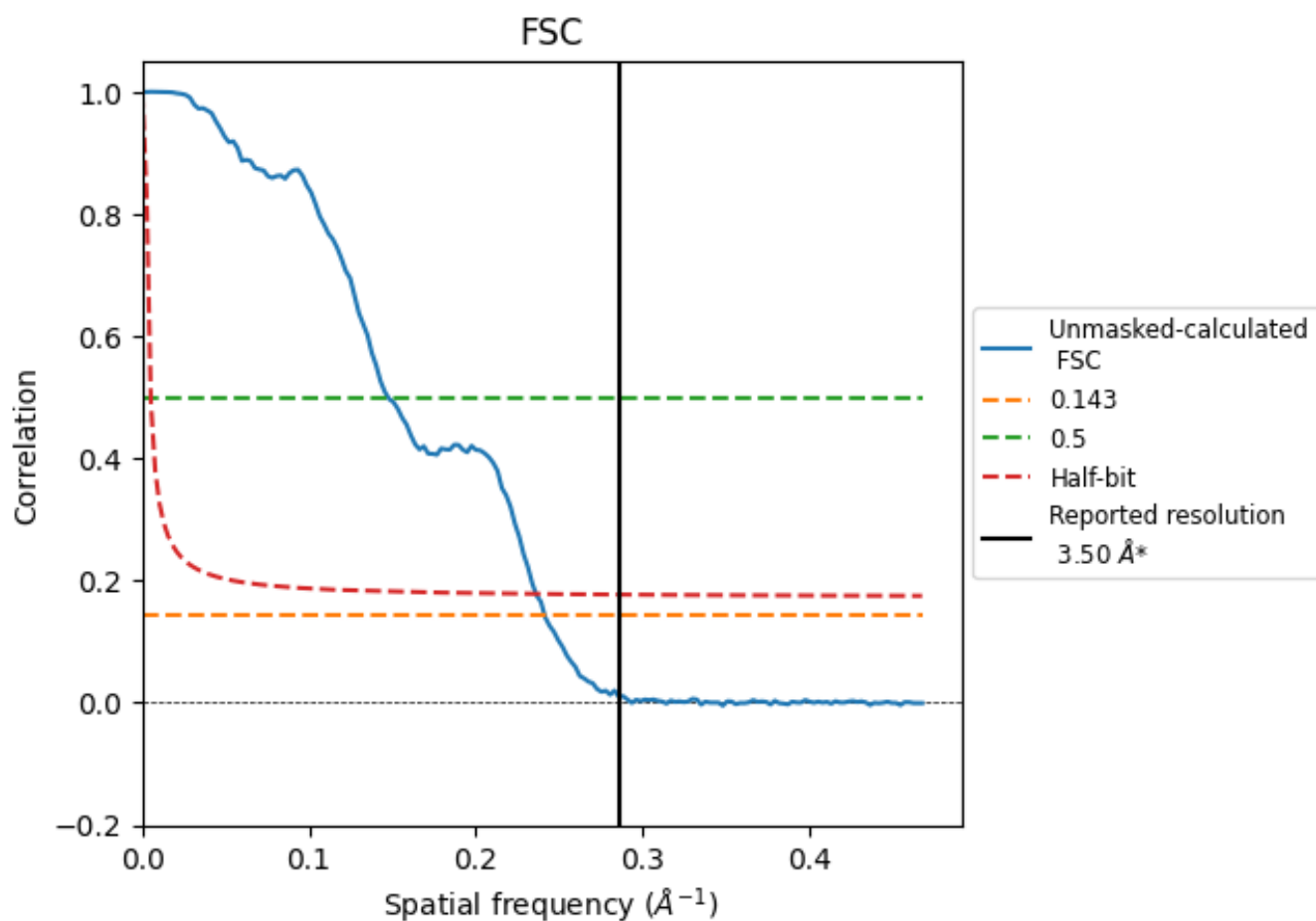


*Reported resolution corresponds to spatial frequency of 0.286 \AA^{-1}

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 \AA^{-1}

8.2 Resolution estimates [i](#)

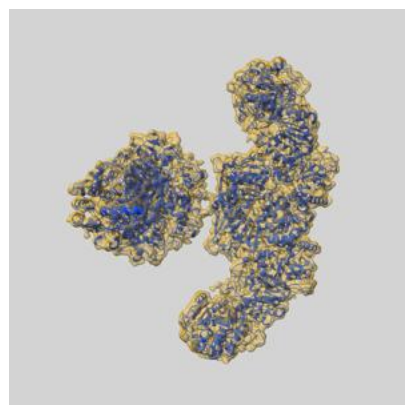
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.14	6.78	4.24

*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 %

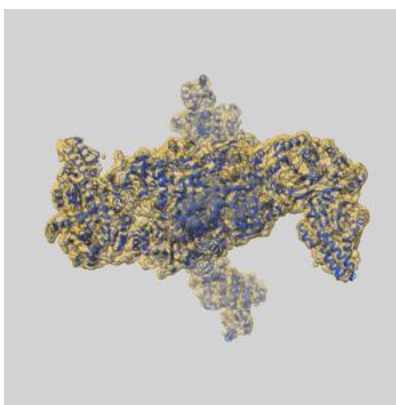
9 Map-model fit [i](#)

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.

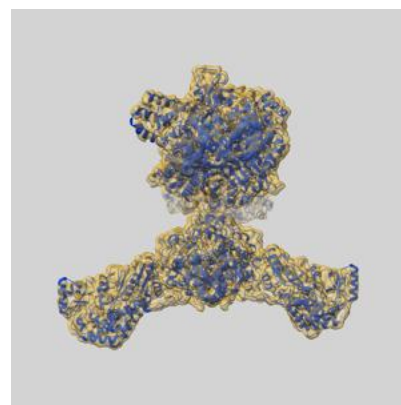
9.1 Map-model overlay [i](#)



X



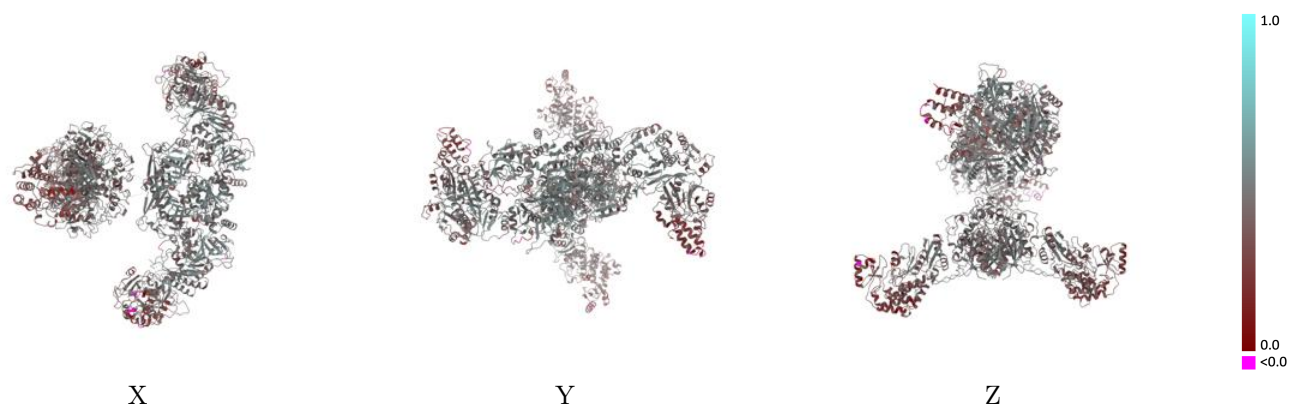
Y



Z

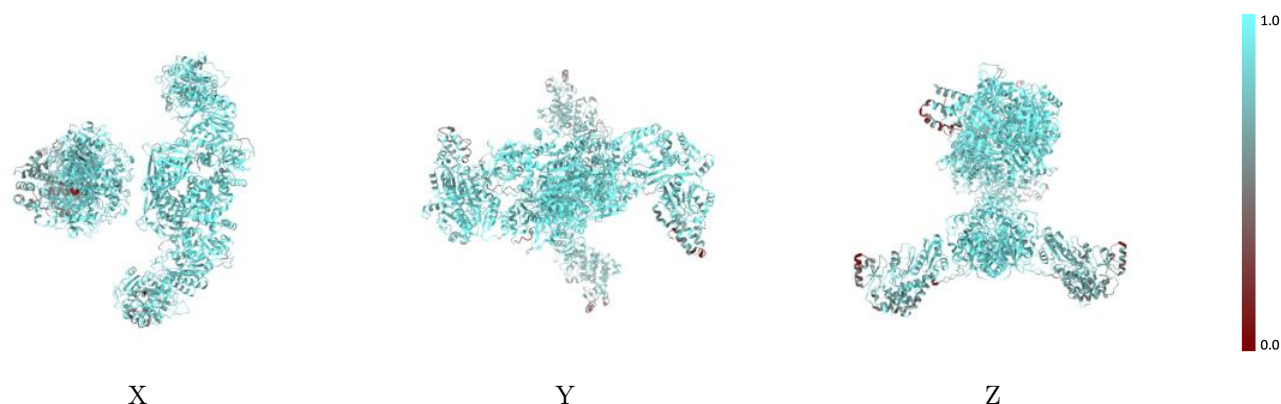
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



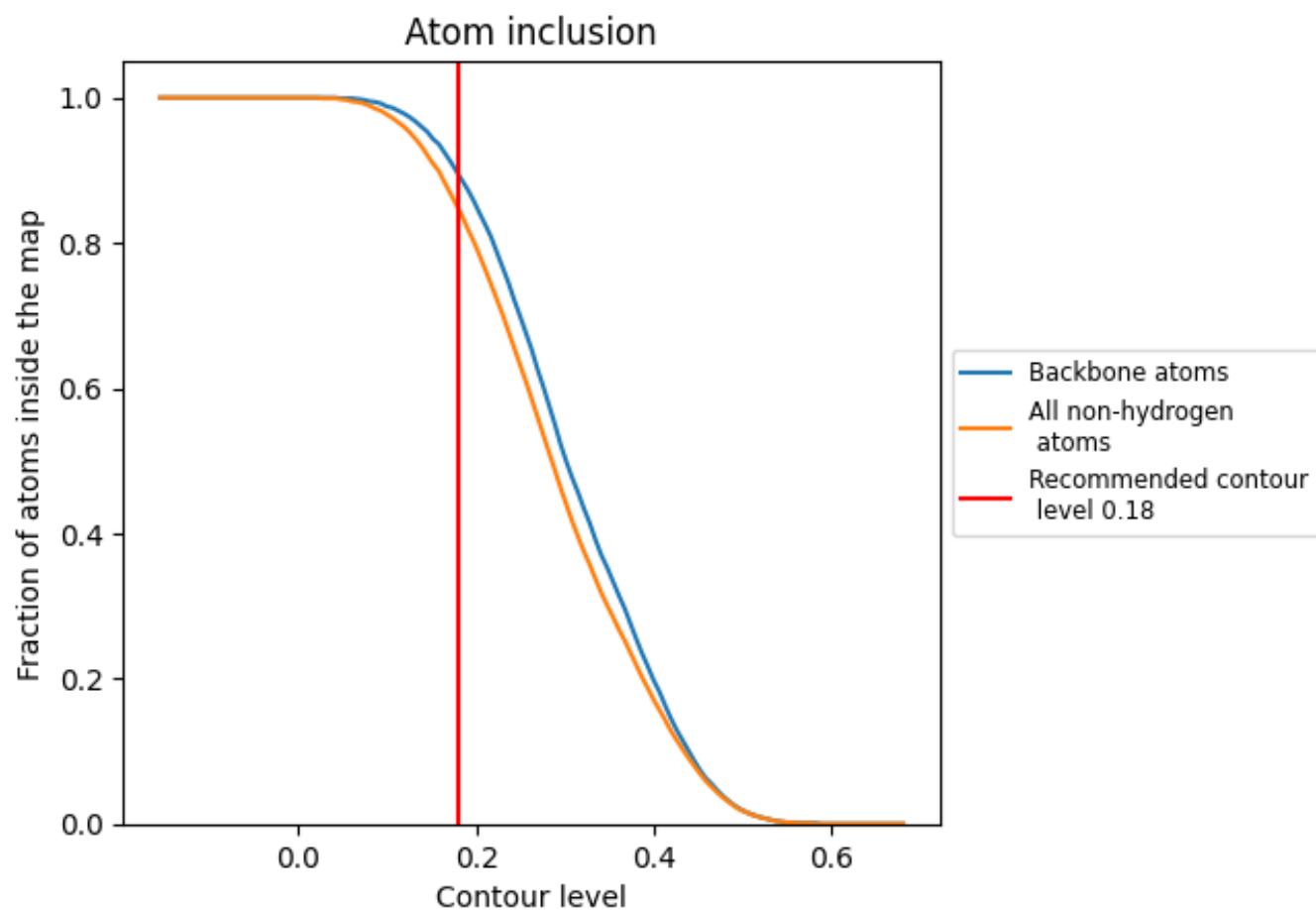
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

