



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 07:39 PM UTC

PDB ID : 8E6U / pdb_00008e6u
EMDB ID : EMD-27926
Title : Human TRPM2 ion channel in 1 mM F-dADPR
Authors : Wang, L.; Fu, T.M.; Xia, S.; Wu, H.
Deposited on : 2022-08-23
Resolution : 3.20 Å(reported)

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 EMD 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

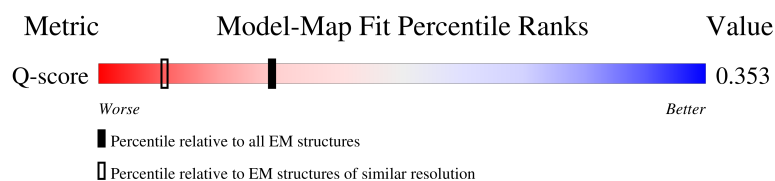
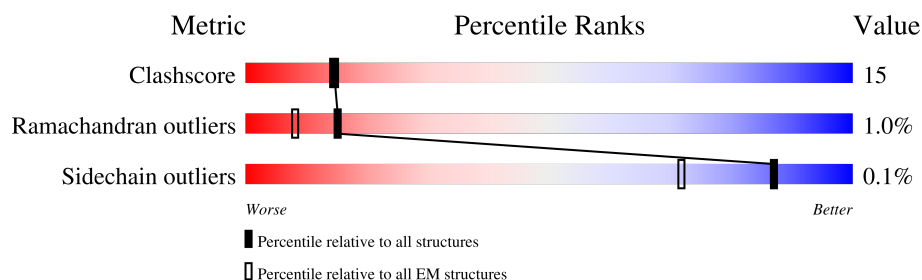
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

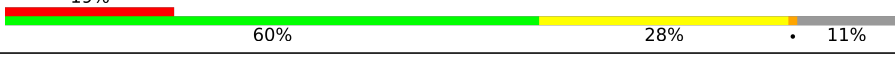
The reported resolution of this entry is 3.20 Å.

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	15020 (2.70 - 3.70)

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	1503	
1	B	1503	
1	C	1503	
1	D	1503	

2 Entry composition [i](#)

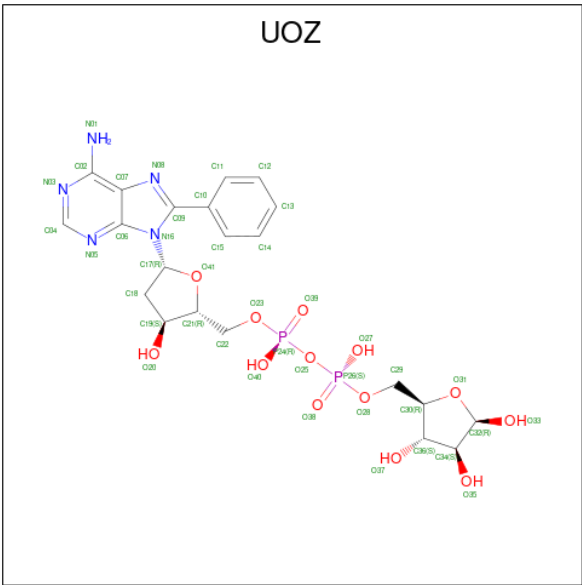
There are 2 unique types of molecules in this entry. The entry contains 43388 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Transient receptor potential cation channel subfamily M member 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1337	Total	C	N	O	S	0	0
			10774	6939	1862	1919	54		
1	B	1337	Total	C	N	O	S	0	0
			10774	6939	1862	1919	54		
1	C	1337	Total	C	N	O	S	0	0
			10774	6939	1862	1919	54		
1	D	1337	Total	C	N	O	S	0	0
			10774	6939	1862	1919	54		

- Molecule 2 is [(2R,3S,5R)-5-(6-amino-8-phenyl-9H-purin-9-yl)-3-hydroxyoxolan-2-yl]methyl [(2R,3S,4S,5R)-3,4,5-trihydroxyoxolan-2-yl]methyl dihydrogen diphosphate (non-preferred name) (CCD ID: UOZ) (formula: C₂₁H₂₇N₅O₁₃P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			41	21	5	13	2	

Continued on next page...

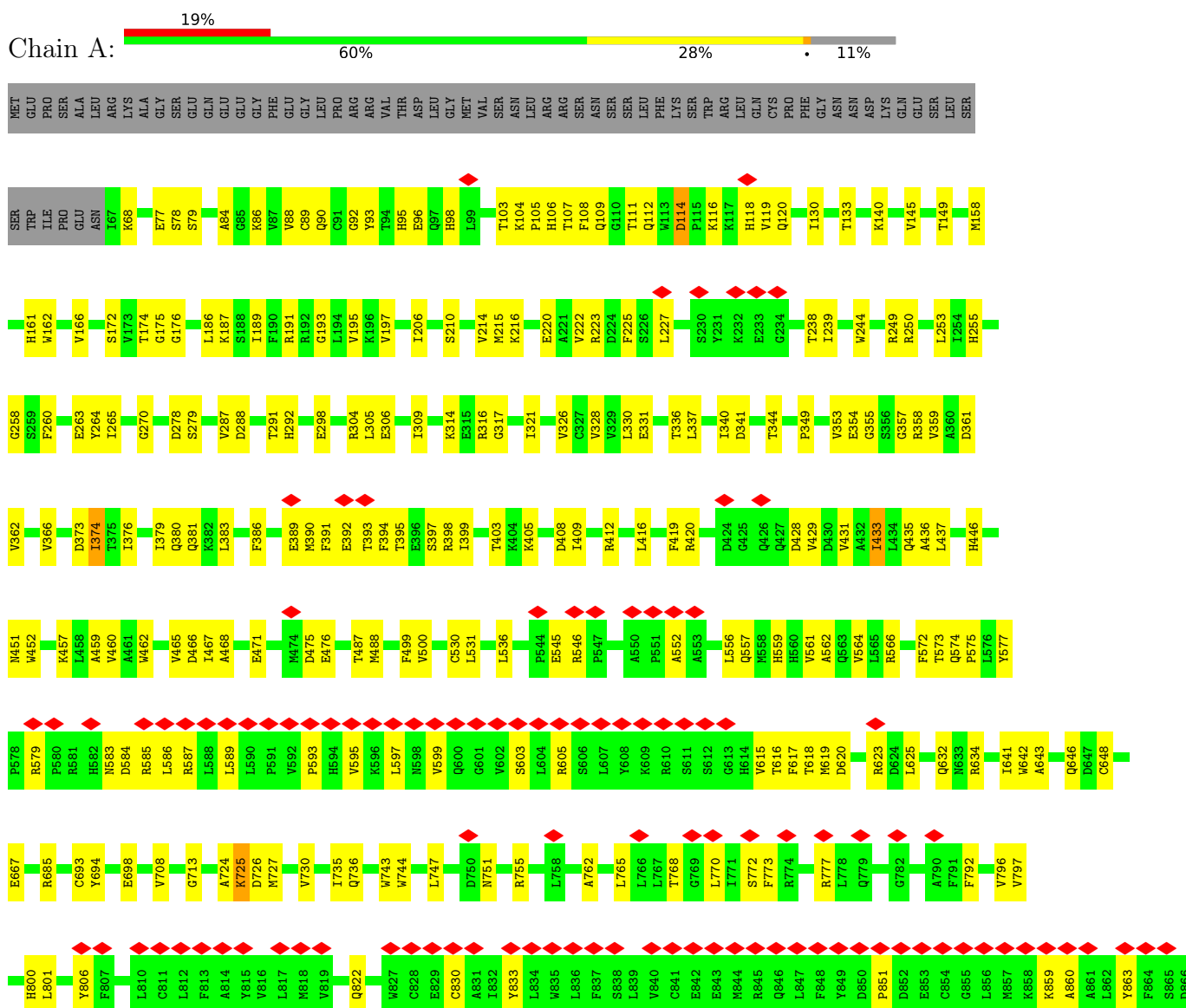
Continued from previous page...

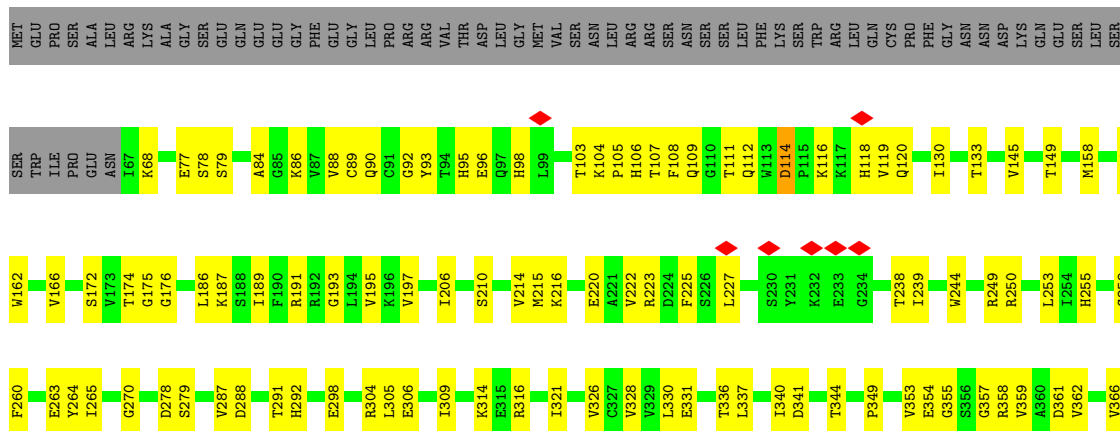
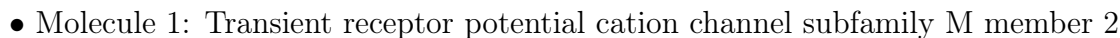
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			32	16	5	9	2	
2	B	1	Total	C	N	O	P	0
			41	21	5	13	2	
2	B	1	Total	C	N	O	P	0
			32	16	5	9	2	
2	C	1	Total	C	N	O	P	0
			41	21	5	13	2	
2	C	1	Total	C	N	O	P	0
			32	16	5	9	2	
2	D	1	Total	C	N	O	P	0
			41	21	5	13	2	
2	D	1	Total	C	N	O	P	0
			32	16	5	9	2	

3 Residue-property plots

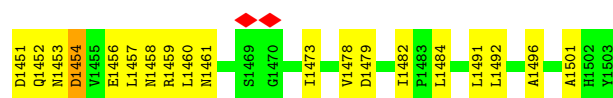
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Transient receptor potential cation channel subfamily M member 2

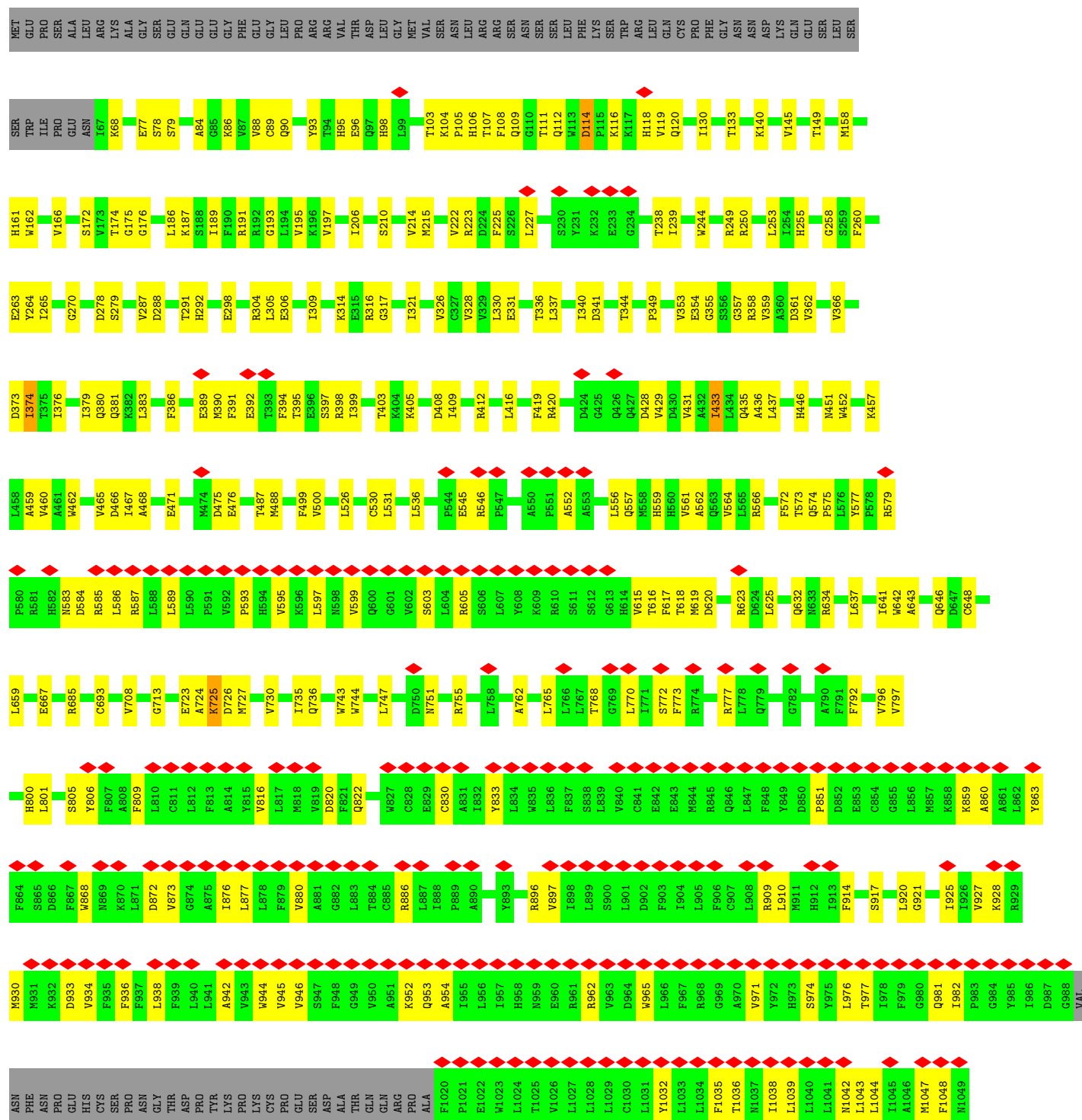


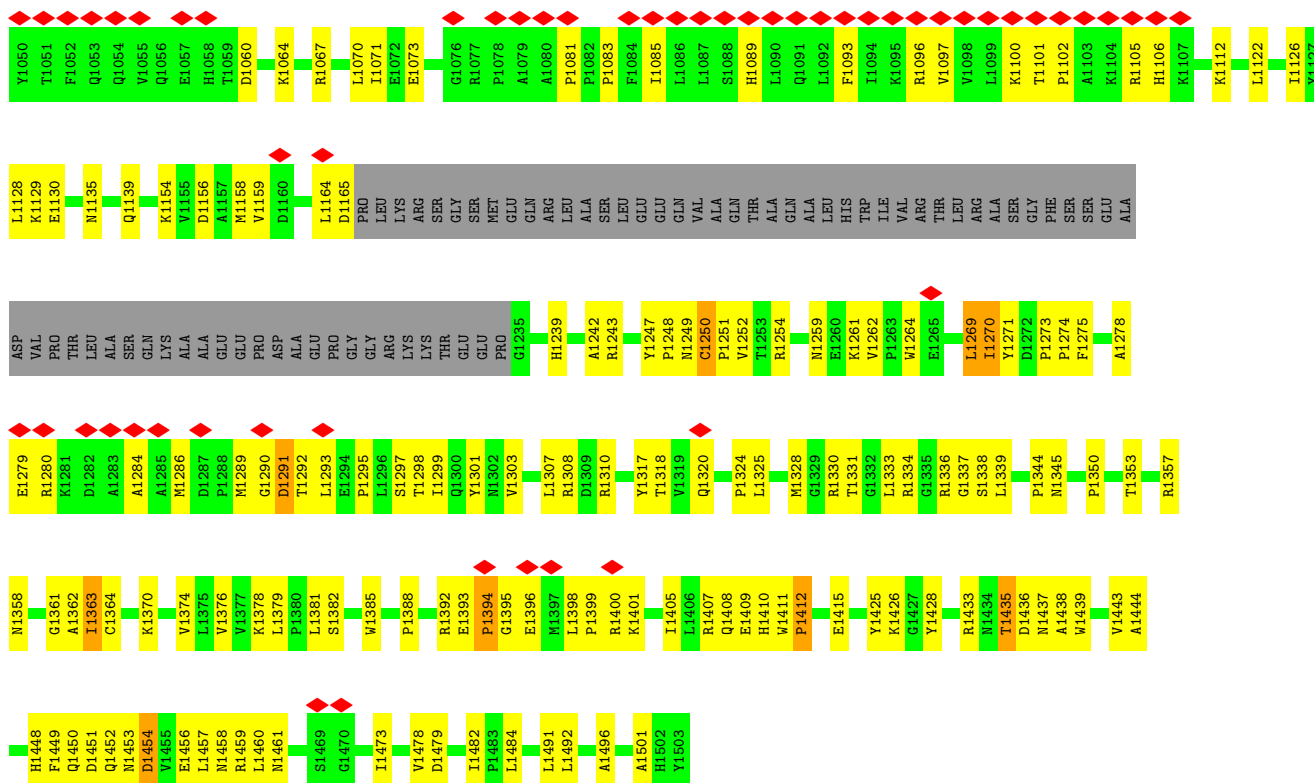


I1363	C1364	K1370	V1374	L1375	V1376	L1379	Q380	Q381	L1467	L1383	F386	E389	M390	F391	E392	T393	F394	T395	E397	R398	L399	T403	K404	K405	D408	I409	R412	L416	F419	R420	D424	Q425	Q426	Q427	D428	V429	D430	V431	A432	I433	L434	Q435	A436	L437	H446	M451	W452																																																																	
K457	L458	A459	V460	A461	V462	V465	D466	A468	E471	M474	D475	E476	T487	M488	F499	V500	L526	C530	L531	L536	P544	E545	R546	P547	A550	P551	A552	A553	L556	Q557	M558	H559	H560	V561	A562	Q563	V564	L565	R566	F572	T573	Q574	P575	L576	Y577	P578																																																																		
R579	P580	R581	H582	N583	D584	R585	L586	R587	L588	L589	L590	P591	V592	P593	H594	V595	K596	L597	N598	V599	Q600	G601	V602	S603	L604	R605	S606	L607	Y608	R609	R610	S611	S612	G613	H614	V615	T616	F617	T618	M619	D620	R623	D624	L625	Q632	N633	R634	T641	W642	A643	Q646	D647	C648	E667																																																										
R685	C693	V708	G713	A724	K725	D726	M727	V730	I735	Q736	W743	W744	L747	D750	N751	R755	L758	A762	L765	L766	L767	T768	G769	L770	I771	S772	F773	R774	R777	L778	Q779	G782	R789	A790	F791	F792	V796	V797	H800	L801	S805	Y806	F807	A808	F809	L810	C811	L812	F813	A814	Y815	V816	L817	M818	V819	D820	Q822	W827	C828	E829	C830	A831	I832	Y833	L834	W835	L836	F837	S838	L839	V840	C841	E842	E843	M844	R845	Q846	L847	F848	Y849	D850	P851	D852	E853	C854	G855	L856	M857	K858	K859	A860	A861	R862	Y863	F864	S865	D866															
F867	W868	N869	L871	D872	V873	G874	A875	L876	L877	L878	F879	V880	A881	G882	L883	T884	C885	R886	L887	T888	P889	A890	Y893	R896	V897	L898	L899	S900	L901	D902	F903	L904	L905	F906	C907	L908	R909	L910	W911	H912	T913	F914	S917	L920	G921	I925	V926	Y927	K928	R929	Y930	N931	K932	D933	Y934	F935	F936	F937	L938	F939	L940	L941	A942	Y943	W944	Y945	Y946	S947	F948	G949	Y950	A951	K952	Q953	A954	I955	L956	I957	H958	N959	E960	R961	R962	D964	Y965	L966	F967	A968	G969	A970	Y971	Y972	H973	S974	Y975	L976	T977	L978	F979	G980	Q981	I982	F983	G984	Y985	I986	D987	G988	VAL	ASN	PHE	ASN
PRO	GLU	HIS	CYS	SER	PRO	ASN	GLY	THR	ASP	ASP	THR	LYS	PRO	LYS	CYS	PRO	GLU	GLY	SER	ASP	ALA	THR	GLN	GLN	ARG	PRO	ALA	F1020	P1021	E1022	W1023	L1024	T1025	V1026	L1027	L1028	L1029	C1030	L1031	Y1032	L1033	L1034	F1035	T1036	N1037	I1038	L1039	L1040	L1041	N1042	L1043	L1044	I1045	A1046	M1047	F1048	N1049	Y1050	T1051	F1052																																																				
Q1053	Q1054	V1055	Q1056	E1057	H1058	T1059	D1060	K1064	R1067	L1070	I1071	E1072	E1073	G1076	P1077	P1078	A1079	A1080	F1081	P1082	F1083	F1084	I1085	L1086	L1087	S1088	H1089	L1090	Q1091	F1093	I1094	R1095	V1097	V1098	L1099	K1100	T1101	P1102	A1103	K1104	R1105	H1106	K1107	K1112	L1122	I1126	Y1127	L1128	K1129	E1130																																																														
N1135	Q1139	K1154	V1155	D1156	M1158	V1159	D1160	L1164	D1165	PRO	LEU	ARG	LYS	SER	GLY	SER	ARG	GLN	LEU	ALA	P1084	I1085	L1086	L1087	S1088	H1089	L1090	Q1091	F1093	I1094	R1095	V1097	V1098	L1099	K1100	T1101	P1102	A1103	K1104	R1105	H1106	K1107	K1112	L1122	I1126	Y1127	L1128	K1129	E1130																																																															
THR	LEU	ALA	SER	GLN	LYS	ALA	ALA	GLU	PRO	ASP	ALA	GLU	PRO	GLY	ARG	LYS	LYS	THR	GLU	GLU	PRO	G1235	H1239	A1242	R1243	Y1247	P1248	M1249	C1250	P1251	V1252	T1253	R1254	N1259	E1260	K1261	V1262	F1263	W1264	E1265	L1269	I1270	Y1271	D1272	P1273	P1274	F1275	A1278	E1279	L1280	K1281																																																													
D1282	A1283	A1284	A1285	M1286	D1287	P1288	M1289	G1290	D1291	T1292	L1293	E1294	P1295	L1296	S1297	T1298	I1299	Q1300	P1301	N1302	V1303	R1308	D1309	R1310	Y1317	T1318	V1319	Q1320	P1324	L1325	M1328	G1329	R1330	T1331	G1332	L1333	R1334	G1335	G1336	G1337	S1338	L1339	P1344	N1345	P1350	T1353	R1357	N1358	G1361	A1362																																																														
I1405	L1406	R1407	Q1408	E1409	H1410	W1411	P1412	E1415	Y1425	K1426	G1427	Y1428	R1433	W1434	T1435	D1436	N1437	A1438	W1439	V1443	A1444	H1448	F1449	Q1450																																																																																								

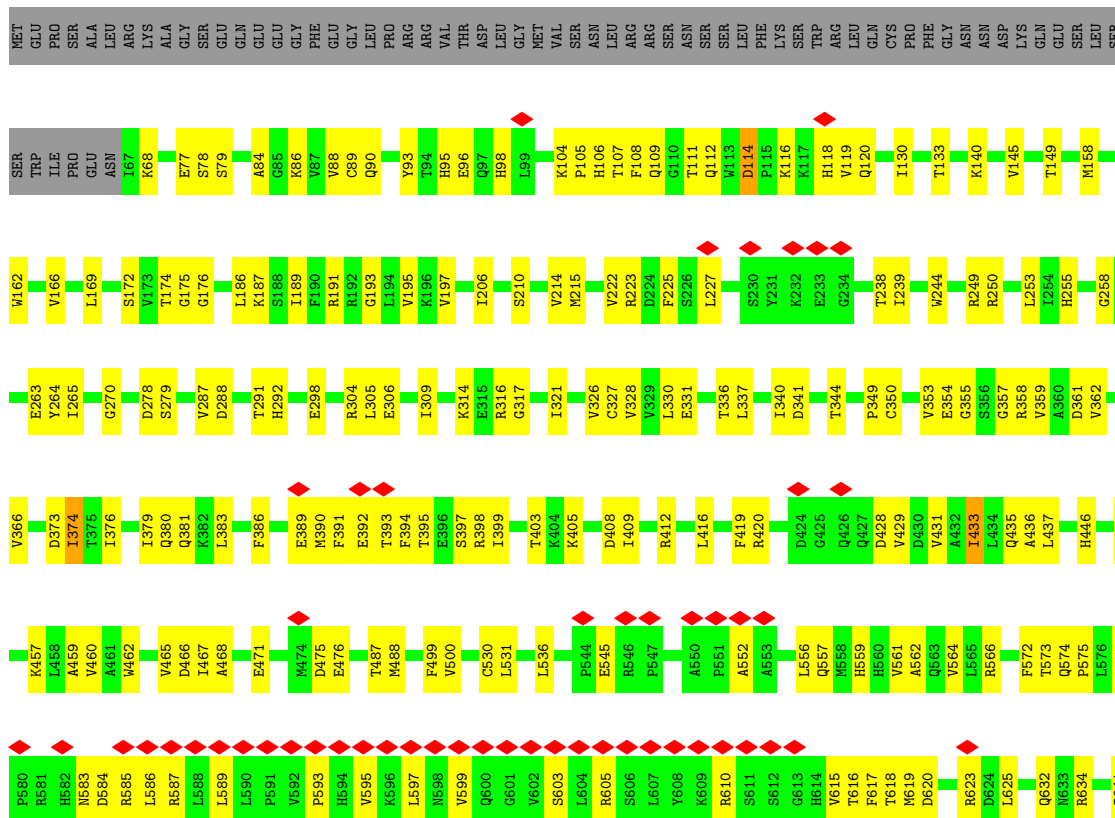


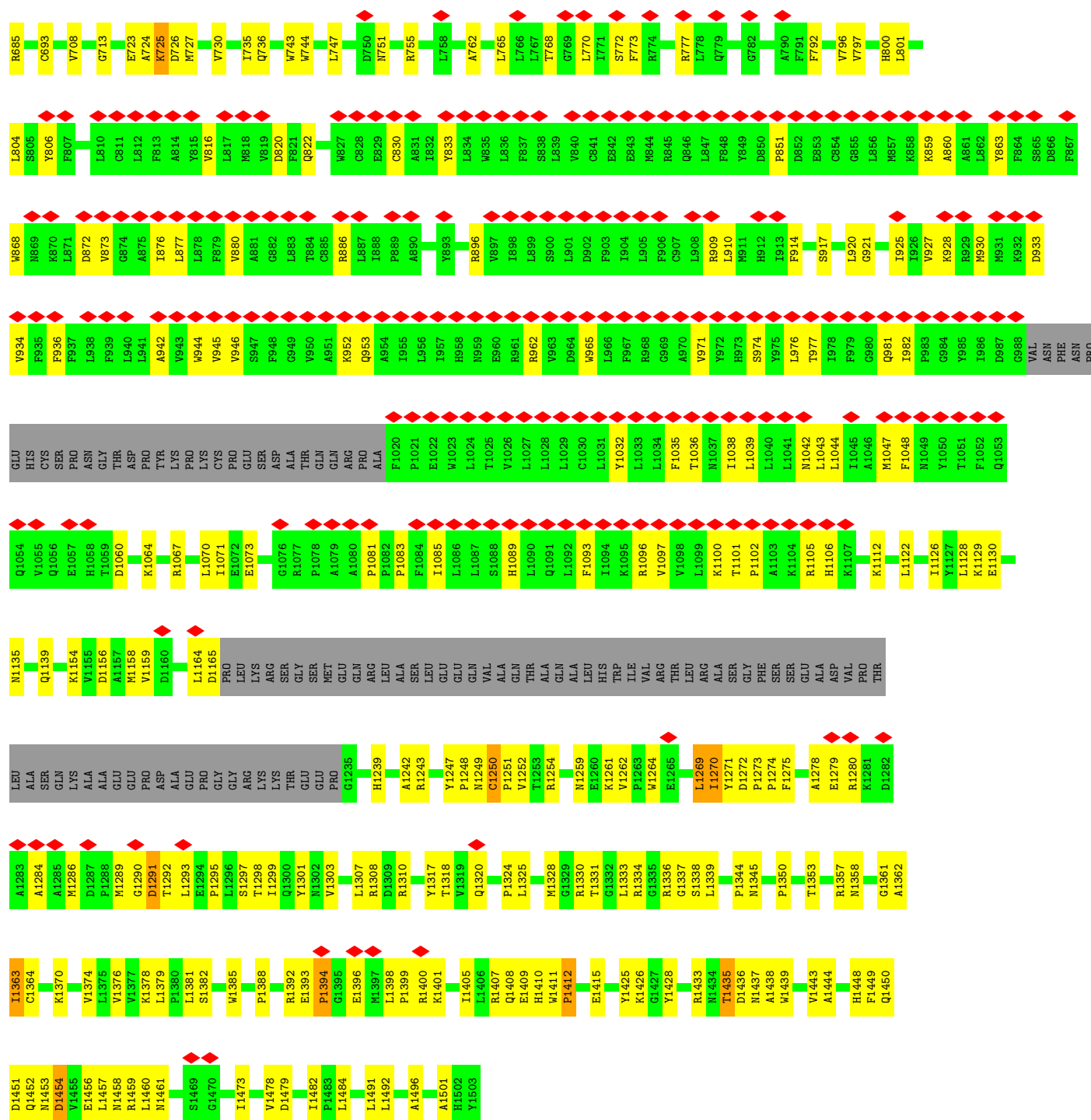
● Molecule 1: Transient receptor potential cation channel subfamily M member 2





• Molecule 1: Transient receptor potential cation channel subfamily M member 2





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	61503	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.163	Depositor
Minimum map value	-1.247	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.076	Depositor
Recommended contour level	0.234	Depositor
Map size (Å)	317.99997, 317.99997, 317.99997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.19	0/11044	0.55	3/14983 (0.0%)
1	B	0.19	0/11044	0.55	3/14983 (0.0%)
1	C	0.19	0/11044	0.55	3/14983 (0.0%)
1	D	0.19	0/11044	0.55	3/14983 (0.0%)
All	All	0.19	0/44176	0.55	12/59932 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	4
1	C	0	4
1	D	0	4
All	All	0	16

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	357	GLY	N-CA-C	7.68	119.99	111.85
1	C	357	GLY	N-CA-C	7.65	119.96	111.85
1	A	357	GLY	N-CA-C	7.65	119.96	111.85
1	D	357	GLY	N-CA-C	7.65	119.96	111.85
1	A	1269	LEU	CA-C-N	5.77	132.36	121.97
1	A	1269	LEU	C-N-CA	5.77	132.36	121.97
1	B	1269	LEU	CA-C-N	5.77	132.36	121.97
1	B	1269	LEU	C-N-CA	5.77	132.36	121.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1269	LEU	CA-C-N	5.77	132.36	121.97
1	C	1269	LEU	C-N-CA	5.77	132.36	121.97
1	D	1269	LEU	CA-C-N	5.76	132.34	121.97
1	D	1269	LEU	C-N-CA	5.76	132.34	121.97

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	114	ASP	Peptide
1	A	1291	ASP	Peptide
1	A	1435	THR	Peptide
1	A	725	LYS	Peptide
1	B	114	ASP	Peptide
1	B	1291	ASP	Peptide
1	B	1435	THR	Peptide
1	B	725	LYS	Peptide
1	C	114	ASP	Peptide
1	C	1291	ASP	Peptide
1	C	1435	THR	Peptide
1	C	725	LYS	Peptide
1	D	114	ASP	Peptide
1	D	1291	ASP	Peptide
1	D	1435	THR	Peptide
1	D	725	LYS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10774	0	10813	341	0
1	B	10774	0	10813	342	0
1	C	10774	0	10813	344	0
1	D	10774	0	10813	339	0
2	A	73	0	0	2	0
2	B	73	0	0	2	0
2	C	73	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	73	0	0	2	0
All	All	43388	0	43252	1319	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (1319) 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:D:1453:ASN:O	1:D:1457:LEU:HB2	1.44	1.17
1:C:1453:ASN:O	1:C:1457:LEU:HB2	1.44	1.16
1:A:1453:ASN:O	1:A:1457:LEU:HB2	1.44	1.13
1:B:1453:ASN:O	1:B:1457:LEU:HB2	1.44	1.13
1:D:376:ILE:HA	1:D:379:ILE:HG22	1.58	0.84
1:C:376:ILE:HA	1:C:379:ILE:HG22	1.58	0.84
1:B:376:ILE:HA	1:B:379:ILE:HG22	1.58	0.84
1:A:376:ILE:HA	1:A:379:ILE:HG22	1.58	0.83
1:D:244:TRP:HB3	1:D:288:ASP:HB3	1.62	0.81
1:C:244:TRP:HB3	1:C:288:ASP:HB3	1.62	0.81
1:A:244:TRP:HB3	1:A:288:ASP:HB3	1.62	0.81
1:C:605:ARG:HE	1:C:615:VAL:HG22	1.46	0.80
1:B:605:ARG:HE	1:B:615:VAL:HG22	1.46	0.80
1:A:1286:MET:HG2	1:A:1336:ARG:NH2	1.97	0.80
1:A:605:ARG:HE	1:A:615:VAL:HG22	1.46	0.80
1:B:244:TRP:HB3	1:B:288:ASP:HB3	1.62	0.80
1:C:593:PRO:HB2	1:C:597:LEU:HB2	1.65	0.80
1:A:796:VAL:HG12	1:A:800:HIS:CE1	2.18	0.79
1:C:1286:MET:HG2	1:C:1336:ARG:NH2	1.97	0.79
1:D:1286:MET:HG2	1:D:1336:ARG:NH2	1.97	0.79
1:C:796:VAL:HG12	1:C:800:HIS:CE1	2.18	0.79
1:B:593:PRO:HB2	1:B:597:LEU:HB2	1.65	0.79
1:B:796:VAL:HG12	1:B:800:HIS:CE1	2.18	0.79
1:D:605:ARG:HE	1:D:615:VAL:HG22	1.46	0.79
1:A:593:PRO:HB2	1:A:597:LEU:HB2	1.65	0.78
1:B:1286:MET:HG2	1:B:1336:ARG:NH2	1.97	0.78
1:D:796:VAL:HG12	1:D:800:HIS:CE1	2.18	0.78
1:A:114:ASP:O	1:A:116:LYS:N	2.16	0.78
1:D:593:PRO:HB2	1:D:597:LEU:HB2	1.65	0.77
1:B:114:ASP:O	1:B:116:LYS:N	2.16	0.76
1:A:1273:PRO:HB2	1:A:1334:ARG:HG3	1.67	0.76
1:B:1273:PRO:HB2	1:B:1334:ARG:HG3	1.67	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1273:PRO:HB2	1:D:1334:ARG:HG3	1.67	0.76
1:A:536:LEU:HD13	1:A:556:LEU:HD11	1.68	0.76
1:D:536:LEU:HD13	1:D:556:LEU:HD11	1.67	0.76
1:A:1426:LYS:HG2	1:A:1443:VAL:HG12	1.68	0.76
1:D:114:ASP:O	1:D:116:LYS:N	2.16	0.76
1:B:536:LEU:HD13	1:B:556:LEU:HD11	1.68	0.76
1:D:1426:LYS:HG2	1:D:1443:VAL:HG12	1.68	0.76
1:C:1273:PRO:HB2	1:C:1334:ARG:HG3	1.67	0.75
1:A:1324:PRO:HG2	1:A:1437:ASN:HB2	1.69	0.75
1:B:1324:PRO:HG2	1:B:1437:ASN:HB2	1.69	0.75
1:B:1426:LYS:HG2	1:B:1443:VAL:HG12	1.68	0.74
1:C:536:LEU:HD13	1:C:556:LEU:HD11	1.67	0.74
1:C:1426:LYS:HG2	1:C:1443:VAL:HG12	1.68	0.74
1:C:114:ASP:O	1:C:116:LYS:N	2.16	0.74
1:D:1324:PRO:HG2	1:D:1437:ASN:HB2	1.69	0.74
1:A:976:LEU:HB3	1:A:981:GLN:HB3	1.70	0.73
1:D:976:LEU:HB3	1:D:981:GLN:HB3	1.70	0.73
1:B:111:THR:HG22	1:B:112:GLN:HG2	1.71	0.73
1:D:111:THR:HG22	1:D:112:GLN:HG2	1.70	0.73
1:C:1324:PRO:HG2	1:C:1437:ASN:HB2	1.69	0.73
1:C:1363:ILE:HG22	1:C:1364:CYS:H	1.53	0.73
1:C:111:THR:HG22	1:C:112:GLN:HG2	1.70	0.73
1:C:1038:ILE:HG23	1:D:1044:LEU:HD21	1.71	0.73
1:D:1363:ILE:HG22	1:D:1364:CYS:H	1.54	0.72
1:B:1038:ILE:HG23	1:C:1044:LEU:HD21	1.70	0.72
1:C:1279:GLU:OE1	1:C:1338:SER:OG	2.08	0.72
1:A:1044:LEU:HD21	1:D:1038:ILE:HG23	1.71	0.72
1:C:976:LEU:HB3	1:C:981:GLN:HB3	1.70	0.72
1:B:976:LEU:HB3	1:B:981:GLN:HB3	1.70	0.72
1:A:111:THR:HG22	1:A:112:GLN:HG2	1.71	0.72
1:A:1279:GLU:OE1	1:A:1338:SER:OG	2.08	0.72
1:C:214:VAL:HG23	1:C:330:LEU:HD12	1.72	0.72
1:B:1333:LEU:HB3	1:B:1435:THR:HB	1.72	0.72
1:D:1333:LEU:HB3	1:D:1435:THR:HB	1.72	0.71
1:A:1333:LEU:HB3	1:A:1435:THR:HB	1.72	0.71
1:A:214:VAL:HG23	1:A:330:LEU:HD12	1.72	0.71
1:B:214:VAL:HG23	1:B:330:LEU:HD12	1.72	0.71
1:A:1038:ILE:HG23	1:B:1044:LEU:HD21	1.71	0.71
1:D:1279:GLU:OE1	1:D:1338:SER:OG	2.08	0.71
1:A:1363:ILE:HG22	1:A:1364:CYS:H	1.53	0.71
1:D:214:VAL:HG23	1:D:330:LEU:HD12	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:GLN:NE2	1:A:577:TYR:O	2.23	0.71
1:B:1363:ILE:HG22	1:B:1364:CYS:H	1.53	0.71
1:A:358:ARG:HB3	1:A:383:LEU:HG	1.73	0.70
1:B:1279:GLU:OE1	1:B:1338:SER:OG	2.08	0.70
1:C:68:LYS:HG3	1:C:161:HIS:CE1	2.27	0.70
1:B:358:ARG:HB3	1:B:383:LEU:HG	1.72	0.70
1:C:1333:LEU:HB3	1:C:1435:THR:HB	1.72	0.70
1:D:574:GLN:NE2	1:D:577:TYR:O	2.23	0.70
1:B:68:LYS:HG3	1:B:161:HIS:CE1	2.27	0.70
1:D:68:LYS:HG3	1:D:161:HIS:CE1	2.27	0.70
1:C:962:ARG:HB2	1:C:965:TRP:HB2	1.74	0.70
1:D:358:ARG:HB3	1:D:383:LEU:HG	1.72	0.70
1:A:68:LYS:HG3	1:A:161:HIS:CE1	2.27	0.70
1:C:358:ARG:HB3	1:C:383:LEU:HG	1.73	0.70
1:D:962:ARG:HB2	1:D:965:TRP:HB2	1.74	0.69
1:B:574:GLN:NE2	1:B:577:TYR:O	2.23	0.69
1:D:1393:GLU:HB3	1:D:1394:PRO:HD2	1.75	0.69
1:C:574:GLN:NE2	1:C:577:TYR:O	2.23	0.69
1:C:1451:ASP:OD1	1:C:1452:GLN:N	2.24	0.69
1:D:358:ARG:NH2	2:D:2001:UOZ:O39	2.26	0.69
1:D:1339:LEU:HD11	1:D:1433:ARG:HB3	1.75	0.69
1:A:77:GLU:HB2	1:A:119:VAL:HA	1.75	0.69
1:A:386:PHE:HB3	1:A:390:MET:HA	1.75	0.69
1:A:1393:GLU:HB3	1:A:1394:PRO:HD2	1.75	0.69
1:B:77:GLU:HB2	1:B:119:VAL:HA	1.75	0.69
1:B:962:ARG:HB2	1:B:965:TRP:HB2	1.74	0.69
1:C:1339:LEU:HD11	1:C:1433:ARG:HB3	1.75	0.69
1:A:358:ARG:NH2	2:A:2001:UOZ:O39	2.26	0.69
1:D:431:VAL:O	1:D:435:GLN:HG2	1.93	0.69
1:A:962:ARG:HB2	1:A:965:TRP:HB2	1.74	0.69
1:D:1451:ASP:OD1	1:D:1452:GLN:N	2.24	0.68
1:B:358:ARG:NH2	2:B:2001:UOZ:O39	2.26	0.68
1:B:1393:GLU:HB3	1:B:1394:PRO:HD2	1.75	0.68
1:B:1039:LEU:HD12	1:C:927:VAL:HG12	1.76	0.68
1:B:386:PHE:HB3	1:B:390:MET:HA	1.75	0.68
1:B:431:VAL:O	1:B:435:GLN:HG2	1.93	0.68
1:C:358:ARG:NH2	2:C:2001:UOZ:O39	2.26	0.68
1:C:1361:GLY:O	1:C:1363:ILE:N	2.26	0.68
1:C:1393:GLU:HB3	1:C:1394:PRO:HD2	1.75	0.68
1:B:1339:LEU:HD11	1:B:1433:ARG:HB3	1.75	0.68
1:B:1451:ASP:OD1	1:B:1452:GLN:N	2.24	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1039:LEU:HD12	1:D:927:VAL:HG12	1.76	0.68
1:A:431:VAL:O	1:A:435:GLN:HG2	1.93	0.68
1:C:77:GLU:HB2	1:C:119:VAL:HA	1.75	0.68
1:C:386:PHE:HB3	1:C:390:MET:HA	1.75	0.68
1:B:743:TRP:HB2	1:B:1071:ILE:HD12	1.76	0.68
1:C:431:VAL:O	1:C:435:GLN:HG2	1.93	0.68
1:C:743:TRP:HB2	1:C:1071:ILE:HD12	1.76	0.68
1:A:743:TRP:HB2	1:A:1071:ILE:HD12	1.76	0.67
1:A:927:VAL:HG12	1:D:1039:LEU:HD12	1.76	0.67
1:D:77:GLU:HB2	1:D:119:VAL:HA	1.75	0.67
1:D:386:PHE:HB3	1:D:390:MET:HA	1.75	0.67
1:A:1361:GLY:O	1:A:1363:ILE:N	2.26	0.67
1:B:1361:GLY:O	1:B:1363:ILE:N	2.26	0.67
1:D:743:TRP:HB2	1:D:1071:ILE:HD12	1.76	0.67
1:A:744:TRP:CD1	1:A:796:VAL:HG21	2.30	0.67
1:B:648:CYS:SG	1:B:1129:LYS:HD3	2.35	0.67
1:C:744:TRP:CD1	1:C:796:VAL:HG21	2.30	0.67
1:D:648:CYS:SG	1:D:1129:LYS:HD3	2.35	0.67
1:A:1039:LEU:HD12	1:B:927:VAL:HG12	1.76	0.67
1:A:1451:ASP:OD1	1:A:1452:GLN:N	2.24	0.67
1:A:1339:LEU:HD11	1:A:1433:ARG:HB3	1.74	0.67
1:D:1361:GLY:O	1:D:1363:ILE:N	2.26	0.67
1:D:1428:TYR:HE1	1:D:1439:TRP:HB2	1.60	0.67
1:C:648:CYS:SG	1:C:1129:LYS:HD3	2.35	0.67
1:A:1428:TYR:HE1	1:A:1439:TRP:HB2	1.60	0.67
1:B:744:TRP:CD1	1:B:796:VAL:HG21	2.30	0.67
1:C:95:HIS:CG	1:C:96:GLU:H	2.13	0.66
1:C:1425:TYR:H	1:C:1444:ALA:HB3	1.60	0.66
1:D:95:HIS:CG	1:D:96:GLU:H	2.13	0.66
1:A:95:HIS:CG	1:A:96:GLU:H	2.13	0.66
1:A:648:CYS:SG	1:A:1129:LYS:HD3	2.35	0.66
1:D:743:TRP:CD1	1:D:744:TRP:HD1	2.14	0.66
1:D:796:VAL:HG12	1:D:800:HIS:HE1	1.61	0.66
1:A:743:TRP:CD1	1:A:744:TRP:HD1	2.14	0.66
1:A:1425:TYR:H	1:A:1444:ALA:HB3	1.60	0.66
1:C:743:TRP:CD1	1:C:744:TRP:HD1	2.14	0.66
1:C:796:VAL:HG12	1:C:800:HIS:HE1	1.60	0.66
1:C:1428:TYR:HE1	1:C:1439:TRP:HB2	1.60	0.66
1:D:744:TRP:CD1	1:D:796:VAL:HG21	2.30	0.66
1:B:1291:ASP:O	1:B:1292:THR:OG1	2.14	0.66
1:D:1425:TYR:H	1:D:1444:ALA:HB3	1.60	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:HIS:CG	1:B:96:GLU:H	2.13	0.66
1:D:1353:THR:HG1	1:D:1448:HIS:HD1	1.44	0.66
1:B:1428:TYR:HE1	1:B:1439:TRP:HB2	1.60	0.65
1:A:451:ASN:OD1	1:A:452:TRP:N	2.30	0.65
1:C:376:ILE:HD12	1:C:403:THR:HG22	1.78	0.65
1:A:796:VAL:HG12	1:A:800:HIS:HE1	1.61	0.65
1:B:451:ASN:OD1	1:B:452:TRP:N	2.30	0.65
1:B:743:TRP:CD1	1:B:744:TRP:HD1	2.14	0.65
1:B:176:GLY:N	1:B:331:GLU:O	2.30	0.65
1:B:982:ILE:O	1:C:981:GLN:NE2	2.30	0.65
1:C:982:ILE:O	1:D:981:GLN:NE2	2.30	0.65
1:B:376:ILE:HD12	1:B:403:THR:HG22	1.78	0.65
1:C:176:GLY:N	1:C:331:GLU:O	2.30	0.65
1:A:172:SER:OG	1:A:306:GLU:OE2	2.14	0.64
1:B:1425:TYR:H	1:B:1444:ALA:HB3	1.60	0.64
1:C:1291:ASP:O	1:C:1292:THR:OG1	2.14	0.64
1:C:1363:ILE:HG21	1:C:1370:LYS:HD3	1.80	0.64
1:D:376:ILE:HD12	1:D:403:THR:HG22	1.78	0.64
1:D:451:ASN:OD1	1:D:452:TRP:N	2.30	0.64
1:A:977:THR:HG22	1:A:982:ILE:HA	1.80	0.64
1:A:1242:ALA:O	1:A:1254:ARG:NH1	2.31	0.64
1:C:977:THR:HG22	1:C:982:ILE:HA	1.80	0.64
1:C:1278:ALA:HB2	1:C:1336:ARG:HH22	1.62	0.64
1:D:1278:ALA:HB2	1:D:1336:ARG:HH22	1.62	0.64
1:A:1291:ASP:O	1:A:1292:THR:OG1	2.14	0.64
1:A:1353:THR:HG1	1:A:1448:HIS:HD1	1.46	0.64
1:D:176:GLY:N	1:D:331:GLU:O	2.30	0.64
1:A:1278:ALA:HB2	1:A:1336:ARG:HH22	1.61	0.64
1:B:796:VAL:HG12	1:B:800:HIS:HE1	1.60	0.64
1:C:451:ASN:OD1	1:C:452:TRP:N	2.30	0.64
1:B:977:THR:HG22	1:B:982:ILE:HA	1.80	0.64
1:C:1242:ALA:O	1:C:1254:ARG:NH1	2.31	0.64
1:D:977:THR:HG22	1:D:982:ILE:HA	1.80	0.64
1:A:176:GLY:N	1:A:331:GLU:O	2.30	0.64
1:A:981:GLN:NE2	1:D:982:ILE:O	2.30	0.64
1:C:172:SER:OG	1:C:306:GLU:OE2	2.14	0.64
1:B:1242:ALA:O	1:B:1254:ARG:NH1	2.31	0.64
1:C:1353:THR:HG1	1:C:1448:HIS:HD1	1.46	0.64
1:D:1363:ILE:HG21	1:D:1370:LYS:HD3	1.80	0.64
1:B:1363:ILE:HG21	1:B:1370:LYS:HD3	1.80	0.63
1:D:620:ASP:HB2	1:D:623:ARG:HB2	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:982:ILE:O	1:B:981:GLN:NE2	2.30	0.63
1:A:1156:ASP:OD1	1:B:1154:LYS:NZ	2.30	0.63
1:D:1242:ALA:O	1:D:1254:ARG:NH1	2.31	0.63
1:A:270:GLY:O	1:B:1358:ASN:ND2	2.32	0.63
1:A:1358:ASN:ND2	1:D:270:GLY:O	2.32	0.63
1:C:270:GLY:O	1:D:1358:ASN:ND2	2.32	0.63
1:A:376:ILE:HD12	1:A:403:THR:HG22	1.78	0.63
1:B:1278:ALA:HB2	1:B:1336:ARG:HH22	1.61	0.63
1:B:1297:SER:O	1:B:1299:ILE:N	2.32	0.63
1:C:620:ASP:HB2	1:C:623:ARG:HB2	1.80	0.63
1:A:326:VAL:HB	1:A:437:LEU:HD21	1.81	0.63
1:A:1363:ILE:HG21	1:A:1370:LYS:HD3	1.80	0.63
1:B:314:LYS:HE3	1:B:316:ARG:HH11	1.64	0.63
1:B:971:VAL:O	1:B:974:SER:OG	2.17	0.63
1:D:326:VAL:HB	1:D:437:LEU:HD21	1.81	0.63
1:B:95:HIS:O	1:B:98:HIS:ND1	2.32	0.62
1:B:408:ASP:OD1	1:B:412:ARG:NH2	2.33	0.62
1:A:1297:SER:O	1:A:1299:ILE:N	2.32	0.62
1:D:559:HIS:HD1	1:D:586:LEU:HD21	1.63	0.62
1:A:344:THR:OG1	1:A:412:ARG:NH2	2.33	0.62
1:A:559:HIS:HD1	1:A:586:LEU:HD21	1.63	0.62
1:B:435:GLN:NE2	1:B:471:GLU:OE1	2.32	0.62
1:C:326:VAL:HB	1:C:437:LEU:HD21	1.81	0.62
1:A:408:ASP:OD1	1:A:412:ARG:NH2	2.33	0.62
1:B:559:HIS:HD1	1:B:586:LEU:HD21	1.63	0.62
1:C:314:LYS:HE3	1:C:316:ARG:HH11	1.64	0.62
1:C:1297:SER:O	1:C:1299:ILE:N	2.32	0.62
1:D:917:SER:HB3	1:D:920:LEU:HB3	1.82	0.62
1:D:1297:SER:O	1:D:1299:ILE:N	2.32	0.62
1:A:314:LYS:HE3	1:A:316:ARG:HH11	1.64	0.62
1:A:971:VAL:O	1:A:974:SER:OG	2.17	0.62
1:A:1357:ARG:HE	1:A:1452:GLN:HA	1.65	0.62
1:C:917:SER:HB3	1:C:920:LEU:HB3	1.82	0.62
1:D:68:LYS:HG3	1:D:161:HIS:HE1	1.63	0.62
1:A:917:SER:HB3	1:A:920:LEU:HB3	1.82	0.62
1:B:326:VAL:HB	1:B:437:LEU:HD21	1.81	0.62
1:B:344:THR:OG1	1:B:412:ARG:NH2	2.33	0.62
1:D:314:LYS:HE3	1:D:316:ARG:HH11	1.64	0.62
1:C:331:GLU:OE2	1:C:358:ARG:NH1	2.33	0.62
1:D:331:GLU:OE2	1:D:358:ARG:NH1	2.33	0.62
1:B:620:ASP:HB2	1:B:623:ARG:HB2	1.80	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:408:ASP:OD1	1:C:412:ARG:NH2	2.33	0.62
1:A:68:LYS:HG3	1:A:161:HIS:HE1	1.63	0.61
1:C:133:THR:HG21	1:C:265:ILE:HD13	1.82	0.61
1:D:408:ASP:OD1	1:D:412:ARG:NH2	2.33	0.61
1:A:118:HIS:ND1	1:A:120:GLN:OE1	2.32	0.61
1:D:971:VAL:O	1:D:974:SER:OG	2.17	0.61
1:B:270:GLY:O	1:C:1358:ASN:ND2	2.32	0.61
1:D:344:THR:OG1	1:D:412:ARG:NH2	2.33	0.61
1:A:95:HIS:O	1:A:98:HIS:ND1	2.32	0.61
1:B:331:GLU:OE2	1:B:358:ARG:NH1	2.33	0.61
1:C:559:HIS:HD1	1:C:586:LEU:HD21	1.63	0.61
1:C:971:VAL:O	1:C:974:SER:OG	2.17	0.61
1:C:344:THR:OG1	1:C:412:ARG:NH2	2.33	0.61
1:D:133:THR:HG21	1:D:265:ILE:HD13	1.82	0.61
1:A:133:THR:HG21	1:A:265:ILE:HD13	1.82	0.61
1:A:620:ASP:HB2	1:A:623:ARG:HB2	1.81	0.61
1:B:133:THR:HG21	1:B:265:ILE:HD13	1.82	0.61
1:D:118:HIS:ND1	1:D:120:GLN:OE1	2.32	0.61
1:D:391:PHE:HA	1:D:394:PHE:CE2	2.36	0.61
1:D:751:ASN:ND2	1:D:772:SER:OG	2.34	0.61
1:A:391:PHE:HA	1:A:394:PHE:CE2	2.36	0.61
1:B:751:ASN:ND2	1:B:772:SER:OG	2.34	0.61
1:C:435:GLN:NE2	1:C:471:GLU:OE1	2.32	0.61
1:B:391:PHE:HA	1:B:394:PHE:CE2	2.36	0.61
1:B:1353:THR:HG1	1:B:1448:HIS:HD1	1.45	0.61
1:C:86:LYS:HE3	1:C:89:CYS:HA	1.83	0.61
1:C:751:ASN:ND2	1:C:772:SER:OG	2.34	0.61
1:B:1357:ARG:HE	1:B:1452:GLN:HA	1.65	0.61
1:C:391:PHE:HA	1:C:394:PHE:CE2	2.36	0.61
1:D:86:LYS:HE3	1:D:89:CYS:HA	1.83	0.61
1:A:331:GLU:OE2	1:A:358:ARG:NH1	2.33	0.61
1:A:435:GLN:NE2	1:A:471:GLU:OE1	2.32	0.61
1:C:1357:ARG:HE	1:C:1452:GLN:HA	1.65	0.60
1:B:86:LYS:HE3	1:B:89:CYS:HA	1.83	0.60
1:B:917:SER:HB3	1:B:920:LEU:HB3	1.82	0.60
1:C:68:LYS:HG3	1:C:161:HIS:HE1	1.63	0.60
1:A:777:ARG:O	1:A:777:ARG:NH1	2.35	0.60
1:C:1239:HIS:HD2	1:C:1242:ALA:HB3	1.67	0.60
1:D:1357:ARG:HE	1:D:1452:GLN:HA	1.65	0.60
1:A:86:LYS:HE3	1:A:89:CYS:HA	1.83	0.60
1:A:1239:HIS:HD2	1:A:1242:ALA:HB3	1.67	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:LYS:HG3	1:B:161:HIS:HE1	1.63	0.60
1:A:751:ASN:ND2	1:A:772:SER:OG	2.34	0.60
1:D:172:SER:OG	1:D:306:GLU:OE2	2.14	0.60
1:C:118:HIS:ND1	1:C:120:GLN:OE1	2.32	0.60
1:D:95:HIS:O	1:D:98:HIS:ND1	2.32	0.60
1:C:130:ILE:HD11	1:C:264:TYR:HB2	1.84	0.59
1:D:1239:HIS:HD2	1:D:1242:ALA:HB3	1.67	0.59
1:A:130:ILE:HD11	1:A:264:TYR:HB2	1.84	0.59
1:B:118:HIS:ND1	1:B:120:GLN:OE1	2.32	0.59
1:D:130:ILE:HD11	1:D:264:TYR:HB2	1.84	0.59
1:B:187:LYS:NZ	1:C:476:GLU:OE2	2.35	0.59
1:C:187:LYS:NZ	1:D:476:GLU:OE2	2.35	0.59
1:D:331:GLU:HG3	1:D:358:ARG:H	1.67	0.59
1:B:130:ILE:HD11	1:B:264:TYR:HB2	1.84	0.59
1:D:435:GLN:NE2	1:D:471:GLU:OE1	2.32	0.59
1:D:1291:ASP:O	1:D:1292:THR:OG1	2.14	0.59
1:B:409:ILE:HG22	1:B:416:LEU:HD22	1.84	0.59
1:C:409:ILE:HG22	1:C:416:LEU:HD22	1.84	0.59
1:D:1271:TYR:CE1	1:D:1330:ARG:HD3	2.38	0.59
1:C:777:ARG:O	1:C:777:ARG:NH1	2.35	0.59
1:C:331:GLU:HG3	1:C:358:ARG:H	1.67	0.59
1:B:777:ARG:O	1:B:777:ARG:NH1	2.35	0.59
1:B:172:SER:OG	1:B:306:GLU:OE2	2.14	0.59
1:C:1271:TYR:CE1	1:C:1330:ARG:HD3	2.38	0.59
1:A:1271:TYR:CE1	1:A:1330:ARG:HD3	2.38	0.58
1:C:872:ASP:OD2	1:C:909:ARG:NE	2.36	0.58
1:C:1156:ASP:OD1	1:D:1154:LYS:NZ	2.30	0.58
1:D:777:ARG:NH1	1:D:777:ARG:O	2.35	0.58
1:A:187:LYS:NZ	1:B:476:GLU:OE2	2.35	0.58
1:A:476:GLU:OE2	1:D:187:LYS:NZ	2.35	0.58
1:B:1392:ARG:HB2	1:B:1396:GLU:HG3	1.86	0.58
1:A:331:GLU:HG3	1:A:358:ARG:H	1.67	0.58
1:A:409:ILE:HG22	1:A:416:LEU:HD22	1.84	0.58
1:B:331:GLU:HG3	1:B:358:ARG:H	1.67	0.58
1:B:1239:HIS:HD2	1:B:1242:ALA:HB3	1.67	0.58
1:D:373:ASP:O	1:D:374:ILE:HG22	2.04	0.58
1:B:1105:ARG:HH11	1:B:1106:HIS:H	1.52	0.58
1:B:1271:TYR:CE1	1:B:1330:ARG:HD3	2.38	0.58
1:B:1357:ARG:NH2	1:B:1450:GLN:O	2.37	0.58
1:C:1105:ARG:HH11	1:C:1106:HIS:H	1.52	0.58
1:D:693:CYS:HA	1:D:1128:LEU:HD23	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:LEU:HB3	1:A:641:ILE:HD13	1.86	0.58
1:C:373:ASP:O	1:C:374:ILE:HG22	2.04	0.58
1:C:952:LYS:HE3	1:C:953:GLN:HE21	1.68	0.58
1:A:373:ASP:O	1:A:374:ILE:HG22	2.04	0.58
1:A:693:CYS:HA	1:A:1128:LEU:HD23	1.86	0.58
1:B:625:LEU:HB3	1:B:641:ILE:HD13	1.86	0.58
1:B:952:LYS:HE3	1:B:953:GLN:HE21	1.68	0.58
1:C:95:HIS:O	1:C:98:HIS:ND1	2.32	0.58
1:C:1392:ARG:HB2	1:C:1396:GLU:HG3	1.86	0.58
1:B:373:ASP:O	1:B:374:ILE:HG22	2.04	0.58
1:D:409:ILE:HG22	1:D:416:LEU:HD22	1.84	0.58
1:D:1357:ARG:NH2	1:D:1450:GLN:O	2.37	0.58
1:A:1105:ARG:HH11	1:A:1106:HIS:H	1.52	0.58
1:A:872:ASP:OD2	1:A:909:ARG:NE	2.36	0.57
1:C:1353:THR:OG1	1:C:1448:HIS:ND1	2.34	0.57
1:A:1392:ARG:HB2	1:A:1396:GLU:HG3	1.85	0.57
1:D:1339:LEU:O	1:D:1345:ASN:ND2	2.37	0.57
1:C:1357:ARG:NH2	1:C:1450:GLN:O	2.37	0.57
1:D:1250:CYS:HB2	1:D:1251:PRO:HD2	1.86	0.57
1:A:559:HIS:ND1	1:A:586:LEU:HD21	2.20	0.57
1:D:1261:LYS:O	1:D:1330:ARG:NH1	2.38	0.57
1:A:914:PHE:O	1:A:920:LEU:HD21	2.04	0.57
1:A:1261:LYS:O	1:A:1330:ARG:NH1	2.38	0.57
1:D:625:LEU:HB3	1:D:641:ILE:HD13	1.86	0.57
1:D:1105:ARG:HH11	1:D:1106:HIS:H	1.52	0.57
1:A:394:PHE:O	1:A:395:THR:OG1	2.22	0.57
1:B:1081:PRO:HB2	1:B:1083:PRO:HD2	1.86	0.57
1:C:1261:LYS:O	1:C:1330:ARG:NH1	2.38	0.57
1:D:952:LYS:HE3	1:D:953:GLN:HE21	1.68	0.57
1:D:1318:THR:HG22	1:D:1320:GLN:H	1.70	0.57
1:A:1250:CYS:HB2	1:A:1251:PRO:HD2	1.86	0.57
1:C:77:GLU:OE2	1:C:78:SER:OG	2.23	0.57
1:C:914:PHE:O	1:C:920:LEU:HD21	2.04	0.57
1:D:394:PHE:O	1:D:395:THR:OG1	2.22	0.57
1:B:298:GLU:OE1	1:B:298:GLU:N	2.28	0.57
1:D:1392:ARG:HB2	1:D:1396:GLU:HG3	1.86	0.57
1:B:872:ASP:OD2	1:B:909:ARG:NE	2.36	0.57
1:B:1261:LYS:O	1:B:1330:ARG:NH1	2.38	0.57
1:A:952:LYS:HE3	1:A:953:GLN:HE21	1.68	0.57
1:A:1357:ARG:NH2	1:A:1450:GLN:O	2.37	0.57
1:B:559:HIS:ND1	1:B:586:LEU:HD21	2.20	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:693:CYS:HA	1:C:1128:LEU:HD23	1.86	0.57
1:B:914:PHE:O	1:B:920:LEU:HD21	2.04	0.56
1:C:625:LEU:HB3	1:C:641:ILE:HD13	1.86	0.56
1:C:1250:CYS:HB2	1:C:1251:PRO:HD2	1.86	0.56
1:D:77:GLU:OE2	1:D:78:SER:OG	2.23	0.56
1:A:1318:THR:HG22	1:A:1320:GLN:H	1.70	0.56
1:B:394:PHE:O	1:B:395:THR:OG1	2.22	0.56
1:B:693:CYS:HA	1:B:1128:LEU:HD23	1.86	0.56
1:B:1250:CYS:HB2	1:B:1251:PRO:HD2	1.86	0.56
1:B:1339:LEU:O	1:B:1345:ASN:ND2	2.37	0.56
1:B:1458:ASN:OD1	1:B:1459:ARG:N	2.38	0.56
1:C:381:GLN:HA	1:C:386:PHE:HE1	1.70	0.56
1:D:298:GLU:OE1	1:D:298:GLU:N	2.28	0.56
1:D:559:HIS:ND1	1:D:586:LEU:HD21	2.20	0.56
1:D:597:LEU:HG	1:D:599:VAL:H	1.70	0.56
1:D:914:PHE:O	1:D:920:LEU:HD21	2.04	0.56
1:D:1081:PRO:HB2	1:D:1083:PRO:HD2	1.87	0.56
1:A:1154:LYS:NZ	1:D:1156:ASP:OD1	2.30	0.56
1:B:381:GLN:HA	1:B:386:PHE:HE1	1.70	0.56
1:D:872:ASP:OD2	1:D:909:ARG:NE	2.36	0.56
1:A:77:GLU:OE2	1:A:78:SER:OG	2.23	0.56
1:A:1339:LEU:HD22	1:A:1438:ALA:O	2.06	0.56
1:C:1275:PHE:HD2	1:C:1334:ARG:HE	1.53	0.56
1:C:1318:THR:HG22	1:C:1320:GLN:H	1.70	0.56
1:A:1275:PHE:HD2	1:A:1334:ARG:HE	1.53	0.56
1:D:1458:ASN:OD1	1:D:1459:ARG:N	2.38	0.56
1:C:1081:PRO:HB2	1:C:1083:PRO:HD2	1.87	0.56
1:D:933:ASP:HA	1:D:936:PHE:HB3	1.88	0.56
1:C:559:HIS:ND1	1:C:586:LEU:HD21	2.20	0.56
1:C:933:ASP:HA	1:C:936:PHE:HB3	1.88	0.56
1:D:381:GLN:HA	1:D:386:PHE:HE1	1.70	0.56
1:D:1339:LEU:HD22	1:D:1438:ALA:O	2.06	0.56
1:A:381:GLN:HA	1:A:386:PHE:HE1	1.70	0.55
1:D:1479:ASP:H	1:D:1482:ILE:HD11	1.71	0.55
1:A:933:ASP:HA	1:A:936:PHE:HB3	1.88	0.55
1:A:1081:PRO:HB2	1:A:1083:PRO:HD2	1.87	0.55
1:B:77:GLU:OE2	1:B:78:SER:OG	2.23	0.55
1:C:328:VAL:HG22	1:C:433:ILE:HD11	1.88	0.55
1:A:328:VAL:HG22	1:A:433:ILE:HD11	1.88	0.55
1:A:1458:ASN:OD1	1:A:1459:ARG:N	2.38	0.55
1:B:1318:THR:HG22	1:B:1320:GLN:H	1.70	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:796:VAL:CG1	1:C:800:HIS:HE1	2.19	0.55
1:D:328:VAL:HG22	1:D:433:ILE:HD11	1.89	0.55
1:A:597:LEU:HG	1:A:599:VAL:H	1.70	0.55
1:B:597:LEU:HG	1:B:599:VAL:H	1.70	0.55
1:B:337:LEU:HB2	1:B:359:VAL:HG21	1.89	0.55
1:C:1458:ASN:OD1	1:C:1459:ARG:N	2.38	0.55
1:C:337:LEU:HB2	1:C:359:VAL:HG21	1.89	0.55
1:C:792:PHE:HA	1:C:797:VAL:HG21	1.89	0.55
1:C:1339:LEU:HD22	1:C:1438:ALA:O	2.06	0.55
1:D:1275:PHE:HD2	1:D:1334:ARG:HE	1.53	0.55
1:B:851:PRO:HB3	1:B:859:LYS:HD2	1.89	0.55
1:B:1339:LEU:HD22	1:B:1438:ALA:O	2.06	0.55
1:C:755:ARG:HG2	1:C:770:LEU:HD21	1.88	0.55
1:A:1275:PHE:HA	1:A:1334:ARG:HB2	1.89	0.55
1:D:337:LEU:HB2	1:D:359:VAL:HG21	1.89	0.55
1:B:328:VAL:HG22	1:B:433:ILE:HD11	1.88	0.55
1:B:755:ARG:HG2	1:B:770:LEU:HD21	1.88	0.55
1:C:597:LEU:HG	1:C:599:VAL:H	1.70	0.55
1:D:796:VAL:CG1	1:D:800:HIS:HE1	2.20	0.55
1:A:851:PRO:HB3	1:A:859:LYS:HD2	1.89	0.54
1:C:1479:ASP:H	1:C:1482:ILE:HD11	1.71	0.54
1:A:755:ARG:HG2	1:A:770:LEU:HD21	1.88	0.54
1:C:1158:MET:HE2	1:D:1158:MET:HE1	1.89	0.54
1:D:792:PHE:HA	1:D:797:VAL:HG21	1.89	0.54
1:A:566:ARG:NH1	1:A:572:PHE:O	2.41	0.54
1:A:1339:LEU:O	1:A:1345:ASN:ND2	2.37	0.54
1:B:1275:PHE:HD2	1:B:1334:ARG:HE	1.53	0.54
1:C:1339:LEU:O	1:C:1345:ASN:ND2	2.37	0.54
1:D:566:ARG:NH1	1:D:572:PHE:O	2.41	0.54
1:A:593:PRO:HD2	1:A:597:LEU:HD22	1.90	0.54
1:A:1479:ASP:H	1:A:1482:ILE:HD11	1.71	0.54
1:D:755:ARG:HG2	1:D:770:LEU:HD21	1.88	0.54
1:B:796:VAL:CG1	1:B:800:HIS:HE1	2.19	0.54
1:B:933:ASP:HA	1:B:936:PHE:HB3	1.88	0.54
1:B:1158:MET:HE2	1:C:1158:MET:HE1	1.89	0.54
1:C:593:PRO:HD2	1:C:597:LEU:HD22	1.90	0.54
1:C:851:PRO:HB3	1:C:859:LYS:HD2	1.89	0.54
1:C:1275:PHE:HA	1:C:1334:ARG:HB2	1.89	0.54
1:D:593:PRO:HD2	1:D:597:LEU:HD22	1.90	0.54
1:B:593:PRO:HD2	1:B:597:LEU:HD22	1.90	0.54
1:B:1479:ASP:H	1:B:1482:ILE:HD11	1.71	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1286:MET:HE2	1:C:1289:MET:HB2	1.90	0.54
1:A:298:GLU:OE1	1:A:298:GLU:N	2.28	0.54
1:A:792:PHE:HA	1:A:797:VAL:HG21	1.89	0.54
1:B:1096:ARG:HH22	1:B:1102:PRO:HA	1.73	0.54
1:B:1286:MET:HE2	1:B:1289:MET:HB2	1.90	0.54
1:C:174:THR:OG1	2:C:2001:UOZ:O35	2.24	0.54
1:D:1275:PHE:HA	1:D:1334:ARG:HB2	1.89	0.54
1:C:1275:PHE:HB2	1:C:1334:ARG:HD3	1.90	0.54
1:C:1449:PHE:HE2	1:C:1460:LEU:HD23	1.73	0.54
1:A:222:VAL:HG21	1:A:238:THR:HG21	1.90	0.54
1:A:1158:MET:HE2	1:B:1158:MET:HE1	1.89	0.54
1:A:174:THR:OG1	2:A:2001:UOZ:O35	2.24	0.54
1:B:1275:PHE:HB2	1:B:1334:ARG:HD3	1.90	0.54
1:C:84:ALA:O	1:C:86:LYS:HD2	2.08	0.54
1:D:851:PRO:HB3	1:D:859:LYS:HD2	1.89	0.54
1:A:337:LEU:HB2	1:A:359:VAL:HG21	1.89	0.53
1:A:796:VAL:CG1	1:A:800:HIS:HE1	2.20	0.53
1:C:316:ARG:HA	1:C:316:ARG:NE	2.23	0.53
1:D:316:ARG:NE	1:D:316:ARG:HA	2.23	0.53
1:A:1158:MET:HE1	1:D:1158:MET:HE2	1.89	0.53
1:B:1156:ASP:OD1	1:C:1154:LYS:NZ	2.30	0.53
1:B:1394:PRO:O	1:B:1398:LEU:HD12	2.09	0.53
1:D:1449:PHE:HE2	1:D:1460:LEU:HD23	1.73	0.53
1:A:1286:MET:HE2	1:A:1289:MET:HB2	1.90	0.53
1:D:174:THR:OG1	2:D:2001:UOZ:O35	2.24	0.53
1:D:1394:PRO:O	1:D:1398:LEU:HD12	2.09	0.53
1:C:222:VAL:HG21	1:C:238:THR:HG21	1.90	0.53
1:D:1275:PHE:HB2	1:D:1334:ARG:HD3	1.90	0.53
1:A:316:ARG:HA	1:A:316:ARG:NE	2.23	0.53
1:A:1096:ARG:HH22	1:A:1102:PRO:HA	1.73	0.53
1:B:475:ASP:OD1	1:B:476:GLU:N	2.42	0.53
1:B:792:PHE:HA	1:B:797:VAL:HG21	1.89	0.53
1:A:84:ALA:O	1:A:86:LYS:HA	2.09	0.53
1:B:1275:PHE:HA	1:B:1334:ARG:HB2	1.89	0.53
1:B:1363:ILE:HG22	1:B:1364:CYS:N	2.23	0.53
1:C:193:GLY:O	1:C:197:VAL:HG23	2.09	0.53
1:C:321:ILE:HG22	1:C:457:LYS:HB3	1.91	0.53
1:A:475:ASP:OD1	1:A:476:GLU:N	2.42	0.53
1:A:1275:PHE:HB2	1:A:1334:ARG:HD3	1.90	0.53
1:B:321:ILE:HG22	1:B:457:LYS:HB3	1.91	0.53
1:B:566:ARG:NH1	1:B:572:PHE:O	2.41	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1096:ARG:HH22	1:C:1102:PRO:HA	1.73	0.53
1:D:222:VAL:HG21	1:D:238:THR:HG21	1.90	0.53
1:D:321:ILE:HG22	1:D:457:LYS:HB3	1.91	0.53
1:D:488:MET:HE1	1:D:500:VAL:HA	1.90	0.53
1:D:1376:VAL:HG11	1:D:1484:LEU:HD21	1.91	0.53
1:A:84:ALA:O	1:A:86:LYS:HD2	2.09	0.53
1:C:1376:VAL:HG11	1:C:1484:LEU:HD21	1.91	0.53
1:D:193:GLY:O	1:D:197:VAL:HG23	2.09	0.53
1:D:475:ASP:OD1	1:D:476:GLU:N	2.42	0.53
1:A:321:ILE:HG22	1:A:457:LYS:HB3	1.91	0.53
1:B:84:ALA:O	1:B:86:LYS:HD2	2.09	0.53
1:B:106:HIS:ND1	1:B:107:THR:O	2.42	0.53
1:B:1449:PHE:HE2	1:B:1460:LEU:HD23	1.73	0.53
1:C:84:ALA:O	1:C:86:LYS:HA	2.09	0.53
1:D:1286:MET:HE2	1:D:1289:MET:HB2	1.90	0.53
1:A:1376:VAL:HG11	1:A:1484:LEU:HD21	1.91	0.53
1:A:1394:PRO:O	1:A:1398:LEU:HD12	2.09	0.53
1:B:222:VAL:HG21	1:B:238:THR:HG21	1.90	0.53
1:D:84:ALA:O	1:D:86:LYS:HD2	2.08	0.53
1:A:1449:PHE:HE2	1:A:1460:LEU:HD23	1.73	0.52
1:C:394:PHE:O	1:C:395:THR:OG1	2.22	0.52
1:D:1405:ILE:O	1:D:1409:GLU:N	2.43	0.52
1:A:106:HIS:ND1	1:A:107:THR:O	2.42	0.52
1:A:1284:ALA:O	1:A:1292:THR:HG21	2.10	0.52
1:B:316:ARG:HA	1:B:316:ARG:NE	2.23	0.52
1:C:566:ARG:NH1	1:C:572:PHE:O	2.41	0.52
1:C:1394:PRO:O	1:C:1398:LEU:HD12	2.09	0.52
1:D:84:ALA:O	1:D:86:LYS:HA	2.09	0.52
1:A:488:MET:HE1	1:A:500:VAL:HA	1.90	0.52
1:B:193:GLY:O	1:B:197:VAL:HG23	2.09	0.52
1:C:106:HIS:ND1	1:C:107:THR:O	2.42	0.52
1:C:1291:ASP:OD1	1:C:1308:ARG:NH1	2.43	0.52
1:C:1363:ILE:HG22	1:C:1364:CYS:N	2.23	0.52
1:D:1291:ASP:OD1	1:D:1308:ARG:NH1	2.43	0.52
1:A:573:THR:OG1	1:A:713:GLY:O	2.28	0.52
1:B:1376:VAL:HG11	1:B:1484:LEU:HD21	1.91	0.52
1:D:1096:ARG:HH22	1:D:1102:PRO:HA	1.73	0.52
1:D:1284:ALA:O	1:D:1292:THR:HG21	2.10	0.52
1:B:488:MET:HE1	1:B:500:VAL:HA	1.90	0.52
1:C:475:ASP:OD1	1:C:476:GLU:N	2.42	0.52
1:A:1405:ILE:O	1:A:1409:GLU:N	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:ALA:O	1:B:86:LYS:HA	2.09	0.52
1:B:860:ALA:HA	1:B:863:TYR:HD2	1.75	0.52
1:B:1291:ASP:OD1	1:B:1308:ARG:NH1	2.43	0.52
1:B:573:THR:OG1	1:B:713:GLY:O	2.28	0.52
1:C:488:MET:HE1	1:C:500:VAL:HA	1.90	0.52
1:C:860:ALA:HA	1:C:863:TYR:HD2	1.75	0.52
1:A:193:GLY:O	1:A:197:VAL:HG23	2.09	0.52
1:A:1291:ASP:OD1	1:A:1308:ARG:NH1	2.43	0.52
1:B:1284:ALA:O	1:B:1292:THR:HG21	2.10	0.52
1:D:362:VAL:O	1:D:366:VAL:HG12	2.10	0.52
1:C:460:VAL:HG21	1:C:487:THR:HG23	1.92	0.51
1:D:106:HIS:ND1	1:D:107:THR:O	2.42	0.51
1:D:460:VAL:HG21	1:D:487:THR:HG23	1.92	0.51
1:D:574:GLN:HG2	1:D:575:PRO:HD2	1.91	0.51
1:A:362:VAL:O	1:A:366:VAL:HG12	2.10	0.51
1:A:1350:PRO:HD2	1:A:1388:PRO:O	2.11	0.51
1:B:362:VAL:O	1:B:366:VAL:HG12	2.10	0.51
1:B:1350:PRO:HD2	1:B:1388:PRO:O	2.11	0.51
1:C:355:GLY:HA2	1:C:361:ASP:OD1	2.10	0.51
1:C:1122:LEU:O	1:C:1126:ILE:HG12	2.11	0.51
1:C:1284:ALA:O	1:C:1292:THR:HG21	2.10	0.51
1:C:1350:PRO:HD2	1:C:1388:PRO:O	2.11	0.51
1:D:573:THR:OG1	1:D:713:GLY:O	2.27	0.51
1:A:258:GLY:HA2	1:A:260:PHE:CD1	2.45	0.51
1:B:557:GLN:HG2	1:B:585:ARG:HB3	1.93	0.51
1:C:1344:PRO:HG3	1:C:1439:TRP:CZ2	2.46	0.51
1:A:1363:ILE:HG22	1:A:1364:CYS:N	2.23	0.51
1:B:1278:ALA:O	1:B:1280:ARG:N	2.44	0.51
1:B:1353:THR:OG1	1:B:1448:HIS:ND1	2.34	0.51
1:A:460:VAL:HG21	1:A:487:THR:HG23	1.92	0.51
1:B:1269:LEU:O	1:B:1270:ILE:HG12	2.10	0.51
1:C:258:GLY:HA2	1:C:260:PHE:CD1	2.46	0.51
1:C:557:GLN:HG2	1:C:585:ARG:HB3	1.93	0.51
1:D:1344:PRO:HG3	1:D:1439:TRP:CZ2	2.46	0.51
1:B:355:GLY:HA2	1:B:361:ASP:OD1	2.11	0.51
1:C:574:GLN:HG2	1:C:575:PRO:HD2	1.92	0.51
1:D:460:VAL:HA	1:D:499:PHE:HE2	1.76	0.51
1:D:1269:LEU:O	1:D:1270:ILE:HG12	2.10	0.51
1:D:1353:THR:HG22	1:D:1374:VAL:HG12	1.92	0.51
1:A:78:SER:OG	1:A:103:THR:OG1	2.28	0.51
1:A:355:GLY:HA2	1:A:361:ASP:OD1	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:GLN:HG2	1:A:585:ARG:HB3	1.93	0.51
1:A:1122:LEU:O	1:A:1126:ILE:HG12	2.11	0.51
1:A:1269:LEU:O	1:A:1270:ILE:HG12	2.10	0.51
1:B:460:VAL:HA	1:B:499:PHE:CE2	2.46	0.51
1:B:1353:THR:HG22	1:B:1374:VAL:HG12	1.92	0.51
1:C:362:VAL:O	1:C:366:VAL:HG12	2.10	0.51
1:D:557:GLN:HG2	1:D:585:ARG:HB3	1.93	0.51
1:A:796:VAL:CG1	1:A:800:HIS:CE1	2.92	0.50
1:A:859:LYS:NZ	1:A:863:TYR:OH	2.44	0.50
1:B:258:GLY:HA2	1:B:260:PHE:CD1	2.46	0.50
1:C:1278:ALA:O	1:C:1280:ARG:N	2.44	0.50
1:D:859:LYS:NZ	1:D:863:TYR:OH	2.45	0.50
1:A:860:ALA:HA	1:A:863:TYR:HD2	1.75	0.50
1:C:460:VAL:HA	1:C:499:PHE:CE2	2.47	0.50
1:C:1269:LEU:O	1:C:1270:ILE:HG12	2.10	0.50
1:D:166:VAL:O	1:D:314:LYS:NZ	2.45	0.50
1:D:1363:ILE:HG22	1:D:1364:CYS:N	2.23	0.50
1:A:1398:LEU:HB3	1:A:1399:PRO:HD2	1.94	0.50
1:B:291:THR:HG22	1:B:292:HIS:H	1.77	0.50
1:B:1398:LEU:HB3	1:B:1399:PRO:HD2	1.94	0.50
1:D:355:GLY:HA2	1:D:361:ASP:OD1	2.10	0.50
1:D:435:GLN:HE22	1:D:471:GLU:CD	2.18	0.50
1:D:1122:LEU:O	1:D:1126:ILE:HG12	2.11	0.50
1:A:574:GLN:HG2	1:A:575:PRO:HD2	1.91	0.50
1:A:1344:PRO:HG3	1:A:1439:TRP:CZ2	2.46	0.50
1:B:354:GLU:HB2	1:B:420:ARG:HA	1.94	0.50
1:B:1344:PRO:HG3	1:B:1439:TRP:CZ2	2.46	0.50
1:C:166:VAL:O	1:C:314:LYS:NZ	2.45	0.50
1:C:573:THR:OG1	1:C:713:GLY:O	2.28	0.50
1:C:1353:THR:HG22	1:C:1374:VAL:HG12	1.92	0.50
1:A:354:GLU:HB2	1:A:420:ARG:HA	1.94	0.50
1:B:1122:LEU:O	1:B:1126:ILE:HG12	2.11	0.50
1:C:354:GLU:HB2	1:C:420:ARG:HA	1.94	0.50
1:C:859:LYS:NZ	1:C:863:TYR:OH	2.44	0.50
1:D:460:VAL:HA	1:D:499:PHE:CE2	2.46	0.50
1:A:341:ASP:HA	1:A:409:ILE:HD11	1.93	0.50
1:A:1278:ALA:O	1:A:1280:ARG:N	2.44	0.50
1:B:341:ASP:HA	1:B:409:ILE:HD11	1.93	0.50
1:B:460:VAL:HG21	1:B:487:THR:HG23	1.92	0.50
1:B:643:ALA:O	1:B:1129:LYS:NZ	2.30	0.50
1:C:435:GLN:HE22	1:C:471:GLU:CD	2.18	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1398:LEU:HB3	1:C:1399:PRO:HD2	1.94	0.50
1:D:860:ALA:HA	1:D:863:TYR:HD2	1.75	0.50
1:D:1350:PRO:HD2	1:D:1388:PRO:O	2.11	0.50
1:A:291:THR:HG22	1:A:292:HIS:H	1.77	0.50
1:C:349:PRO:HB2	1:C:436:ALA:HB1	1.94	0.50
1:D:258:GLY:HA2	1:D:260:PHE:CD1	2.46	0.50
1:A:187:LYS:O	1:A:191:ARG:HG2	2.12	0.50
1:C:145:VAL:O	1:C:287:VAL:HA	2.12	0.50
1:D:806:TYR:HE2	1:D:910:LEU:HB2	1.77	0.50
1:D:1278:ALA:O	1:D:1280:ARG:N	2.44	0.50
1:A:460:VAL:HA	1:A:499:PHE:CE2	2.46	0.50
1:A:460:VAL:HA	1:A:499:PHE:HE2	1.76	0.50
1:A:1453:ASN:O	1:A:1457:LEU:CB	2.38	0.50
1:B:349:PRO:HB2	1:B:436:ALA:HB1	1.94	0.50
1:B:435:GLN:HE22	1:B:471:GLU:CD	2.18	0.50
1:B:574:GLN:HG2	1:B:575:PRO:HD2	1.92	0.50
1:C:291:THR:HG22	1:C:292:HIS:H	1.77	0.50
1:C:1405:ILE:O	1:C:1409:GLU:N	2.43	0.50
1:D:187:LYS:O	1:D:191:ARG:HG2	2.12	0.50
1:D:341:ASP:HA	1:D:409:ILE:HD11	1.93	0.50
1:A:1278:ALA:HB2	1:A:1336:ARG:NH2	2.26	0.49
1:A:1347:THR:OG1	1:A:1390:GLY:O	2.19	0.49
1:D:291:THR:HG22	1:D:292:HIS:H	1.77	0.49
1:D:354:GLU:HB2	1:D:420:ARG:HA	1.94	0.49
1:A:1353:THR:HG22	1:A:1374:VAL:HG12	1.92	0.49
1:B:1405:ILE:O	1:B:1409:GLU:N	2.43	0.49
1:D:1398:LEU:HB3	1:D:1399:PRO:HD2	1.94	0.49
1:A:166:VAL:O	1:A:314:LYS:NZ	2.45	0.49
1:B:145:VAL:O	1:B:287:VAL:HA	2.12	0.49
1:B:460:VAL:HA	1:B:499:PHE:HE2	1.76	0.49
1:B:806:TYR:HE2	1:B:910:LEU:HB2	1.77	0.49
1:B:1278:ALA:HB2	1:B:1336:ARG:NH2	2.26	0.49
1:D:349:PRO:HB2	1:D:436:ALA:HB1	1.94	0.49
1:D:399:ILE:O	1:D:403:THR:HG23	2.13	0.49
1:A:145:VAL:O	1:A:287:VAL:HA	2.12	0.49
1:A:399:ILE:O	1:A:403:THR:HG23	2.13	0.49
1:B:765:LEU:O	1:B:768:THR:OG1	2.27	0.49
1:D:1278:ALA:HB2	1:D:1336:ARG:NH2	2.26	0.49
1:A:806:TYR:HE2	1:A:910:LEU:HB2	1.77	0.49
1:B:859:LYS:NZ	1:B:863:TYR:OH	2.44	0.49
1:C:1042:ASN:HB2	1:D:1048:PHE:HD2	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1339:LEU:HB3	1:B:1345:ASN:ND2	2.27	0.49
1:C:341:ASP:HA	1:C:409:ILE:HD11	1.93	0.49
1:D:643:ALA:O	1:D:1129:LYS:NZ	2.30	0.49
1:A:349:PRO:HB2	1:A:436:ALA:HB1	1.94	0.49
1:A:747:LEU:HD22	1:A:773:PHE:CE1	2.47	0.49
1:B:747:LEU:HD22	1:B:773:PHE:CE1	2.47	0.49
1:D:796:VAL:CG1	1:D:800:HIS:CE1	2.92	0.49
1:A:1328:MET:HG3	1:A:1428:TYR:CD2	2.48	0.49
1:B:930:MET:O	1:B:934:VAL:HG23	2.13	0.49
1:B:1328:MET:HG3	1:B:1428:TYR:CD2	2.48	0.49
1:C:187:LYS:O	1:C:191:ARG:HG2	2.12	0.49
1:C:460:VAL:HA	1:C:499:PHE:HE2	1.76	0.49
1:C:751:ASN:HD22	1:C:772:SER:H	1.61	0.49
1:C:1379:LEU:HB2	1:C:1382:SER:HB3	1.95	0.49
1:A:765:LEU:O	1:A:768:THR:OG1	2.27	0.49
1:A:930:MET:O	1:A:934:VAL:HG23	2.13	0.49
1:A:1339:LEU:HB3	1:A:1345:ASN:ND2	2.27	0.49
1:A:1401:LYS:HD2	1:A:1415:GLU:HB2	1.95	0.49
1:B:166:VAL:O	1:B:314:LYS:NZ	2.45	0.49
1:B:1392:ARG:NH1	1:B:1400:ARG:HA	2.28	0.49
1:B:1401:LYS:HD2	1:B:1415:GLU:HB2	1.95	0.49
1:D:751:ASN:HD22	1:D:772:SER:H	1.61	0.49
1:A:708:VAL:HG21	1:A:1112:LYS:HD2	1.95	0.49
1:A:1048:PHE:HD2	1:D:1042:ASN:HB2	1.78	0.49
1:A:1392:ARG:NH1	1:A:1400:ARG:HA	2.28	0.49
1:B:187:LYS:O	1:B:191:ARG:HG2	2.12	0.49
1:C:806:TYR:HE2	1:C:910:LEU:HB2	1.77	0.49
1:C:1401:LYS:HD2	1:C:1415:GLU:HB2	1.95	0.49
1:D:145:VAL:O	1:D:287:VAL:HA	2.12	0.49
1:D:743:TRP:CD1	1:D:744:TRP:CD1	3.00	0.49
1:D:876:ILE:O	1:D:880:VAL:HG23	2.13	0.49
1:D:1401:LYS:HD2	1:D:1415:GLU:HB2	1.95	0.49
1:A:465:VAL:HA	1:A:499:PHE:HE1	1.78	0.48
1:A:1042:ASN:HB2	1:B:1048:PHE:HD2	1.78	0.48
1:B:708:VAL:HG21	1:B:1112:LYS:HD2	1.95	0.48
1:C:1392:ARG:NH1	1:C:1400:ARG:HA	2.28	0.48
1:C:1453:ASN:O	1:C:1457:LEU:CB	2.38	0.48
1:D:459:ALA:HB1	1:D:468:ALA:HB2	1.95	0.48
1:A:459:ALA:HB1	1:A:468:ALA:HB2	1.95	0.48
1:A:632:GLN:OE1	1:A:634:ARG:NE	2.46	0.48
1:C:390:MET:SD	1:C:392:GLU:N	2.86	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1262:VAL:O	1:C:1330:ARG:N	2.33	0.48
1:D:390:MET:SD	1:D:392:GLU:N	2.86	0.48
1:D:465:VAL:HA	1:D:499:PHE:HE1	1.78	0.48
1:D:1328:MET:HG3	1:D:1428:TYR:CD2	2.48	0.48
1:D:1379:LEU:HB2	1:D:1382:SER:HB3	1.95	0.48
1:A:435:GLN:HE22	1:A:471:GLU:CD	2.18	0.48
1:C:1278:ALA:HB2	1:C:1336:ARG:NH2	2.26	0.48
1:A:876:ILE:O	1:A:880:VAL:HG23	2.13	0.48
1:B:95:HIS:CG	1:B:96:GLU:N	2.81	0.48
1:B:465:VAL:HA	1:B:499:PHE:HE1	1.78	0.48
1:B:1339:LEU:HB3	1:B:1345:ASN:HD21	1.79	0.48
1:C:399:ILE:O	1:C:403:THR:HG23	2.13	0.48
1:C:747:LEU:HD22	1:C:773:PHE:CE1	2.47	0.48
1:C:765:LEU:O	1:C:768:THR:OG1	2.27	0.48
1:B:1408:GLN:HE21	1:B:1473:ILE:HG12	1.79	0.48
1:C:1328:MET:HG3	1:C:1428:TYR:CD2	2.48	0.48
1:D:1339:LEU:HB3	1:D:1345:ASN:ND2	2.28	0.48
1:A:390:MET:SD	1:A:392:GLU:N	2.86	0.48
1:A:643:ALA:O	1:A:1129:LYS:NZ	2.30	0.48
1:A:1339:LEU:HB3	1:A:1345:ASN:HD21	1.79	0.48
1:C:561:VAL:HA	1:C:564:VAL:HG12	1.96	0.48
1:C:743:TRP:CD1	1:C:744:TRP:CD1	3.00	0.48
1:C:876:ILE:O	1:C:880:VAL:HG23	2.13	0.48
1:C:1339:LEU:HB3	1:C:1345:ASN:ND2	2.28	0.48
1:D:561:VAL:HA	1:D:564:VAL:HG12	1.96	0.48
1:B:390:MET:SD	1:B:392:GLU:N	2.86	0.48
1:B:876:ILE:O	1:B:880:VAL:HG23	2.13	0.48
1:B:1379:LEU:HB2	1:B:1382:SER:HB3	1.95	0.48
1:C:78:SER:OG	1:C:103:THR:OG1	2.28	0.48
1:C:465:VAL:HA	1:C:499:PHE:HE1	1.78	0.48
1:C:930:MET:O	1:C:934:VAL:HG23	2.13	0.48
1:C:1408:GLN:HE21	1:C:1473:ILE:HG12	1.79	0.48
1:D:1392:ARG:NH1	1:D:1400:ARG:HA	2.28	0.48
1:D:1408:GLN:HE21	1:D:1473:ILE:HG12	1.79	0.48
1:A:1262:VAL:O	1:A:1330:ARG:N	2.33	0.48
1:A:1379:LEU:HB2	1:A:1382:SER:HB3	1.95	0.48
1:B:395:THR:HG22	1:B:397:SER:H	1.78	0.48
1:D:747:LEU:HD22	1:D:773:PHE:CE1	2.47	0.48
1:A:743:TRP:CD1	1:A:744:TRP:CD1	3.00	0.48
1:A:1408:GLN:HE21	1:A:1473:ILE:HG12	1.79	0.48
1:B:206:ILE:HD13	1:B:239:ILE:HB	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1299:ILE:HD11	1:B:1310:ARG:CZ	2.44	0.48
1:C:1299:ILE:HD11	1:C:1310:ARG:CZ	2.44	0.48
1:A:1299:ILE:HD11	1:A:1310:ARG:CZ	2.44	0.48
1:B:399:ILE:O	1:B:403:THR:HG23	2.13	0.48
1:B:561:VAL:HA	1:B:564:VAL:HG12	1.96	0.48
1:C:708:VAL:HG21	1:C:1112:LYS:HD2	1.95	0.48
1:D:395:THR:HG22	1:D:397:SER:H	1.78	0.48
1:D:930:MET:O	1:D:934:VAL:HG23	2.13	0.48
1:D:1299:ILE:HD11	1:D:1310:ARG:CZ	2.44	0.48
1:A:751:ASN:HD22	1:A:772:SER:H	1.61	0.47
1:A:1100:LYS:HG3	1:A:1101:THR:HG23	1.96	0.47
1:A:1392:ARG:HH22	1:A:1400:ARG:HE	1.62	0.47
1:B:381:GLN:HA	1:B:386:PHE:CE1	2.48	0.47
1:C:1381:LEU:HD23	1:C:1381:LEU:H	1.79	0.47
1:D:1381:LEU:HD23	1:D:1381:LEU:H	1.79	0.47
1:A:1444:ALA:HB2	1:A:1491:LEU:HD11	1.96	0.47
1:B:88:VAL:HG12	1:B:88:VAL:O	2.14	0.47
1:B:459:ALA:HB1	1:B:468:ALA:HB2	1.95	0.47
1:B:1042:ASN:HB2	1:C:1048:PHE:HD2	1.78	0.47
1:B:1381:LEU:H	1:B:1381:LEU:HD23	1.79	0.47
1:C:395:THR:HG22	1:C:397:SER:H	1.78	0.47
1:C:1100:LYS:HG3	1:C:1101:THR:HG23	1.96	0.47
1:D:206:ILE:HD13	1:D:239:ILE:HB	1.96	0.47
1:A:1286:MET:HE2	1:A:1289:MET:CB	2.45	0.47
1:B:78:SER:OG	1:B:103:THR:OG1	2.28	0.47
1:B:1444:ALA:HB2	1:B:1491:LEU:HD11	1.96	0.47
1:C:459:ALA:HB1	1:C:468:ALA:HB2	1.95	0.47
1:C:616:THR:OG1	1:C:617:PHE:N	2.48	0.47
1:D:1100:LYS:HG3	1:D:1101:THR:HG23	1.96	0.47
1:A:561:VAL:HA	1:A:564:VAL:HG12	1.96	0.47
1:C:796:VAL:CG1	1:C:800:HIS:CE1	2.92	0.47
1:C:1286:MET:HE2	1:C:1289:MET:CB	2.45	0.47
1:D:1339:LEU:HB3	1:D:1345:ASN:HD21	1.79	0.47
1:D:1444:ALA:HB2	1:D:1491:LEU:HD11	1.96	0.47
1:A:616:THR:OG1	1:A:617:PHE:N	2.48	0.47
1:A:1381:LEU:HD23	1:A:1381:LEU:H	1.79	0.47
1:B:562:ALA:HB2	1:B:577:TYR:HD2	1.80	0.47
1:C:801:LEU:HD21	1:C:1081:PRO:HB3	1.97	0.47
1:C:1247:TYR:OH	1:C:1337:GLY:HA3	2.15	0.47
1:D:88:VAL:HG12	1:D:88:VAL:O	2.14	0.47
1:D:616:THR:OG1	1:D:617:PHE:N	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:708:VAL:HG21	1:D:1112:LYS:HD2	1.95	0.47
1:D:1247:TYR:OH	1:D:1337:GLY:HA3	2.15	0.47
1:A:88:VAL:HG12	1:A:88:VAL:O	2.14	0.47
1:A:562:ALA:HB2	1:A:577:TYR:HD2	1.80	0.47
1:A:1247:TYR:OH	1:A:1337:GLY:HA3	2.15	0.47
1:B:174:THR:OG1	2:B:2001:UOZ:O35	2.24	0.47
1:B:751:ASN:HD22	1:B:772:SER:H	1.61	0.47
1:C:1339:LEU:HB3	1:C:1345:ASN:HD21	1.79	0.47
1:A:381:GLN:HA	1:A:386:PHE:CE1	2.48	0.47
1:C:88:VAL:HG12	1:C:88:VAL:O	2.14	0.47
1:C:562:ALA:HB2	1:C:577:TYR:HD2	1.80	0.47
1:D:743:TRP:CE2	1:D:796:VAL:HG22	2.50	0.47
1:D:1292:THR:HG22	1:D:1293:LEU:N	2.30	0.47
1:A:255:HIS:HB3	1:A:260:PHE:CE1	2.50	0.47
1:B:428:ASP:OD1	1:B:429:VAL:N	2.48	0.47
1:B:632:GLN:OE1	1:B:634:ARG:NE	2.46	0.47
1:B:801:LEU:HD21	1:B:1081:PRO:HB3	1.97	0.47
1:B:1286:MET:HE2	1:B:1289:MET:CB	2.45	0.47
1:C:1292:THR:HG22	1:C:1293:LEU:N	2.30	0.47
1:C:1444:ALA:HB2	1:C:1491:LEU:HD11	1.96	0.47
1:D:381:GLN:HA	1:D:386:PHE:CE1	2.48	0.47
1:B:743:TRP:CD1	1:B:744:TRP:CD1	3.00	0.47
1:D:428:ASP:OD1	1:D:429:VAL:N	2.48	0.47
1:D:632:GLN:OE1	1:D:634:ARG:NE	2.46	0.47
1:D:1286:MET:HE2	1:D:1289:MET:CB	2.45	0.47
1:D:1392:ARG:NH1	1:D:1399:PRO:O	2.48	0.47
1:A:86:LYS:HZ1	1:A:92:GLY:HA2	1.80	0.47
1:A:395:THR:HG22	1:A:397:SER:H	1.78	0.47
1:C:206:ILE:HD13	1:C:239:ILE:HB	1.96	0.47
1:D:255:HIS:HB3	1:D:260:PHE:CE1	2.50	0.47
1:D:1392:ARG:HH22	1:D:1400:ARG:HE	1.62	0.47
1:A:743:TRP:CE2	1:A:796:VAL:HG22	2.50	0.46
1:B:1100:LYS:HG3	1:B:1101:THR:HG23	1.96	0.46
1:B:1392:ARG:NH1	1:B:1399:PRO:O	2.48	0.46
1:D:562:ALA:HB2	1:D:577:TYR:HD2	1.80	0.46
1:A:730:VAL:HA	1:A:735:ILE:HG21	1.97	0.46
1:A:1292:THR:HG22	1:A:1293:LEU:N	2.30	0.46
1:A:1392:ARG:NH1	1:A:1399:PRO:O	2.48	0.46
1:B:255:HIS:HB3	1:B:260:PHE:CE1	2.50	0.46
1:B:557:GLN:CG	1:B:585:ARG:HB3	2.45	0.46
1:C:743:TRP:CE2	1:C:796:VAL:HG22	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1039:LEU:O	1:A:1043:LEU:HB2	2.16	0.46
1:B:1292:THR:HG22	1:B:1293:LEU:N	2.30	0.46
1:B:1410:HIS:O	1:B:1410:HIS:ND1	2.49	0.46
1:A:557:GLN:CG	1:A:585:ARG:HB3	2.46	0.46
1:B:616:THR:OG1	1:B:617:PHE:N	2.48	0.46
1:C:79:SER:HB3	1:C:93:TYR:CE2	2.51	0.46
1:C:389:GLU:O	1:C:390:MET:HB3	2.15	0.46
1:C:643:ALA:O	1:C:1129:LYS:NZ	2.30	0.46
1:D:389:GLU:O	1:D:390:MET:HB3	2.15	0.46
1:A:104:LYS:HG2	1:A:105:PRO:HD3	1.98	0.46
1:B:730:VAL:HA	1:B:735:ILE:HG21	1.97	0.46
1:B:1135:ASN:O	1:B:1139:GLN:HG2	2.16	0.46
1:B:1301:TYR:HB3	1:B:1317:TYR:OH	2.16	0.46
1:C:381:GLN:HA	1:C:386:PHE:CE1	2.48	0.46
1:C:751:ASN:ND2	1:C:772:SER:H	2.14	0.46
1:C:1392:ARG:NH1	1:C:1399:PRO:O	2.48	0.46
1:C:1478:VAL:HA	1:C:1482:ILE:HD11	1.98	0.46
1:D:95:HIS:CD2	1:D:96:GLU:H	2.34	0.46
1:D:801:LEU:HD21	1:D:1081:PRO:HB3	1.97	0.46
1:D:1301:TYR:HB3	1:D:1317:TYR:OH	2.16	0.46
1:A:206:ILE:HD13	1:A:239:ILE:HB	1.96	0.46
1:B:249:ARG:HH11	1:B:265:ILE:HB	1.81	0.46
1:B:743:TRP:CE2	1:B:796:VAL:HG22	2.50	0.46
1:C:249:ARG:HH11	1:C:265:ILE:HB	1.81	0.46
1:C:255:HIS:HB3	1:C:260:PHE:CE1	2.50	0.46
1:C:1301:TYR:HB3	1:C:1317:TYR:OH	2.16	0.46
1:D:249:ARG:HH11	1:D:265:ILE:HB	1.81	0.46
1:D:1410:HIS:ND1	1:D:1410:HIS:O	2.49	0.46
1:A:395:THR:O	1:A:399:ILE:HG12	2.16	0.46
1:B:1247:TYR:OH	1:B:1337:GLY:HA3	2.15	0.46
1:D:1135:ASN:O	1:D:1139:GLN:HG2	2.16	0.46
1:D:1264:TRP:HE3	1:D:1330:ARG:HB2	1.81	0.46
1:A:1478:VAL:HA	1:A:1482:ILE:HD11	1.98	0.46
1:B:389:GLU:O	1:B:390:MET:HB3	2.15	0.46
1:C:1264:TRP:HE3	1:C:1330:ARG:HB2	1.81	0.46
1:A:428:ASP:OD1	1:A:429:VAL:N	2.48	0.46
1:B:79:SER:HB3	1:B:93:TYR:CE2	2.51	0.46
1:B:1264:TRP:HE3	1:B:1330:ARG:HB2	1.81	0.46
1:D:104:LYS:HG2	1:D:105:PRO:HD3	1.98	0.46
1:D:395:THR:O	1:D:399:ILE:HG12	2.16	0.46
1:D:921:GLY:O	1:D:925:ILE:HG12	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1478:VAL:HA	1:D:1482:ILE:HD11	1.98	0.46
1:A:389:GLU:O	1:A:390:MET:HB3	2.15	0.46
1:A:801:LEU:HD21	1:A:1081:PRO:HB3	1.97	0.46
1:A:1301:TYR:HB3	1:A:1317:TYR:OH	2.16	0.46
1:B:921:GLY:O	1:B:925:ILE:HG12	2.16	0.46
1:B:1398:LEU:HB3	1:B:1399:PRO:CD	2.46	0.46
1:C:730:VAL:HA	1:C:735:ILE:HG21	1.97	0.46
1:C:1410:HIS:O	1:C:1410:HIS:ND1	2.49	0.46
1:D:725:LYS:O	1:D:727:MET:HE2	2.16	0.46
1:A:95:HIS:CD2	1:A:96:GLU:H	2.34	0.45
1:A:394:PHE:HD1	1:A:398:ARG:HH21	1.64	0.45
1:B:394:PHE:HD1	1:B:398:ARG:HH21	1.64	0.45
1:B:751:ASN:ND2	1:B:772:SER:H	2.14	0.45
1:B:1039:LEU:O	1:B:1043:LEU:HB2	2.16	0.45
1:C:1039:LEU:O	1:C:1043:LEU:HB2	2.16	0.45
1:C:1105:ARG:HD2	1:C:1105:ARG:HA	1.79	0.45
1:C:1392:ARG:NH2	1:C:1400:ARG:HE	2.15	0.45
1:A:725:LYS:O	1:A:727:MET:HE2	2.16	0.45
1:B:1392:ARG:HH22	1:B:1400:ARG:HE	1.62	0.45
1:C:395:THR:O	1:C:399:ILE:HG12	2.16	0.45
1:C:1392:ARG:HH22	1:C:1400:ARG:HE	1.62	0.45
1:D:394:PHE:HD1	1:D:398:ARG:HH21	1.64	0.45
1:D:557:GLN:CG	1:D:585:ARG:HB3	2.46	0.45
1:D:730:VAL:HA	1:D:735:ILE:HG21	1.97	0.45
1:D:751:ASN:ND2	1:D:772:SER:H	2.14	0.45
1:D:765:LEU:O	1:D:768:THR:OG1	2.27	0.45
1:A:1264:TRP:HE3	1:A:1330:ARG:HB2	1.81	0.45
1:B:86:LYS:HZ1	1:B:92:GLY:HA2	1.82	0.45
1:C:95:HIS:CD2	1:C:96:GLU:H	2.34	0.45
1:C:921:GLY:O	1:C:925:ILE:HG12	2.16	0.45
1:A:79:SER:HB3	1:A:93:TYR:CE2	2.51	0.45
1:B:104:LYS:HG2	1:B:105:PRO:HD3	1.98	0.45
1:B:353:VAL:HA	1:B:419:PHE:HB3	1.99	0.45
1:B:584:ASP:OD2	1:B:587:ARG:NH1	2.50	0.45
1:C:1496:ALA:HB1	1:C:1501:ALA:HB3	1.98	0.45
1:D:1392:ARG:NH2	1:D:1400:ARG:HE	2.15	0.45
1:B:395:THR:O	1:B:399:ILE:HG12	2.16	0.45
1:C:223:ARG:HG2	1:C:227:LEU:HD13	1.99	0.45
1:C:557:GLN:CG	1:C:585:ARG:HB3	2.46	0.45
1:C:632:GLN:OE1	1:C:634:ARG:NE	2.46	0.45
1:D:79:SER:HB3	1:D:93:TYR:CE2	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1496:ALA:HB1	1:D:1501:ALA:HB3	1.98	0.45
1:A:584:ASP:OD2	1:A:587:ARG:NH1	2.50	0.45
1:A:1135:ASN:O	1:A:1139:GLN:HG2	2.16	0.45
1:A:1398:LEU:HB3	1:A:1399:PRO:CD	2.46	0.45
1:B:1392:ARG:NH2	1:B:1400:ARG:HE	2.15	0.45
1:C:428:ASP:OD1	1:C:429:VAL:N	2.48	0.45
1:C:1093:PHE:O	1:C:1097:VAL:HG23	2.17	0.45
1:C:1135:ASN:O	1:C:1139:GLN:HG2	2.16	0.45
1:C:1398:LEU:HB3	1:C:1399:PRO:CD	2.46	0.45
1:D:149:THR:O	1:D:304:ARG:NH2	2.50	0.45
1:D:223:ARG:HG2	1:D:227:LEU:HD13	1.99	0.45
1:D:340:ILE:HG22	1:D:409:ILE:HD12	1.99	0.45
1:D:1039:LEU:O	1:D:1043:LEU:HB2	2.16	0.45
1:A:921:GLY:O	1:A:925:ILE:HG12	2.16	0.45
1:B:223:ARG:HG2	1:B:227:LEU:HD13	1.99	0.45
1:B:1093:PHE:O	1:B:1097:VAL:HG23	2.17	0.45
1:B:1478:VAL:HA	1:B:1482:ILE:HD11	1.98	0.45
1:C:394:PHE:HD1	1:C:398:ARG:HH21	1.64	0.45
1:D:1398:LEU:HB3	1:D:1399:PRO:CD	2.46	0.45
1:A:278:ASP:OD1	1:A:279:SER:N	2.50	0.45
1:A:1410:HIS:O	1:A:1410:HIS:ND1	2.49	0.45
1:B:95:HIS:CD2	1:B:96:GLU:H	2.34	0.45
1:C:725:LYS:O	1:C:727:MET:HE2	2.16	0.45
1:A:223:ARG:HG2	1:A:227:LEU:HD13	1.99	0.45
1:B:725:LYS:O	1:B:727:MET:HE2	2.16	0.45
1:B:1164:LEU:HD23	1:B:1164:LEU:H	1.82	0.45
1:C:298:GLU:OE1	1:C:298:GLU:N	2.28	0.45
1:C:584:ASP:OD2	1:C:587:ARG:NH1	2.50	0.45
1:D:1273:PRO:HA	1:D:1274:PRO:HD3	1.85	0.45
1:A:149:THR:O	1:A:304:ARG:NH2	2.50	0.45
1:A:249:ARG:HH11	1:A:265:ILE:HB	1.81	0.45
1:A:751:ASN:ND2	1:A:772:SER:H	2.14	0.45
1:A:1496:ALA:HB1	1:A:1501:ALA:HB3	1.98	0.45
1:B:305:LEU:O	1:B:309:ILE:HG13	2.17	0.45
1:B:446:HIS:CG	1:B:451:ASN:HB3	2.52	0.45
1:C:1301:TYR:CE2	1:C:1324:PRO:HD3	2.52	0.45
1:D:873:VAL:O	1:D:877:LEU:HG	2.17	0.45
1:A:353:VAL:HA	1:A:419:PHE:HB3	1.99	0.44
1:C:79:SER:HB3	1:C:93:TYR:CD2	2.52	0.44
1:C:278:ASP:OD1	1:C:279:SER:N	2.50	0.44
1:D:79:SER:HB3	1:D:93:TYR:CD2	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:584:ASP:OD2	1:D:587:ARG:NH1	2.49	0.44
1:A:1105:ARG:HA	1:A:1105:ARG:HD2	1.79	0.44
1:B:79:SER:HB3	1:B:93:TYR:CD2	2.52	0.44
1:B:278:ASP:OD1	1:B:279:SER:N	2.50	0.44
1:B:340:ILE:HG22	1:B:409:ILE:HD12	1.99	0.44
1:B:405:LYS:O	1:B:409:ILE:HG12	2.17	0.44
1:B:552:ALA:HB3	1:B:589:LEU:HB3	2.00	0.44
1:B:796:VAL:CG1	1:B:800:HIS:CE1	2.92	0.44
1:D:1301:TYR:CE2	1:D:1324:PRO:HD3	2.52	0.44
1:A:1093:PHE:O	1:A:1097:VAL:HG23	2.17	0.44
1:A:1353:THR:OG1	1:A:1448:HIS:ND1	2.34	0.44
1:A:1392:ARG:NH2	1:A:1400:ARG:HE	2.15	0.44
1:B:149:THR:O	1:B:304:ARG:NH2	2.50	0.44
1:C:104:LYS:HG2	1:C:105:PRO:HD3	1.98	0.44
1:C:873:VAL:O	1:C:877:LEU:HG	2.17	0.44
1:C:1164:LEU:HD23	1:C:1164:LEU:H	1.82	0.44
1:D:175:GLY:O	1:D:336:THR:OG1	2.36	0.44
1:D:405:LYS:O	1:D:409:ILE:HG12	2.17	0.44
1:A:405:LYS:O	1:A:409:ILE:HG12	2.17	0.44
1:A:446:HIS:CG	1:A:451:ASN:HB3	2.52	0.44
1:C:353:VAL:HA	1:C:419:PHE:HB3	1.99	0.44
1:D:305:LEU:O	1:D:309:ILE:HG13	2.17	0.44
1:A:873:VAL:O	1:A:877:LEU:HG	2.17	0.44
1:A:1273:PRO:HA	1:A:1274:PRO:HD3	1.85	0.44
1:A:1408:GLN:NE2	1:A:1473:ILE:HG12	2.32	0.44
1:B:873:VAL:O	1:B:877:LEU:HG	2.17	0.44
1:D:1239:HIS:NE2	1:D:1331:THR:HB	2.33	0.44
1:C:546:ARG:HA	1:C:546:ARG:HD3	1.87	0.44
1:C:552:ALA:HB3	1:C:589:LEU:HB3	2.00	0.44
1:D:353:VAL:HA	1:D:419:PHE:HB3	1.99	0.44
1:D:1093:PHE:O	1:D:1097:VAL:HG23	2.17	0.44
1:D:1408:GLN:NE2	1:D:1473:ILE:HG12	2.32	0.44
1:A:95:HIS:CG	1:A:96:GLU:N	2.81	0.44
1:A:291:THR:HG22	1:A:292:HIS:N	2.33	0.44
1:B:291:THR:HG22	1:B:292:HIS:N	2.33	0.44
1:B:1044:LEU:HA	1:B:1047:MET:HG3	2.00	0.44
1:B:1435:THR:OG1	1:B:1436:ASP:N	2.51	0.44
1:B:1496:ALA:HB1	1:B:1501:ALA:HB3	1.98	0.44
1:C:175:GLY:O	1:C:336:THR:OG1	2.36	0.44
1:C:340:ILE:HG22	1:C:409:ILE:HD12	1.99	0.44
1:C:1408:GLN:NE2	1:C:1473:ILE:HG12	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1454:ASP:HB3	1:C:1456:GLU:CD	2.43	0.44
1:D:278:ASP:OD1	1:D:279:SER:N	2.50	0.44
1:D:446:HIS:CG	1:D:451:ASN:HB3	2.53	0.44
1:A:340:ILE:HG22	1:A:409:ILE:HD12	1.99	0.44
1:C:195:VAL:HG21	1:C:225:PHE:CG	2.53	0.44
1:C:868:TRP:HZ2	1:C:928:LYS:HE3	1.83	0.44
1:C:1435:THR:OG1	1:C:1436:ASP:N	2.51	0.44
1:D:158:MET:O	1:D:162:TRP:HB2	2.18	0.44
1:A:133:THR:HG22	1:A:263:GLU:HB2	2.00	0.43
1:A:822:GLN:O	1:A:886:ARG:NH1	2.51	0.43
1:B:822:GLN:O	1:B:886:ARG:NH1	2.51	0.43
1:B:1408:GLN:NE2	1:B:1473:ILE:HG12	2.32	0.43
1:C:158:MET:O	1:C:162:TRP:HB2	2.18	0.43
1:C:1239:HIS:NE2	1:C:1331:THR:HB	2.33	0.43
1:C:1264:TRP:CZ2	1:C:1325:LEU:HB3	2.53	0.43
1:D:195:VAL:HG21	1:D:225:PHE:CG	2.53	0.43
1:A:1264:TRP:CZ2	1:A:1325:LEU:HB3	2.53	0.43
1:A:1301:TYR:CE2	1:A:1324:PRO:HD3	2.52	0.43
1:B:1396:GLU:O	1:B:1400:ARG:NH2	2.51	0.43
1:C:149:THR:O	1:C:304:ARG:NH2	2.50	0.43
1:C:291:THR:HG22	1:C:292:HIS:N	2.33	0.43
1:C:305:LEU:O	1:C:309:ILE:HG13	2.17	0.43
1:C:405:LYS:O	1:C:409:ILE:HG12	2.17	0.43
1:C:762:ALA:HB1	1:C:765:LEU:HD13	2.01	0.43
1:D:1243:ARG:NH2	1:D:1259:ASN:OD1	2.51	0.43
1:A:667:GLU:CD	1:A:667:GLU:H	2.26	0.43
1:A:1044:LEU:HA	1:A:1047:MET:HG3	2.00	0.43
1:A:1396:GLU:O	1:A:1400:ARG:NH2	2.51	0.43
1:B:667:GLU:CD	1:B:667:GLU:H	2.26	0.43
1:B:1126:ILE:O	1:B:1130:GLU:HG3	2.19	0.43
1:B:1239:HIS:NE2	1:B:1331:THR:HB	2.33	0.43
1:B:1301:TYR:CE2	1:B:1324:PRO:HD3	2.52	0.43
1:C:559:HIS:NE2	1:C:579:ARG:HG2	2.33	0.43
1:D:291:THR:HG22	1:D:292:HIS:N	2.33	0.43
1:A:79:SER:HB3	1:A:93:TYR:CD2	2.52	0.43
1:A:210:SER:O	1:A:215:MET:HG3	2.18	0.43
1:A:1165:ASP:OD1	1:A:1165:ASP:N	2.52	0.43
1:A:1239:HIS:NE2	1:A:1331:THR:HB	2.33	0.43
1:B:175:GLY:O	1:B:336:THR:OG1	2.36	0.43
1:B:210:SER:O	1:B:215:MET:HG3	2.18	0.43
1:B:762:ALA:HB1	1:B:765:LEU:HD13	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:667:GLU:H	1:C:667:GLU:CD	2.26	0.43
1:C:822:GLN:O	1:C:886:ARG:NH1	2.51	0.43
1:C:1243:ARG:NH2	1:C:1259:ASN:OD1	2.51	0.43
1:D:822:GLN:O	1:D:886:ARG:NH1	2.51	0.43
1:D:1262:VAL:O	1:D:1330:ARG:N	2.33	0.43
1:A:305:LEU:O	1:A:309:ILE:HG13	2.17	0.43
1:A:762:ALA:HB1	1:A:765:LEU:HD13	2.01	0.43
1:A:868:TRP:HZ2	1:A:928:LYS:HE3	1.83	0.43
1:B:459:ALA:HA	1:B:462:TRP:CD1	2.54	0.43
1:B:559:HIS:NE2	1:B:579:ARG:HG2	2.33	0.43
1:B:1243:ARG:NH2	1:B:1259:ASN:OD1	2.51	0.43
1:C:446:HIS:CG	1:C:451:ASN:HB3	2.53	0.43
1:A:559:HIS:NE2	1:A:579:ARG:HG2	2.33	0.43
1:B:1262:VAL:O	1:B:1330:ARG:N	2.33	0.43
1:B:1454:ASP:HB3	1:B:1456:GLU:CD	2.43	0.43
1:D:559:HIS:NE2	1:D:579:ARG:HG2	2.33	0.43
1:A:195:VAL:HG21	1:A:225:PHE:CG	2.53	0.43
1:A:1126:ILE:O	1:A:1130:GLU:HG3	2.19	0.43
1:B:133:THR:HG22	1:B:263:GLU:HB2	2.00	0.43
1:B:287:VAL:HG11	1:B:298:GLU:HA	2.00	0.43
1:B:944:TRP:CD1	1:B:1036:THR:HG22	2.54	0.43
1:D:95:HIS:CG	1:D:96:GLU:N	2.81	0.43
1:D:287:VAL:HG11	1:D:298:GLU:HA	2.00	0.43
1:D:552:ALA:HB3	1:D:589:LEU:HB3	2.00	0.43
1:D:667:GLU:CD	1:D:667:GLU:H	2.26	0.43
1:D:868:TRP:HZ2	1:D:928:LYS:HE3	1.83	0.43
1:D:1164:LEU:H	1:D:1164:LEU:HD23	1.82	0.43
1:D:1264:TRP:CZ2	1:D:1325:LEU:HB3	2.53	0.43
1:B:428:ASP:HB3	1:B:431:VAL:H	1.84	0.43
1:B:868:TRP:HZ2	1:B:928:LYS:HE3	1.83	0.43
1:C:936:PHE:CE1	1:D:920:LEU:HB2	2.54	0.43
1:C:945:VAL:HA	1:C:1032:TYR:OH	2.19	0.43
1:C:1396:GLU:O	1:C:1400:ARG:NH2	2.51	0.43
1:D:1165:ASP:OD1	1:D:1165:ASP:N	2.52	0.43
1:A:175:GLY:O	1:A:336:THR:OG1	2.36	0.43
1:A:1412:PRO:HG2	1:A:1459:ARG:NH1	2.34	0.43
1:B:186:LEU:HD23	1:B:186:LEU:HA	1.79	0.43
1:B:380:GLN:NE2	1:B:394:PHE:CE2	2.87	0.43
1:B:945:VAL:HA	1:B:1032:TYR:OH	2.19	0.43
1:C:944:TRP:CD1	1:C:1036:THR:HG22	2.54	0.43
1:C:1165:ASP:N	1:C:1165:ASP:OD1	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:762:ALA:HB1	1:D:765:LEU:HD13	2.00	0.43
1:D:944:TRP:CD1	1:D:1036:THR:HG22	2.54	0.43
1:D:1126:ILE:O	1:D:1130:GLU:HG3	2.19	0.43
1:D:1247:TYR:CG	1:D:1248:PRO:HD2	2.54	0.43
1:D:1454:ASP:HB3	1:D:1456:GLU:CD	2.43	0.43
1:A:380:GLN:NE2	1:A:394:PHE:CE2	2.87	0.43
1:B:158:MET:O	1:B:162:TRP:HB2	2.18	0.43
1:B:195:VAL:HG21	1:B:225:PHE:CG	2.53	0.43
1:B:1264:TRP:CZ2	1:B:1325:LEU:HB3	2.53	0.43
1:B:1290:GLY:HA3	1:B:1308:ARG:HH22	1.84	0.43
1:C:428:ASP:HB3	1:C:431:VAL:H	1.84	0.43
1:C:1044:LEU:HA	1:C:1047:MET:HG3	2.00	0.43
1:C:1290:GLY:HA3	1:C:1308:ARG:HH22	1.84	0.43
1:D:250:ARG:O	1:D:253:LEU:HB3	2.19	0.43
1:D:428:ASP:HB3	1:D:431:VAL:H	1.84	0.43
1:A:158:MET:O	1:A:162:TRP:HB2	2.18	0.42
1:A:936:PHE:CE1	1:B:920:LEU:HB2	2.54	0.42
1:A:1039:LEU:HA	1:A:1043:LEU:HD13	2.01	0.42
1:A:1164:LEU:H	1:A:1164:LEU:HD23	1.82	0.42
1:A:1249:ASN:HB2	1:A:1279:GLU:OE2	2.19	0.42
1:A:1407:ARG:HG3	1:A:1407:ARG:HH11	1.84	0.42
1:B:1412:PRO:HG2	1:B:1459:ARG:NH1	2.34	0.42
1:C:954:ALA:O	1:D:896:ARG:NH2	2.51	0.42
1:D:316:ARG:HB3	1:D:317:GLY:H	1.66	0.42
1:D:1044:LEU:HA	1:D:1047:MET:HG3	2.00	0.42
1:D:1407:ARG:HG3	1:D:1407:ARG:HH11	1.84	0.42
1:D:1457:LEU:O	1:D:1461:ASN:ND2	2.52	0.42
1:A:258:GLY:HA2	1:A:260:PHE:CE1	2.55	0.42
1:A:459:ALA:HA	1:A:462:TRP:CD1	2.54	0.42
1:A:920:LEU:HB2	1:D:936:PHE:CE1	2.54	0.42
1:A:1243:ARG:NH2	1:A:1259:ASN:OD1	2.51	0.42
1:A:1454:ASP:HB3	1:A:1456:GLU:CD	2.43	0.42
1:B:583:ASN:O	1:B:585:ARG:HG2	2.20	0.42
1:B:1165:ASP:OD1	1:B:1165:ASP:N	2.52	0.42
1:C:287:VAL:HG11	1:C:298:GLU:HA	2.00	0.42
1:C:459:ALA:HA	1:C:462:TRP:CD1	2.54	0.42
1:D:1396:GLU:O	1:D:1400:ARG:NH2	2.51	0.42
1:B:258:GLY:HA2	1:B:260:PHE:CE1	2.55	0.42
1:C:210:SER:O	1:C:215:MET:HG3	2.18	0.42
1:C:1126:ILE:O	1:C:1130:GLU:HG3	2.19	0.42
1:D:133:THR:HG22	1:D:263:GLU:HB2	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:186:LEU:HD23	1:D:186:LEU:HA	1.79	0.42
1:D:595:VAL:HG13	1:D:603:SER:O	2.19	0.42
1:D:1249:ASN:HB2	1:D:1279:GLU:OE2	2.19	0.42
1:D:1428:TYR:CE1	1:D:1439:TRP:HB2	2.49	0.42
1:A:583:ASN:O	1:A:585:ARG:HG2	2.19	0.42
1:A:830:CYS:HA	1:A:833:TYR:CD2	2.55	0.42
1:A:1067:ARG:O	1:A:1071:ILE:HG12	2.20	0.42
1:B:936:PHE:CE1	1:C:920:LEU:HB2	2.54	0.42
1:B:954:ALA:O	1:C:896:ARG:NH2	2.51	0.42
1:B:1105:ARG:HD2	1:B:1105:ARG:HA	1.79	0.42
1:B:1247:TYR:CG	1:B:1248:PRO:HD2	2.54	0.42
1:B:1249:ASN:HB2	1:B:1279:GLU:OE2	2.19	0.42
1:C:559:HIS:H	1:C:585:ARG:HB2	1.85	0.42
1:C:1039:LEU:HA	1:C:1043:LEU:HD13	2.01	0.42
1:D:559:HIS:H	1:D:585:ARG:HB2	1.85	0.42
1:A:112:GLN:O	1:A:114:ASP:N	2.53	0.42
1:A:1060:ASP:O	1:A:1064:LYS:HG2	2.19	0.42
1:B:595:VAL:HG13	1:B:603:SER:O	2.19	0.42
1:C:250:ARG:O	1:C:253:LEU:HB3	2.19	0.42
1:C:1412:PRO:HG2	1:C:1459:ARG:NH1	2.34	0.42
1:D:258:GLY:HA2	1:D:260:PHE:CE1	2.55	0.42
1:D:459:ALA:HA	1:D:462:TRP:CD1	2.54	0.42
1:D:804:LEU:HD23	1:D:804:LEU:HA	1.86	0.42
1:D:945:VAL:HA	1:D:1032:TYR:OH	2.19	0.42
1:D:1060:ASP:O	1:D:1064:LYS:HG2	2.19	0.42
1:A:944:TRP:CD1	1:A:1036:THR:HG22	2.54	0.42
1:A:1247:TYR:CG	1:A:1248:PRO:HD2	2.54	0.42
1:A:1290:GLY:HA3	1:A:1308:ARG:HH22	1.84	0.42
1:B:250:ARG:O	1:B:253:LEU:HB3	2.19	0.42
1:B:1060:ASP:O	1:B:1064:LYS:HG2	2.19	0.42
1:C:112:GLN:O	1:C:114:ASP:N	2.53	0.42
1:C:1156:ASP:HA	1:C:1159:VAL:HG22	2.01	0.42
1:D:210:SER:O	1:D:215:MET:HG3	2.18	0.42
1:A:316:ARG:HB3	1:A:317:GLY:H	1.66	0.42
1:A:428:ASP:HB3	1:A:431:VAL:H	1.84	0.42
1:B:789:ARG:HA	1:B:789:ARG:HD3	1.83	0.42
1:B:1039:LEU:HA	1:B:1043:LEU:HD13	2.01	0.42
1:B:1070:LEU:HA	1:B:1073:GLU:OE1	2.20	0.42
1:B:1407:ARG:HG3	1:B:1407:ARG:HH11	1.84	0.42
1:C:1407:ARG:HG3	1:C:1407:ARG:HH11	1.84	0.42
1:C:1457:LEU:O	1:C:1461:ASN:ND2	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:830:CYS:HA	1:D:833:TYR:CD2	2.55	0.42
1:D:1105:ARG:HA	1:D:1105:ARG:HD2	1.79	0.42
1:A:466:ASP:OD1	1:A:467:ILE:HG13	2.20	0.42
1:A:595:VAL:HG13	1:A:603:SER:O	2.19	0.42
1:B:530:CYS:SG	1:B:531:LEU:N	2.93	0.42
1:B:1067:ARG:O	1:B:1071:ILE:HG12	2.20	0.42
1:B:1269:LEU:HB3	1:B:1270:ILE:H	1.71	0.42
1:B:1457:LEU:O	1:B:1461:ASN:ND2	2.52	0.42
1:C:1060:ASP:O	1:C:1064:LYS:HG2	2.19	0.42
1:C:1247:TYR:CG	1:C:1248:PRO:HD2	2.54	0.42
1:D:545:GLU:HB2	1:D:552:ALA:HA	2.02	0.42
1:D:1290:GLY:HA3	1:D:1308:ARG:HH22	1.84	0.42
1:A:250:ARG:O	1:A:253:LEU:HB3	2.19	0.42
1:D:1156:ASP:HA	1:D:1159:VAL:HG22	2.01	0.42
1:B:337:LEU:HD21	1:B:405:LYS:CB	2.50	0.42
1:C:133:THR:HG22	1:C:263:GLU:HB2	2.00	0.42
1:C:316:ARG:HB3	1:C:317:GLY:H	1.66	0.42
1:C:545:GLU:HB2	1:C:552:ALA:HA	2.02	0.42
1:D:112:GLN:O	1:D:114:ASP:N	2.53	0.42
1:D:337:LEU:HD21	1:D:405:LYS:CB	2.50	0.42
1:A:186:LEU:HA	1:A:189:ILE:HG22	2.02	0.41
1:A:287:VAL:HG11	1:A:298:GLU:HA	2.00	0.41
1:A:552:ALA:HB3	1:A:589:LEU:HB3	2.00	0.41
1:A:1392:ARG:HH12	1:A:1400:ARG:NE	2.18	0.41
1:A:1411:TRP:H	1:A:1411:TRP:HE3	1.67	0.41
1:A:1457:LEU:O	1:A:1461:ASN:ND2	2.52	0.41
1:B:806:TYR:CE2	1:B:910:LEU:HB2	2.55	0.41
1:B:830:CYS:HA	1:B:833:TYR:CD2	2.55	0.41
1:C:1067:ARG:O	1:C:1071:ILE:HG12	2.20	0.41
1:C:1070:LEU:HA	1:C:1073:GLU:OE1	2.20	0.41
1:C:1411:TRP:H	1:C:1411:TRP:HE3	1.67	0.41
1:D:1039:LEU:HA	1:D:1043:LEU:HD13	2.01	0.41
1:D:1067:ARG:O	1:D:1071:ILE:HG12	2.20	0.41
1:D:1412:PRO:HG2	1:D:1459:ARG:NH1	2.34	0.41
1:A:546:ARG:HA	1:A:546:ARG:HD3	1.87	0.41
1:A:1070:LEU:HA	1:A:1073:GLU:OE1	2.20	0.41
1:B:186:LEU:HA	1:B:189:ILE:HG22	2.02	0.41
1:B:559:HIS:H	1:B:585:ARG:HB2	1.85	0.41
1:C:186:LEU:HA	1:C:189:ILE:HG22	2.02	0.41
1:C:583:ASN:O	1:C:585:ARG:HG2	2.19	0.41
1:C:595:VAL:HG13	1:C:603:SER:O	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1392:ARG:HH12	1:D:1400:ARG:NE	2.18	0.41
1:A:545:GLU:HB2	1:A:552:ALA:HA	2.02	0.41
1:B:618:THR:O	1:B:619:MET:HG3	2.21	0.41
1:C:337:LEU:HD21	1:C:405:LYS:CB	2.50	0.41
1:C:659:LEU:HD23	1:C:659:LEU:HA	1.83	0.41
1:D:186:LEU:HA	1:D:189:ILE:HG22	2.02	0.41
1:D:466:ASP:OD1	1:D:467:ILE:HG13	2.20	0.41
1:D:583:ASN:O	1:D:585:ARG:HG2	2.20	0.41
1:D:1070:LEU:HA	1:D:1073:GLU:OE1	2.20	0.41
1:D:1435:THR:OG1	1:D:1436:ASP:N	2.51	0.41
1:A:108:PHE:CD1	1:A:109:GLN:HG2	2.56	0.41
1:A:806:TYR:CE2	1:A:910:LEU:HB2	2.54	0.41
1:A:945:VAL:HA	1:A:1032:TYR:OH	2.19	0.41
1:B:108:PHE:CD1	1:B:109:GLN:HG2	2.56	0.41
1:B:112:GLN:O	1:B:114:ASP:N	2.53	0.41
1:C:258:GLY:HA2	1:C:260:PHE:CE1	2.55	0.41
1:C:646:GLN:HA	1:C:1126:ILE:HD11	2.03	0.41
1:C:736:GLN:NE2	1:C:1064:LYS:HB3	2.36	0.41
1:D:1374:VAL:HG11	1:D:1492:LEU:HD11	2.03	0.41
1:A:193:GLY:HA3	1:A:429:VAL:CG1	2.51	0.41
1:A:530:CYS:SG	1:A:531:LEU:N	2.93	0.41
1:A:559:HIS:H	1:A:585:ARG:HB2	1.85	0.41
1:A:1425:TYR:N	1:A:1444:ALA:HB3	2.32	0.41
1:B:724:ALA:HB3	1:B:726:ASP:OD2	2.20	0.41
1:C:724:ALA:HB3	1:C:726:ASP:OD2	2.20	0.41
1:C:1249:ASN:HB2	1:C:1279:GLU:OE2	2.19	0.41
1:C:1392:ARG:HH12	1:C:1400:ARG:HA	1.86	0.41
1:C:1492:LEU:HD12	1:C:1492:LEU:HA	1.90	0.41
1:D:566:ARG:NH1	1:D:573:THR:O	2.54	0.41
1:D:1035:PHE:O	1:D:1039:LEU:HB2	2.21	0.41
1:A:216:LYS:NZ	1:A:220:GLU:OE2	2.47	0.41
1:A:390:MET:HG3	1:A:393:THR:OG1	2.21	0.41
1:A:1378:LYS:HB2	1:A:1385:TRP:CD2	2.56	0.41
1:B:466:ASP:OD1	1:B:467:ILE:HG13	2.20	0.41
1:B:546:ARG:HA	1:B:546:ARG:HD3	1.87	0.41
1:B:566:ARG:NH1	1:B:573:THR:O	2.54	0.41
1:B:1085:ILE:HG23	1:B:1089:HIS:CE1	2.56	0.41
1:B:1156:ASP:HA	1:B:1159:VAL:HG22	2.01	0.41
1:B:1273:PRO:HA	1:B:1274:PRO:HD3	1.85	0.41
1:C:530:CYS:SG	1:C:531:LEU:N	2.93	0.41
1:C:1085:ILE:HG23	1:C:1089:HIS:CE1	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1374:VAL:HG11	1:C:1492:LEU:HD11	2.03	0.41
1:D:806:TYR:CE2	1:D:910:LEU:HB2	2.55	0.41
1:A:1156:ASP:HA	1:A:1159:VAL:HG22	2.01	0.41
1:A:1357:ARG:HH21	1:A:1451:ASP:C	2.29	0.41
1:B:216:LYS:NZ	1:B:220:GLU:OE2	2.47	0.41
1:B:646:GLN:HA	1:B:1126:ILE:HD11	2.03	0.41
1:B:736:GLN:NE2	1:B:1064:LYS:HB3	2.36	0.41
1:C:193:GLY:HA3	1:C:429:VAL:CG1	2.51	0.41
1:C:380:GLN:NE2	1:C:394:PHE:CE2	2.87	0.41
1:C:566:ARG:NH1	1:C:573:THR:O	2.54	0.41
1:C:618:THR:O	1:C:619:MET:HG3	2.21	0.41
1:C:1273:PRO:HA	1:C:1274:PRO:HD3	1.85	0.41
1:D:380:GLN:NE2	1:D:394:PHE:CE2	2.87	0.41
1:D:618:THR:C	1:D:619:MET:HG3	2.46	0.41
1:A:337:LEU:HD21	1:A:405:LYS:CB	2.50	0.41
1:A:373:ASP:HB3	1:A:374:ILE:H	1.76	0.41
1:A:618:THR:O	1:A:619:MET:HG3	2.21	0.41
1:B:1035:PHE:O	1:B:1039:LEU:HB2	2.21	0.41
1:C:1392:ARG:HH12	1:C:1400:ARG:NE	2.18	0.41
1:D:108:PHE:CD1	1:D:109:GLN:HG2	2.56	0.41
1:D:724:ALA:HB3	1:D:726:ASP:OD2	2.20	0.41
1:D:736:GLN:NE2	1:D:1064:LYS:HB3	2.36	0.41
1:D:1357:ARG:HH21	1:D:1451:ASP:C	2.29	0.41
1:D:1411:TRP:HE3	1:D:1411:TRP:H	1.67	0.41
1:A:536:LEU:HD23	1:A:536:LEU:HA	1.92	0.41
1:A:618:THR:C	1:A:619:MET:HG3	2.46	0.41
1:A:936:PHE:HE1	1:B:920:LEU:HD12	1.86	0.41
1:A:942:ALA:O	1:A:946:VAL:HG23	2.21	0.41
1:A:1034:LEU:HD22	1:B:938:LEU:HB2	2.03	0.41
1:A:1336:ARG:H	1:A:1336:ARG:HG2	1.74	0.41
1:B:545:GLU:HB2	1:B:552:ALA:HA	2.02	0.41
1:B:618:THR:C	1:B:619:MET:HG3	2.45	0.41
1:B:1392:ARG:HH12	1:B:1400:ARG:NE	2.18	0.41
1:B:1392:ARG:HH12	1:B:1400:ARG:HA	1.86	0.41
1:C:526:LEU:HA	1:C:632:GLN:NE2	2.36	0.41
1:C:806:TYR:CE2	1:C:910:LEU:HB2	2.55	0.41
1:C:816:VAL:HA	1:C:820:ASP:HB3	2.03	0.41
1:C:1259:ASN:O	1:C:1262:VAL:HG22	2.21	0.41
1:C:1378:LYS:HB2	1:C:1385:TRP:CD2	2.56	0.41
1:D:390:MET:HG3	1:D:393:THR:OG1	2.21	0.41
1:D:530:CYS:SG	1:D:531:LEU:N	2.93	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:816:VAL:HA	1:D:820:ASP:HB3	2.03	0.41
1:D:942:ALA:O	1:D:946:VAL:HG23	2.21	0.41
1:D:1392:ARG:HH12	1:D:1400:ARG:HA	1.86	0.41
1:A:566:ARG:NH1	1:A:573:THR:O	2.54	0.41
1:A:724:ALA:HB3	1:A:726:ASP:OD2	2.20	0.41
1:B:642:TRP:CE3	1:B:685:ARG:HD3	2.56	0.41
1:B:805:SER:O	1:B:809:PHE:HD2	2.04	0.41
1:B:1357:ARG:HH21	1:B:1451:ASP:C	2.29	0.41
1:B:1378:LYS:HB2	1:B:1385:TRP:CD2	2.56	0.41
1:C:642:TRP:CE3	1:C:685:ARG:HD3	2.56	0.41
1:C:830:CYS:HA	1:C:833:TYR:CD2	2.55	0.41
1:C:1269:LEU:HB3	1:C:1270:ILE:H	1.71	0.41
1:B:526:LEU:HA	1:B:632:GLN:NE2	2.36	0.40
1:B:1105:ARG:HB3	1:B:1107:LYS:HE3	2.04	0.40
1:C:466:ASP:OD1	1:C:467:ILE:HG13	2.20	0.40
1:C:942:ALA:O	1:C:946:VAL:HG23	2.21	0.40
1:D:1085:ILE:HG23	1:D:1089:HIS:CE1	2.56	0.40
1:D:1378:LYS:HB2	1:D:1385:TRP:CD2	2.56	0.40
1:D:1425:TYR:N	1:D:1444:ALA:HB3	2.32	0.40
1:A:736:GLN:NE2	1:A:1064:LYS:HB3	2.36	0.40
1:A:1374:VAL:HG11	1:A:1492:LEU:HD11	2.03	0.40
1:B:936:PHE:HE1	1:C:920:LEU:HD12	1.86	0.40
1:C:723:GLU:N	1:C:723:GLU:OE1	2.54	0.40
1:C:805:SER:O	1:C:809:PHE:HD2	2.04	0.40
1:C:928:LYS:HD3	1:C:928:LYS:HA	1.92	0.40
1:C:1357:ARG:HH21	1:C:1451:ASP:C	2.29	0.40
1:D:140:LYS:HE2	1:D:279:SER:O	2.22	0.40
1:D:327:CYS:HB2	1:D:350:CYS:HB3	2.03	0.40
1:D:723:GLU:N	1:D:723:GLU:OE1	2.54	0.40
1:A:955:ILE:HG23	1:B:897:VAL:HG12	2.04	0.40
1:A:1259:ASN:O	1:A:1262:VAL:HG22	2.21	0.40
1:B:390:MET:HG3	1:B:393:THR:OG1	2.21	0.40
1:B:955:ILE:HG23	1:C:897:VAL:HG12	2.04	0.40
1:B:1034:LEU:HD22	1:C:938:LEU:HB2	2.03	0.40
1:C:140:LYS:HE2	1:C:279:SER:O	2.22	0.40
1:C:634:ARG:HD2	1:C:637:LEU:HD23	2.04	0.40
1:D:169:LEU:HB2	1:D:462:TRP:CZ3	2.57	0.40
1:D:610:ARG:HD3	1:D:610:ARG:HA	1.96	0.40
1:D:642:TRP:CE3	1:D:685:ARG:HD3	2.56	0.40
1:D:1272:ASP:OD1	1:D:1272:ASP:N	2.54	0.40
1:A:140:LYS:HE2	1:A:279:SER:O	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:642:TRP:CE3	1:A:685:ARG:HD3	2.56	0.40
1:A:646:GLN:HA	1:A:1126:ILE:HD11	2.03	0.40
1:A:954:ALA:O	1:B:896:ARG:NH2	2.51	0.40
1:B:193:GLY:HA3	1:B:429:VAL:CG1	2.51	0.40
1:B:1374:VAL:HG11	1:B:1492:LEU:HD11	2.03	0.40
1:C:936:PHE:HE1	1:D:920:LEU:HD12	1.86	0.40
1:C:1035:PHE:O	1:C:1039:LEU:HB2	2.21	0.40
1:C:1307:LEU:HD12	1:C:1395:GLY:HA2	2.04	0.40
1:A:694:TYR:CE1	1:A:698:GLU:HB2	2.57	0.40
1:A:920:LEU:HD12	1:D:936:PHE:HE1	1.86	0.40
1:A:1085:ILE:HG23	1:A:1089:HIS:CE1	2.56	0.40
1:B:816:VAL:HA	1:B:820:ASP:HB3	2.03	0.40
1:C:108:PHE:CD1	1:C:109:GLN:HG2	2.56	0.40
1:D:646:GLN:HA	1:D:1126:ILE:HD11	2.03	0.40
1:D:1259:ASN:O	1:D:1262:VAL:HG22	2.21	0.40
1:D:1307:LEU:C	1:D:1308:ARG:HD2	2.47	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	1331/1503 (89%)	1152 (87%)	166 (12%)	13 (1%)	12	45
1	B	1331/1503 (89%)	1151 (86%)	167 (12%)	13 (1%)	12	45
1	C	1331/1503 (89%)	1151 (86%)	167 (12%)	13 (1%)	12	45
1	D	1331/1503 (89%)	1152 (87%)	166 (12%)	13 (1%)	12	45
All	All	5324/6012 (89%)	4606 (86%)	666 (12%)	52 (1%)	15	45

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1270	ILE
1	A	1295	PRO
1	A	1298	THR
1	A	1362	ALA
1	A	1363	ILE
1	A	1394	PRO
1	A	1412	PRO
1	B	1270	ILE
1	B	1295	PRO
1	B	1298	THR
1	B	1362	ALA
1	B	1363	ILE
1	B	1394	PRO
1	B	1412	PRO
1	C	1270	ILE
1	C	1295	PRO
1	C	1298	THR
1	C	1362	ALA
1	C	1363	ILE
1	C	1394	PRO
1	C	1412	PRO
1	D	1270	ILE
1	D	1295	PRO
1	D	1298	THR
1	D	1362	ALA
1	D	1363	ILE
1	D	1394	PRO
1	D	1412	PRO
1	A	1303	VAL
1	A	1454	ASP
1	B	1303	VAL
1	B	1454	ASP
1	C	1303	VAL
1	C	1454	ASP
1	D	1303	VAL
1	D	1454	ASP
1	A	90	GLN
1	B	90	GLN
1	C	90	GLN
1	D	90	GLN
1	A	374	ILE
1	B	374	ILE
1	C	374	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	374	ILE
1	A	1250	CYS
1	B	1250	CYS
1	C	1250	CYS
1	D	1250	CYS
1	A	1252	VAL
1	B	1252	VAL
1	C	1252	VAL
1	D	1252	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1175/1318 (89%)	1174 (100%)	1 (0%)	88	91
1	B	1175/1318 (89%)	1174 (100%)	1 (0%)	88	91
1	C	1175/1318 (89%)	1174 (100%)	1 (0%)	88	91
1	D	1175/1318 (89%)	1174 (100%)	1 (0%)	88	91
All	All	4700/5272 (89%)	4696 (100%)	4 (0%)	87	91

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	433	ILE
1	B	433	ILE
1	C	433	ILE
1	D	433	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	HIS
1	A	454	HIS
1	A	557	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	594	HIS
1	A	751	ASN
1	A	953	GLN
1	A	958	HIS
1	A	959	ASN
1	A	1408	GLN
1	A	1465	HIS
1	B	161	HIS
1	B	414	GLN
1	B	557	GLN
1	B	594	HIS
1	B	732	HIS
1	B	751	ASN
1	B	800	HIS
1	B	912	HIS
1	B	953	GLN
1	B	958	HIS
1	B	959	ASN
1	B	1408	GLN
1	B	1465	HIS
1	C	161	HIS
1	C	454	HIS
1	C	557	GLN
1	C	594	HIS
1	C	751	ASN
1	C	912	HIS
1	C	953	GLN
1	C	958	HIS
1	C	959	ASN
1	C	1408	GLN
1	C	1465	HIS
1	D	161	HIS
1	D	454	HIS
1	D	557	GLN
1	D	594	HIS
1	D	751	ASN
1	D	953	GLN
1	D	958	HIS
1	D	959	ASN
1	D	1075	HIS
1	D	1408	GLN
1	D	1465	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 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	UOZ	A	2002	-	34,35,45	4.34	20 (58%)	49,53,68	2.15	14 (28%)
2	UOZ	C	2002	-	34,35,45	4.35	20 (58%)	49,53,68	2.16	14 (28%)
2	UOZ	A	2001	-	45,45,45	3.76	24 (53%)	62,68,68	2.11	17 (27%)
2	UOZ	B	2002	-	34,35,45	4.34	20 (58%)	49,53,68	2.16	15 (30%)
2	UOZ	D	2002	-	34,35,45	4.35	20 (58%)	49,53,68	2.16	14 (28%)
2	UOZ	B	2001	-	45,45,45	3.76	23 (51%)	62,68,68	2.11	17 (27%)
2	UOZ	C	2001	-	45,45,45	3.76	24 (53%)	62,68,68	2.12	17 (27%)
2	UOZ	D	2001	-	45,45,45	3.76	24 (53%)	62,68,68	2.11	17 (27%)

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	UOZ	A	2002	-	-	8/20/32/54	0/4/4/5
2	UOZ	C	2002	-	-	8/20/32/54	0/4/4/5
2	UOZ	A	2001	-	-	11/26/54/54	0/5/5/5
2	UOZ	B	2002	-	-	8/20/32/54	0/4/4/5
2	UOZ	D	2002	-	-	8/20/32/54	0/4/4/5
2	UOZ	B	2001	-	-	11/26/54/54	0/5/5/5
2	UOZ	C	2001	-	-	11/26/54/54	0/5/5/5
2	UOZ	D	2001	-	-	11/26/54/54	0/5/5/5

All (175) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2002	UOZ	C17-N16	15.83	1.60	1.46
2	C	2002	UOZ	C17-N16	15.83	1.60	1.46
2	D	2002	UOZ	C17-N16	15.83	1.60	1.46
2	A	2002	UOZ	C17-N16	15.73	1.60	1.46
2	A	2001	UOZ	C17-N16	14.17	1.59	1.46
2	B	2001	UOZ	C17-N16	14.17	1.59	1.46
2	C	2001	UOZ	C17-N16	14.17	1.59	1.46
2	D	2001	UOZ	C17-N16	14.17	1.59	1.46
2	C	2002	UOZ	C10-C09	8.50	1.61	1.47
2	A	2002	UOZ	C10-C09	8.50	1.61	1.47
2	D	2002	UOZ	C10-C09	8.47	1.61	1.47
2	B	2002	UOZ	C10-C09	8.46	1.61	1.47
2	A	2001	UOZ	P26-O25	8.46	1.68	1.59
2	B	2001	UOZ	P26-O25	8.46	1.68	1.59
2	D	2001	UOZ	P26-O25	8.46	1.68	1.59
2	C	2001	UOZ	P26-O25	8.40	1.68	1.59
2	A	2001	UOZ	C10-C09	8.04	1.60	1.47
2	B	2001	UOZ	C10-C09	8.04	1.60	1.47
2	D	2001	UOZ	C10-C09	7.99	1.60	1.47
2	C	2001	UOZ	C10-C09	7.96	1.60	1.47
2	A	2002	UOZ	P26-O28	7.47	1.82	1.54
2	B	2002	UOZ	P26-O28	7.47	1.82	1.54
2	C	2002	UOZ	P26-O28	7.47	1.82	1.54
2	D	2002	UOZ	P26-O28	7.45	1.82	1.54
2	D	2002	UOZ	P24-O23	7.26	1.87	1.59
2	B	2002	UOZ	P24-O23	7.26	1.87	1.59
2	A	2002	UOZ	P24-O23	7.24	1.87	1.59
2	C	2002	UOZ	P24-O23	7.22	1.87	1.59
2	B	2001	UOZ	P24-O23	6.95	1.86	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	UOZ	P24-O23	6.92	1.86	1.59
2	D	2001	UOZ	P24-O23	6.92	1.86	1.59
2	C	2001	UOZ	P24-O23	6.91	1.86	1.59
2	C	2002	UOZ	P24-O25	6.74	1.66	1.59
2	D	2002	UOZ	P24-O25	6.69	1.66	1.59
2	A	2002	UOZ	C06-N16	6.69	1.48	1.38
2	A	2002	UOZ	P24-O25	6.68	1.66	1.59
2	C	2002	UOZ	C06-N16	6.66	1.48	1.38
2	D	2002	UOZ	C06-N16	6.66	1.48	1.38
2	B	2002	UOZ	P24-O25	6.62	1.66	1.59
2	B	2002	UOZ	C06-N16	6.61	1.48	1.38
2	D	2001	UOZ	C06-N16	5.98	1.47	1.38
2	A	2001	UOZ	C06-N16	5.92	1.47	1.38
2	B	2001	UOZ	C06-N16	5.92	1.47	1.38
2	C	2001	UOZ	C06-N16	5.89	1.47	1.38
2	A	2001	UOZ	P26-O28	5.57	1.81	1.59
2	C	2001	UOZ	P26-O28	5.57	1.81	1.59
2	B	2001	UOZ	P26-O28	5.57	1.81	1.59
2	D	2001	UOZ	P26-O28	5.56	1.81	1.59
2	C	2001	UOZ	P24-O25	5.40	1.65	1.59
2	A	2001	UOZ	P24-O25	5.32	1.65	1.59
2	B	2001	UOZ	P24-O25	5.32	1.65	1.59
2	D	2001	UOZ	P24-O25	5.32	1.65	1.59
2	A	2002	UOZ	C22-C21	3.85	1.63	1.51
2	B	2002	UOZ	C22-C21	3.85	1.63	1.51
2	C	2002	UOZ	C22-C21	3.85	1.63	1.51
2	D	2002	UOZ	C22-C21	3.85	1.63	1.51
2	A	2001	UOZ	O31-C32	-3.83	1.38	1.43
2	B	2001	UOZ	O31-C32	-3.83	1.38	1.43
2	C	2001	UOZ	O31-C32	-3.83	1.38	1.43
2	D	2001	UOZ	O31-C32	-3.83	1.38	1.43
2	A	2002	UOZ	C06-N05	3.72	1.41	1.34
2	B	2002	UOZ	C06-N05	3.72	1.41	1.34
2	C	2002	UOZ	C06-N05	3.72	1.41	1.34
2	D	2002	UOZ	C06-N05	3.72	1.41	1.34
2	B	2002	UOZ	C04-N03	3.58	1.40	1.33
2	D	2002	UOZ	C04-N03	3.58	1.40	1.33
2	D	2001	UOZ	C04-N03	3.57	1.40	1.33
2	C	2001	UOZ	C29-C30	3.57	1.62	1.51
2	A	2002	UOZ	C04-N03	3.57	1.40	1.33
2	C	2002	UOZ	C04-N03	3.57	1.40	1.33
2	C	2001	UOZ	C04-N03	3.56	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	UOZ	C04-N03	3.56	1.40	1.33
2	B	2001	UOZ	C04-N03	3.55	1.40	1.33
2	B	2001	UOZ	C22-C21	3.55	1.62	1.51
2	C	2001	UOZ	C22-C21	3.55	1.62	1.51
2	A	2001	UOZ	C29-C30	3.55	1.62	1.51
2	B	2001	UOZ	C29-C30	3.55	1.62	1.51
2	D	2001	UOZ	C29-C30	3.55	1.62	1.51
2	A	2001	UOZ	C22-C21	3.52	1.62	1.51
2	D	2001	UOZ	C22-C21	3.52	1.62	1.51
2	A	2001	UOZ	C06-N05	3.50	1.41	1.34
2	C	2001	UOZ	C06-N05	3.50	1.41	1.34
2	B	2001	UOZ	C06-N05	3.47	1.40	1.34
2	D	2001	UOZ	C06-N05	3.44	1.40	1.34
2	D	2001	UOZ	C09-N08	3.22	1.37	1.32
2	A	2002	UOZ	C09-N08	3.21	1.37	1.32
2	D	2002	UOZ	C09-N08	3.21	1.37	1.32
2	B	2002	UOZ	C09-N08	3.20	1.37	1.32
2	A	2001	UOZ	C09-N08	3.18	1.37	1.32
2	C	2001	UOZ	C09-N08	3.18	1.37	1.32
2	B	2001	UOZ	C09-N08	3.16	1.37	1.32
2	C	2002	UOZ	C09-N08	3.14	1.37	1.32
2	B	2002	UOZ	C07-C02	2.80	1.48	1.41
2	C	2002	UOZ	C07-C02	2.80	1.48	1.41
2	A	2002	UOZ	C07-C02	2.79	1.48	1.41
2	D	2002	UOZ	C07-C02	2.77	1.48	1.41
2	C	2001	UOZ	C07-C02	2.73	1.48	1.41
2	D	2001	UOZ	C07-C02	2.73	1.48	1.41
2	A	2001	UOZ	C07-C02	2.71	1.48	1.41
2	B	2001	UOZ	C07-C02	2.71	1.48	1.41
2	D	2002	UOZ	C07-N08	2.66	1.44	1.39
2	B	2001	UOZ	C07-N08	2.65	1.44	1.39
2	C	2001	UOZ	C07-N08	2.65	1.44	1.39
2	A	2002	UOZ	C07-N08	2.64	1.44	1.39
2	A	2001	UOZ	C07-N08	2.62	1.44	1.39
2	C	2002	UOZ	C07-N08	2.62	1.44	1.39
2	B	2002	UOZ	C07-N08	2.60	1.44	1.39
2	D	2001	UOZ	C07-N08	2.58	1.44	1.39
2	A	2002	UOZ	C07-C06	2.55	1.43	1.39
2	B	2002	UOZ	C07-C06	2.55	1.43	1.39
2	C	2002	UOZ	C07-C06	2.55	1.43	1.39
2	B	2002	UOZ	C11-C10	2.53	1.43	1.39
2	D	2002	UOZ	C07-C06	2.52	1.43	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2002	UOZ	C11-C10	2.51	1.43	1.39
2	B	2002	UOZ	C02-N01	2.49	1.40	1.34
2	D	2002	UOZ	C02-N01	2.48	1.40	1.34
2	A	2002	UOZ	C02-N01	2.47	1.40	1.34
2	C	2002	UOZ	C02-N01	2.47	1.40	1.34
2	A	2002	UOZ	C11-C10	2.45	1.43	1.39
2	A	2001	UOZ	C02-N01	2.45	1.40	1.34
2	D	2002	UOZ	C11-C10	2.44	1.43	1.39
2	B	2001	UOZ	C02-N01	2.44	1.40	1.34
2	D	2001	UOZ	C02-N01	2.44	1.40	1.34
2	C	2001	UOZ	C02-N01	2.43	1.40	1.34
2	D	2001	UOZ	O28-C29	-2.36	1.35	1.44
2	B	2001	UOZ	O28-C29	-2.35	1.35	1.44
2	C	2001	UOZ	O28-C29	-2.35	1.35	1.44
2	A	2001	UOZ	O28-C29	-2.34	1.35	1.44
2	C	2001	UOZ	C07-C06	2.33	1.43	1.39
2	A	2001	UOZ	C07-C06	2.33	1.43	1.39
2	B	2001	UOZ	C07-C06	2.33	1.43	1.39
2	D	2002	UOZ	C15-C10	2.33	1.42	1.39
2	D	2001	UOZ	C07-C06	2.32	1.43	1.39
2	A	2002	UOZ	C15-C10	2.30	1.42	1.39
2	B	2001	UOZ	C11-C10	2.30	1.42	1.39
2	C	2001	UOZ	C11-C10	2.30	1.42	1.39
2	D	2001	UOZ	C11-C10	2.30	1.42	1.39
2	C	2001	UOZ	O23-C22	-2.28	1.36	1.44
2	B	2002	UOZ	C15-C10	2.28	1.42	1.39
2	C	2002	UOZ	C15-C10	2.28	1.42	1.39
2	B	2001	UOZ	O23-C22	-2.27	1.36	1.44
2	D	2001	UOZ	C36-C34	2.27	1.59	1.53
2	A	2001	UOZ	O23-C22	-2.25	1.36	1.44
2	D	2001	UOZ	O23-C22	-2.25	1.36	1.44
2	C	2002	UOZ	C09-N16	2.25	1.42	1.38
2	C	2001	UOZ	C36-C34	2.25	1.59	1.53
2	A	2001	UOZ	C36-C34	2.24	1.59	1.53
2	B	2001	UOZ	C36-C34	2.24	1.59	1.53
2	B	2002	UOZ	C09-N16	2.23	1.42	1.38
2	A	2001	UOZ	C11-C10	2.23	1.42	1.39
2	A	2002	UOZ	C14-C15	2.23	1.42	1.38
2	C	2002	UOZ	C14-C15	2.22	1.42	1.38
2	A	2002	UOZ	C09-N16	2.21	1.42	1.38
2	D	2001	UOZ	C15-C10	2.20	1.42	1.39
2	D	2002	UOZ	C09-N16	2.19	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2002	UOZ	C14-C15	2.19	1.42	1.38
2	D	2002	UOZ	C14-C15	2.19	1.42	1.38
2	A	2002	UOZ	O23-C22	-2.18	1.36	1.44
2	B	2002	UOZ	O23-C22	-2.18	1.36	1.44
2	C	2002	UOZ	O23-C22	-2.18	1.36	1.44
2	D	2002	UOZ	O23-C22	-2.18	1.36	1.44
2	C	2001	UOZ	C15-C10	2.17	1.42	1.39
2	A	2001	UOZ	C15-C10	2.14	1.42	1.39
2	B	2001	UOZ	C15-C10	2.14	1.42	1.39
2	D	2002	UOZ	C12-C11	2.12	1.42	1.38
2	A	2001	UOZ	C14-C15	2.11	1.42	1.38
2	B	2001	UOZ	C14-C15	2.11	1.42	1.38
2	C	2001	UOZ	C14-C15	2.11	1.42	1.38
2	A	2002	UOZ	C12-C11	2.09	1.42	1.38
2	B	2002	UOZ	C12-C11	2.09	1.42	1.38
2	C	2002	UOZ	C12-C11	2.09	1.42	1.38
2	C	2001	UOZ	C12-C11	2.07	1.42	1.38
2	D	2001	UOZ	C14-C15	2.06	1.42	1.38
2	D	2001	UOZ	C12-C11	2.04	1.42	1.38
2	A	2001	UOZ	C12-C11	2.02	1.42	1.38

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	UOZ	O41-C17-N16	7.96	117.05	108.29
2	B	2001	UOZ	O41-C17-N16	7.96	117.05	108.29
2	C	2001	UOZ	O41-C17-N16	7.96	117.05	108.29
2	D	2001	UOZ	O41-C17-N16	7.96	117.05	108.29
2	B	2002	UOZ	O41-C17-N16	7.55	116.59	108.29
2	A	2002	UOZ	O41-C17-N16	7.54	116.58	108.29
2	C	2002	UOZ	O41-C17-N16	7.52	116.56	108.29
2	D	2002	UOZ	O41-C17-N16	7.52	116.56	108.29
2	C	2002	UOZ	C07-N08-C09	6.09	110.22	104.29
2	B	2002	UOZ	C07-N08-C09	6.06	110.18	104.29
2	D	2002	UOZ	C07-N08-C09	6.04	110.17	104.29
2	A	2002	UOZ	C07-N08-C09	6.00	110.13	104.29
2	D	2001	UOZ	C07-N08-C09	5.89	110.02	104.29
2	C	2001	UOZ	C07-N08-C09	5.89	110.02	104.29
2	A	2001	UOZ	C07-N08-C09	5.88	110.01	104.29
2	B	2001	UOZ	C07-N08-C09	5.87	110.00	104.29
2	A	2001	UOZ	C18-C17-N16	-5.27	110.26	116.01
2	B	2001	UOZ	C18-C17-N16	-5.27	110.26	116.01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2001	UOZ	C18-C17-N16	-5.27	110.26	116.01
2	D	2001	UOZ	C18-C17-N16	-5.27	110.26	116.01
2	C	2002	UOZ	C18-C17-N16	-4.17	111.45	116.01
2	B	2002	UOZ	C18-C17-N16	-4.15	111.48	116.01
2	D	2002	UOZ	C18-C17-N16	-4.15	111.48	116.01
2	A	2002	UOZ	C18-C17-N16	-4.13	111.50	116.01
2	D	2002	UOZ	C07-C06-N05	-3.90	121.35	126.72
2	A	2002	UOZ	C07-C06-N05	-3.88	121.38	126.72
2	B	2002	UOZ	C07-C06-N05	-3.88	121.38	126.72
2	C	2002	UOZ	C07-C06-N05	-3.88	121.38	126.72
2	A	2002	UOZ	N05-C06-N16	3.77	132.77	127.33
2	B	2002	UOZ	N05-C06-N16	3.76	132.76	127.33
2	C	2002	UOZ	N05-C06-N16	3.75	132.74	127.33
2	D	2002	UOZ	N05-C06-N16	3.75	132.74	127.33
2	C	2001	UOZ	C07-C06-N05	-3.65	121.69	126.72
2	A	2001	UOZ	C07-C06-N05	-3.63	121.71	126.72
2	B	2001	UOZ	C07-C06-N05	-3.62	121.73	126.72
2	D	2001	UOZ	C07-C06-N05	-3.58	121.78	126.72
2	C	2001	UOZ	C06-C07-N08	-3.48	107.35	110.91
2	B	2001	UOZ	C06-C07-N08	-3.46	107.38	110.91
2	A	2001	UOZ	C06-C07-N08	-3.45	107.38	110.91
2	D	2001	UOZ	C06-C07-N08	-3.40	107.43	110.91
2	A	2001	UOZ	N05-C06-N16	3.39	132.22	127.33
2	C	2001	UOZ	N05-C06-N16	3.39	132.21	127.33
2	B	2001	UOZ	N05-C06-N16	3.38	132.20	127.33
2	D	2001	UOZ	N05-C06-N16	3.37	132.19	127.33
2	D	2002	UOZ	C06-C07-N08	-3.32	107.52	110.91
2	C	2002	UOZ	C06-C07-N08	-3.31	107.52	110.91
2	B	2002	UOZ	C06-C07-N08	-3.28	107.56	110.91
2	A	2002	UOZ	C06-C07-N08	-3.26	107.58	110.91
2	D	2001	UOZ	C10-C09-N08	3.07	126.70	122.89
2	A	2001	UOZ	C10-C09-N08	3.05	126.68	122.89
2	C	2001	UOZ	C10-C09-N08	3.05	126.68	122.89
2	B	2001	UOZ	C10-C09-N08	3.04	126.67	122.89
2	C	2002	UOZ	C10-C09-N08	3.00	126.62	122.89
2	B	2002	UOZ	C10-C09-N08	2.98	126.60	122.89
2	C	2001	UOZ	O35-C34-C32	-2.96	103.61	111.85
2	D	2001	UOZ	O35-C34-C32	-2.95	103.64	111.85
2	D	2002	UOZ	C10-C09-N08	2.94	126.55	122.89
2	B	2001	UOZ	O35-C34-C32	-2.94	103.67	111.85
2	A	2002	UOZ	C10-C09-N08	2.94	126.54	122.89
2	A	2001	UOZ	O35-C34-C32	-2.93	103.69	111.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	UOZ	O41-C21-C22	2.92	118.70	109.33
2	D	2001	UOZ	O41-C21-C22	2.92	118.69	109.33
2	B	2001	UOZ	O41-C21-C22	2.91	118.65	109.33
2	C	2001	UOZ	O41-C21-C22	2.91	118.65	109.33
2	A	2002	UOZ	O41-C21-C22	2.79	118.28	109.33
2	B	2002	UOZ	O41-C21-C22	2.79	118.28	109.33
2	C	2002	UOZ	O41-C21-C22	2.78	118.25	109.33
2	D	2002	UOZ	O41-C21-C22	2.78	118.25	109.33
2	D	2001	UOZ	O33-C32-O31	2.75	114.62	111.12
2	C	2001	UOZ	O33-C32-O31	2.74	114.61	111.12
2	A	2001	UOZ	O33-C32-O31	2.72	114.59	111.12
2	B	2001	UOZ	O33-C32-O31	2.71	114.58	111.12
2	A	2001	UOZ	O31-C30-C29	2.57	117.56	109.33
2	B	2001	UOZ	O31-C30-C29	2.57	117.56	109.33
2	D	2001	UOZ	O31-C30-C29	2.56	117.52	109.33
2	D	2001	UOZ	N16-C09-N08	-2.55	108.59	113.26
2	C	2001	UOZ	N16-C09-N08	-2.55	108.59	113.26
2	C	2001	UOZ	O31-C30-C29	2.55	117.50	109.33
2	A	2001	UOZ	N16-C09-N08	-2.54	108.61	113.26
2	B	2001	UOZ	N16-C09-N08	-2.53	108.63	113.26
2	D	2002	UOZ	C11-C10-C15	-2.51	115.38	118.57
2	C	2002	UOZ	C11-C10-C15	-2.51	115.38	118.57
2	B	2002	UOZ	C11-C10-C15	-2.51	115.38	118.57
2	C	2001	UOZ	C14-C15-C10	2.50	122.83	120.36
2	C	2001	UOZ	C11-C10-C15	-2.50	115.39	118.57
2	A	2002	UOZ	C11-C10-C15	-2.50	115.39	118.57
2	B	2002	UOZ	N16-C09-N08	-2.49	108.71	113.26
2	D	2001	UOZ	C11-C10-C15	-2.47	115.42	118.57
2	C	2002	UOZ	N16-C09-N08	-2.47	108.75	113.26
2	D	2002	UOZ	N16-C09-N08	-2.47	108.75	113.26
2	A	2001	UOZ	C11-C10-C15	-2.46	115.44	118.57
2	B	2001	UOZ	C11-C10-C15	-2.46	115.44	118.57
2	A	2001	UOZ	C14-C15-C10	2.45	122.77	120.36
2	B	2001	UOZ	C14-C15-C10	2.45	122.77	120.36
2	D	2001	UOZ	C14-C15-C10	2.45	122.77	120.36
2	A	2002	UOZ	N16-C09-N08	-2.44	108.79	113.26
2	C	2002	UOZ	C14-C15-C10	2.41	122.73	120.36
2	D	2002	UOZ	C14-C15-C10	2.39	122.72	120.36
2	B	2002	UOZ	C14-C15-C10	2.39	122.71	120.36
2	C	2001	UOZ	C02-C07-N08	2.33	134.03	131.72
2	A	2002	UOZ	C14-C15-C10	2.32	122.64	120.36
2	B	2001	UOZ	C02-C07-N08	2.31	134.02	131.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	UOZ	C02-C07-N08	2.31	134.01	131.72
2	D	2001	UOZ	C02-C07-N08	2.30	134.01	131.72
2	A	2002	UOZ	C12-C11-C10	2.24	122.56	120.36
2	D	2002	UOZ	C12-C11-C10	2.19	122.51	120.36
2	C	2002	UOZ	C12-C11-C10	2.16	122.49	120.36
2	C	2002	UOZ	C02-C07-N08	2.16	133.86	131.72
2	B	2002	UOZ	C12-C11-C10	2.15	122.48	120.36
2	D	2002	UOZ	C02-C07-N08	2.14	133.85	131.72
2	D	2001	UOZ	C29-C30-C36	-2.12	107.57	115.21
2	B	2002	UOZ	C02-C07-N08	2.12	133.83	131.72
2	A	2001	UOZ	C29-C30-C36	-2.12	107.58	115.21
2	B	2001	UOZ	C29-C30-C36	-2.12	107.58	115.21
2	C	2001	UOZ	C29-C30-C36	-2.12	107.59	115.21
2	A	2001	UOZ	C12-C11-C10	2.11	122.44	120.36
2	C	2001	UOZ	C12-C11-C10	2.09	122.42	120.36
2	B	2001	UOZ	C12-C11-C10	2.08	122.41	120.36
2	A	2002	UOZ	C02-C07-N08	2.07	133.78	131.72
2	D	2001	UOZ	C12-C11-C10	2.06	122.39	120.36
2	A	2002	UOZ	O27-P26-O38	2.03	118.75	110.83
2	B	2002	UOZ	O27-P26-O38	2.03	118.75	110.83
2	C	2002	UOZ	O27-P26-O38	2.03	118.75	110.83
2	D	2002	UOZ	O27-P26-O38	2.03	118.74	110.83
2	B	2002	UOZ	O40-P24-O23	-2.00	98.49	107.57

There are no chirality outliers.

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2001	UOZ	O41-C21-C22-O23
2	A	2001	UOZ	O28-C29-C30-O31
2	A	2001	UOZ	C29-O28-P26-O25
2	A	2001	UOZ	C29-O28-P26-O27
2	A	2001	UOZ	C29-O28-P26-O38
2	A	2002	UOZ	C18-C17-N16-C09
2	A	2002	UOZ	C22-O23-P24-O25
2	A	2002	UOZ	C22-O23-P24-O39
2	A	2002	UOZ	C22-O23-P24-O40
2	B	2001	UOZ	O41-C21-C22-O23
2	B	2001	UOZ	O28-C29-C30-O31
2	B	2001	UOZ	C29-O28-P26-O25
2	B	2001	UOZ	C29-O28-P26-O27
2	B	2001	UOZ	C29-O28-P26-O38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	2002	UOZ	C18-C17-N16-C09
2	B	2002	UOZ	C22-O23-P24-O25
2	B	2002	UOZ	C22-O23-P24-O39
2	B	2002	UOZ	C22-O23-P24-O40
2	C	2001	UOZ	O41-C21-C22-O23
2	C	2001	UOZ	O28-C29-C30-O31
2	C	2001	UOZ	C29-O28-P26-O25
2	C	2001	UOZ	C29-O28-P26-O27
2	C	2001	UOZ	C29-O28-P26-O38
2	C	2002	UOZ	C18-C17-N16-C09
2	C	2002	UOZ	C22-O23-P24-O25
2	C	2002	UOZ	C22-O23-P24-O39
2	C	2002	UOZ	C22-O23-P24-O40
2	D	2001	UOZ	O41-C21-C22-O23
2	D	2001	UOZ	O28-C29-C30-O31
2	D	2001	UOZ	C29-O28-P26-O25
2	D	2001	UOZ	C29-O28-P26-O27
2	D	2001	UOZ	C29-O28-P26-O38
2	D	2002	UOZ	C18-C17-N16-C09
2	D	2002	UOZ	C22-O23-P24-O25
2	D	2002	UOZ	C22-O23-P24-O39
2	D	2002	UOZ	C22-O23-P24-O40
2	A	2001	UOZ	C19-C21-C22-O23
2	A	2001	UOZ	O28-C29-C30-C36
2	B	2001	UOZ	C19-C21-C22-O23
2	B	2001	UOZ	O28-C29-C30-C36
2	C	2001	UOZ	C19-C21-C22-O23
2	C	2001	UOZ	O28-C29-C30-C36
2	D	2001	UOZ	C19-C21-C22-O23
2	D	2001	UOZ	O28-C29-C30-C36
2	A	2002	UOZ	O41-C21-C22-O23
2	B	2002	UOZ	O41-C21-C22-O23
2	C	2002	UOZ	O41-C21-C22-O23
2	D	2002	UOZ	O41-C21-C22-O23
2	A	2002	UOZ	C19-C21-C22-O23
2	B	2002	UOZ	C19-C21-C22-O23
2	C	2002	UOZ	C19-C21-C22-O23
2	D	2002	UOZ	C19-C21-C22-O23
2	A	2001	UOZ	N16-C09-C10-C11
2	B	2001	UOZ	N16-C09-C10-C11
2	C	2001	UOZ	N16-C09-C10-C11
2	D	2001	UOZ	N16-C09-C10-C11

Continued on next page...

Continued from previous page...

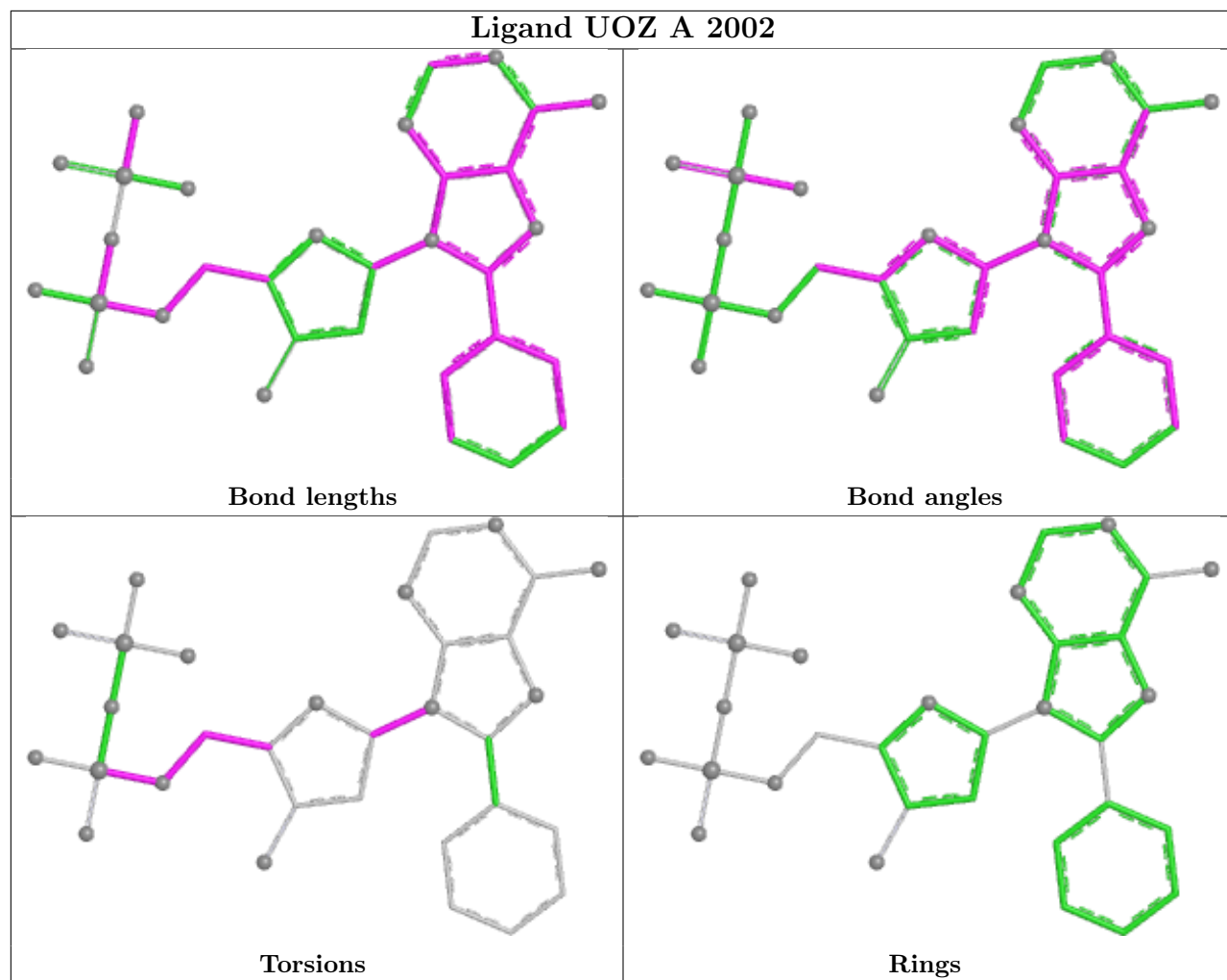
Mol	Chain	Res	Type	Atoms
2	A	2002	UOZ	C18-C17-N16-C06
2	B	2002	UOZ	C18-C17-N16-C06
2	C	2002	UOZ	C18-C17-N16-C06
2	D	2002	UOZ	C18-C17-N16-C06
2	A	2001	UOZ	N08-C09-C10-C11
2	B	2001	UOZ	N08-C09-C10-C11
2	C	2001	UOZ	N08-C09-C10-C11
2	D	2001	UOZ	N08-C09-C10-C11
2	A	2001	UOZ	N16-C09-C10-C15
2	B	2001	UOZ	N16-C09-C10-C15
2	C	2001	UOZ	N16-C09-C10-C15
2	D	2001	UOZ	N16-C09-C10-C15
2	B	2001	UOZ	N08-C09-C10-C15
2	C	2001	UOZ	N08-C09-C10-C15
2	D	2001	UOZ	N08-C09-C10-C15
2	A	2001	UOZ	N08-C09-C10-C15
2	A	2002	UOZ	C21-C22-O23-P24
2	B	2002	UOZ	C21-C22-O23-P24
2	C	2002	UOZ	C21-C22-O23-P24
2	D	2002	UOZ	C21-C22-O23-P24

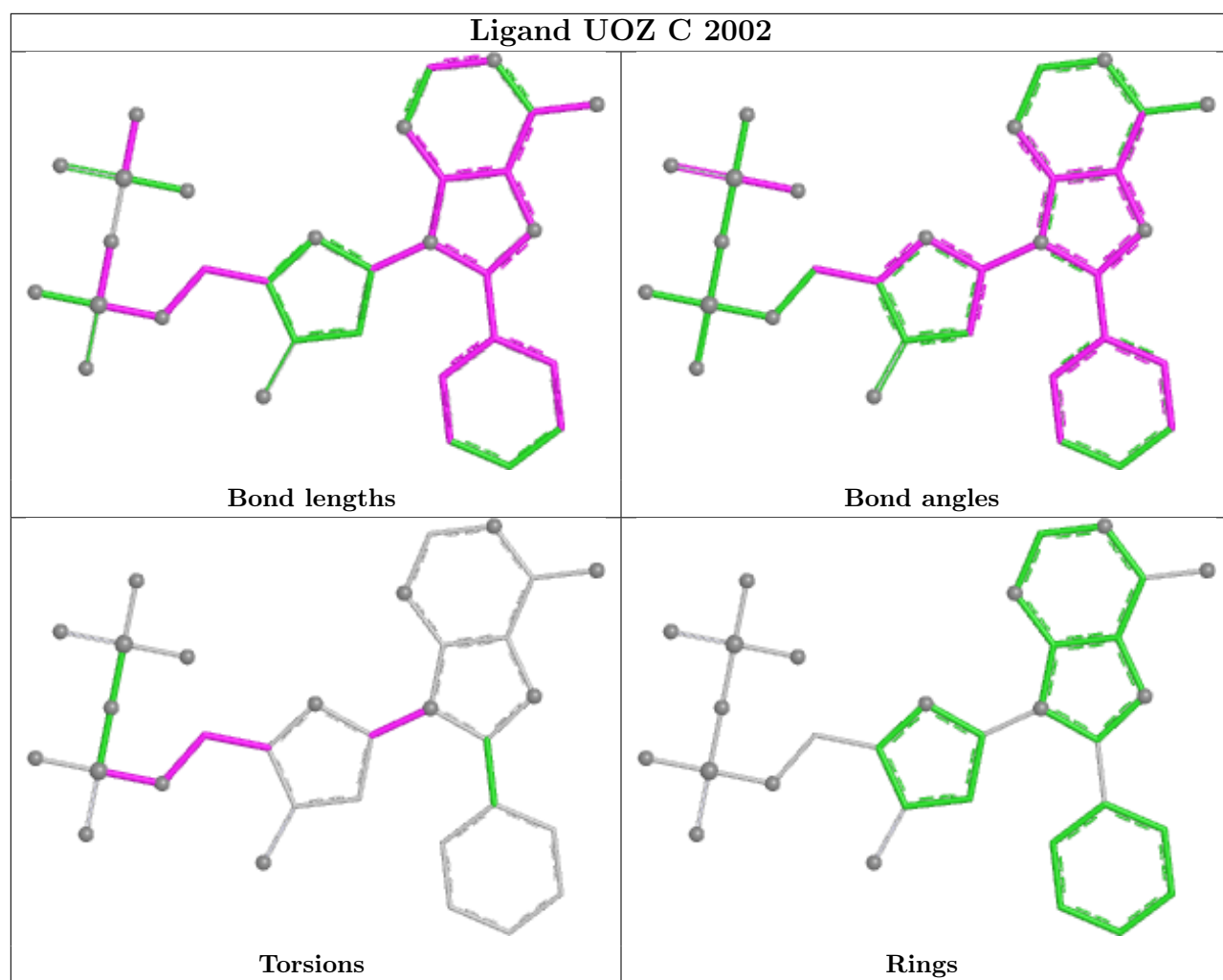
There are no ring outliers.

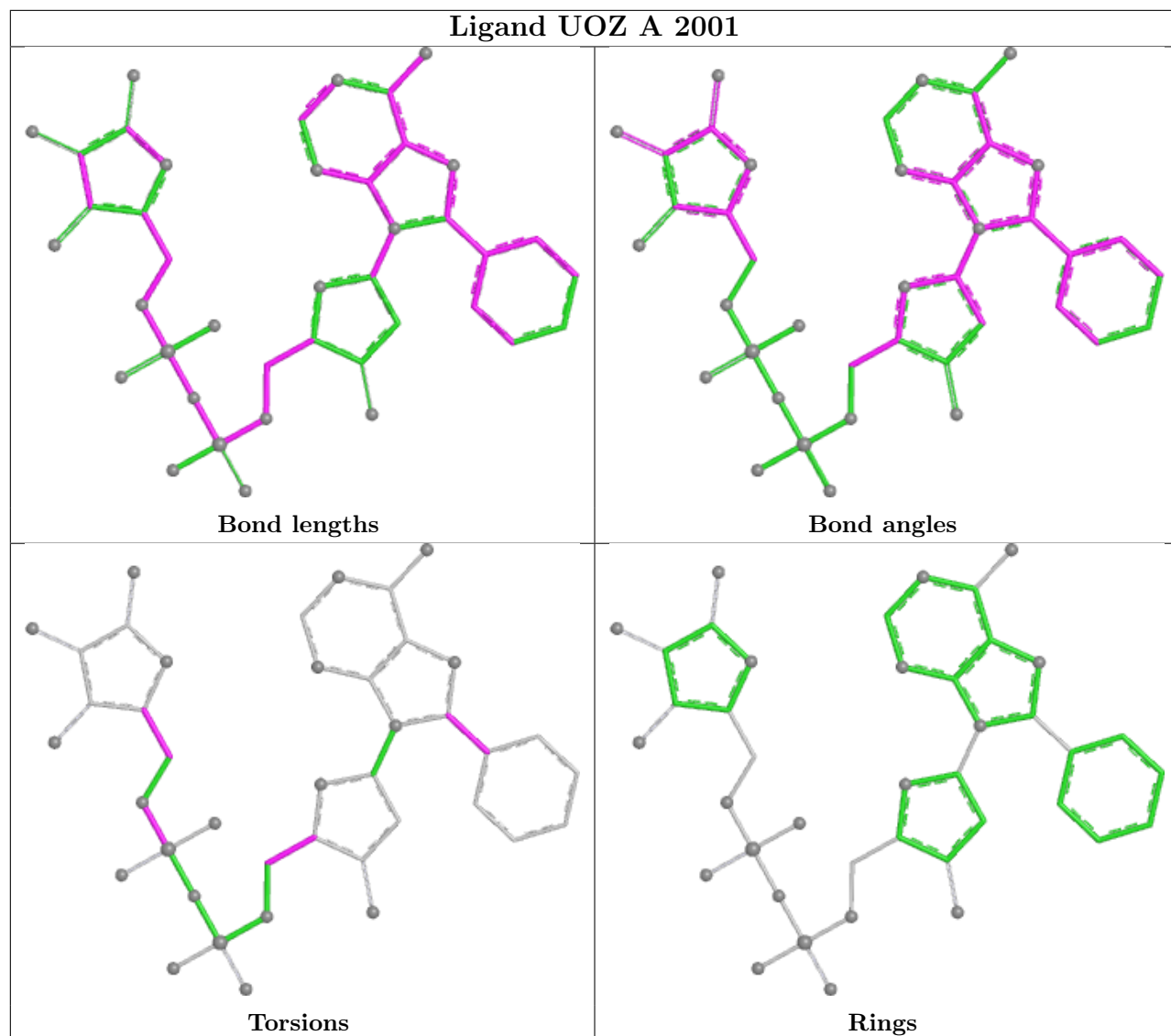
4 monomers are involved in 8 short contacts:

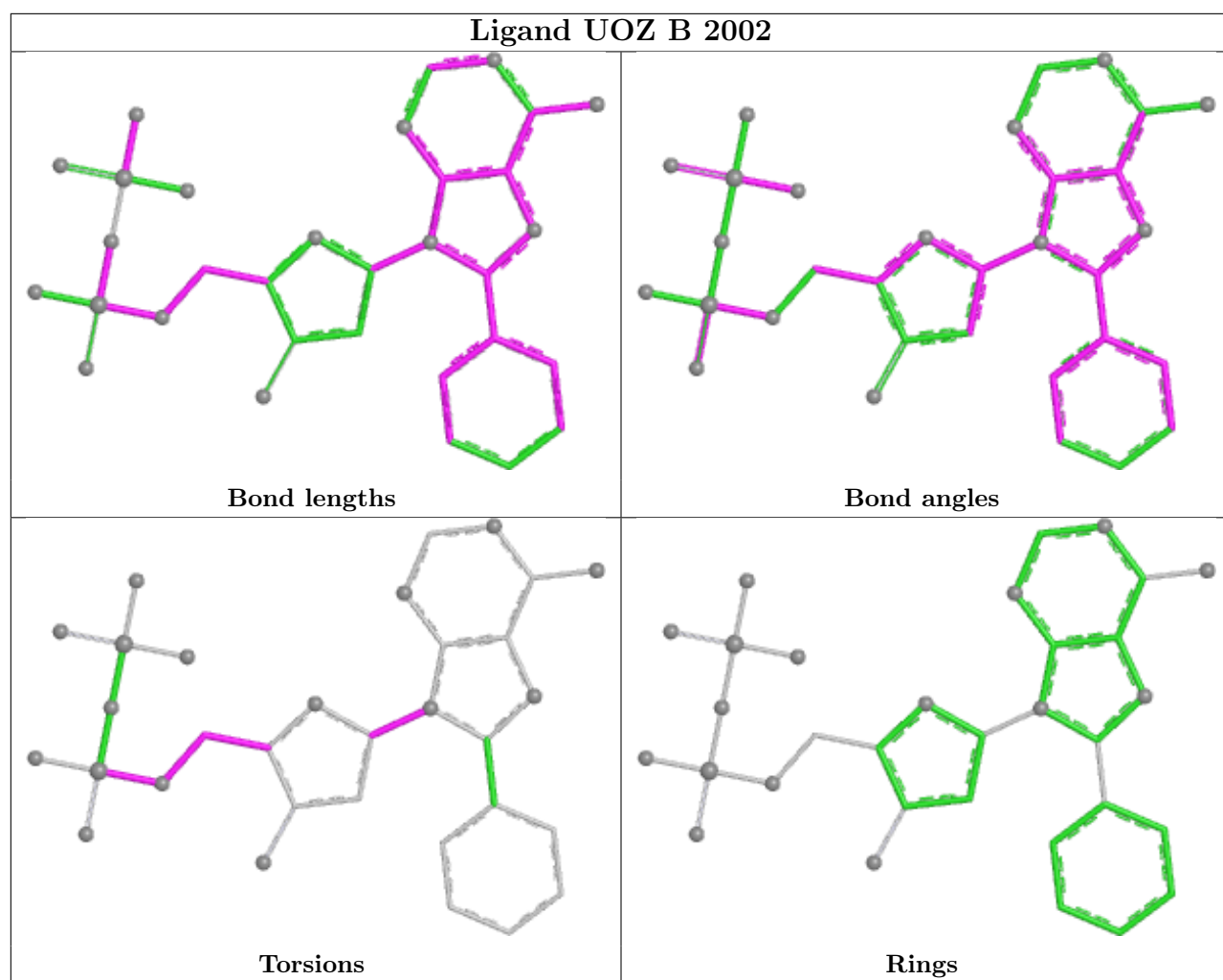
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	UOZ	2	0
2	B	2001	UOZ	2	0
2	C	2001	UOZ	2	0
2	D	2001	UOZ	2	0

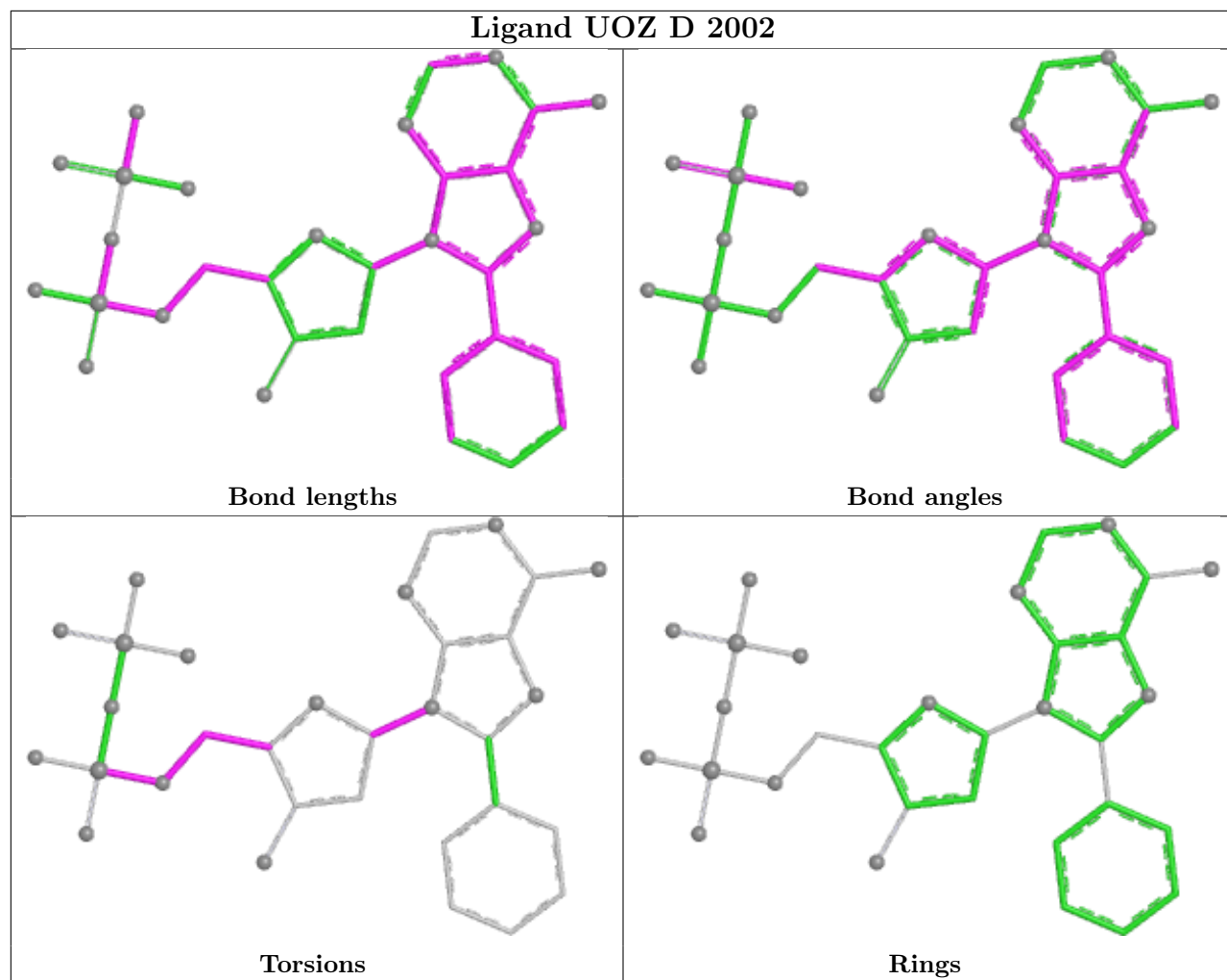
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

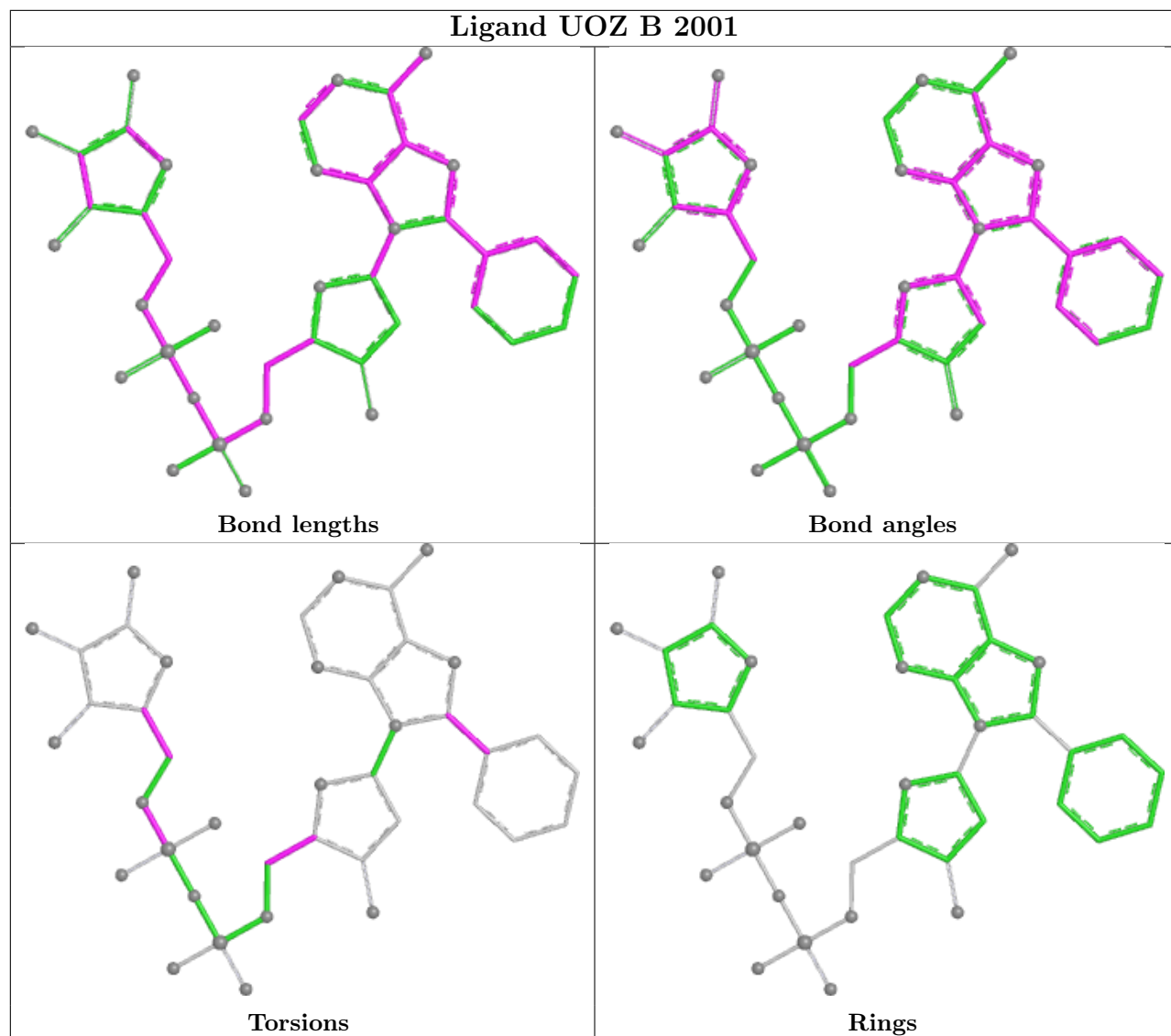


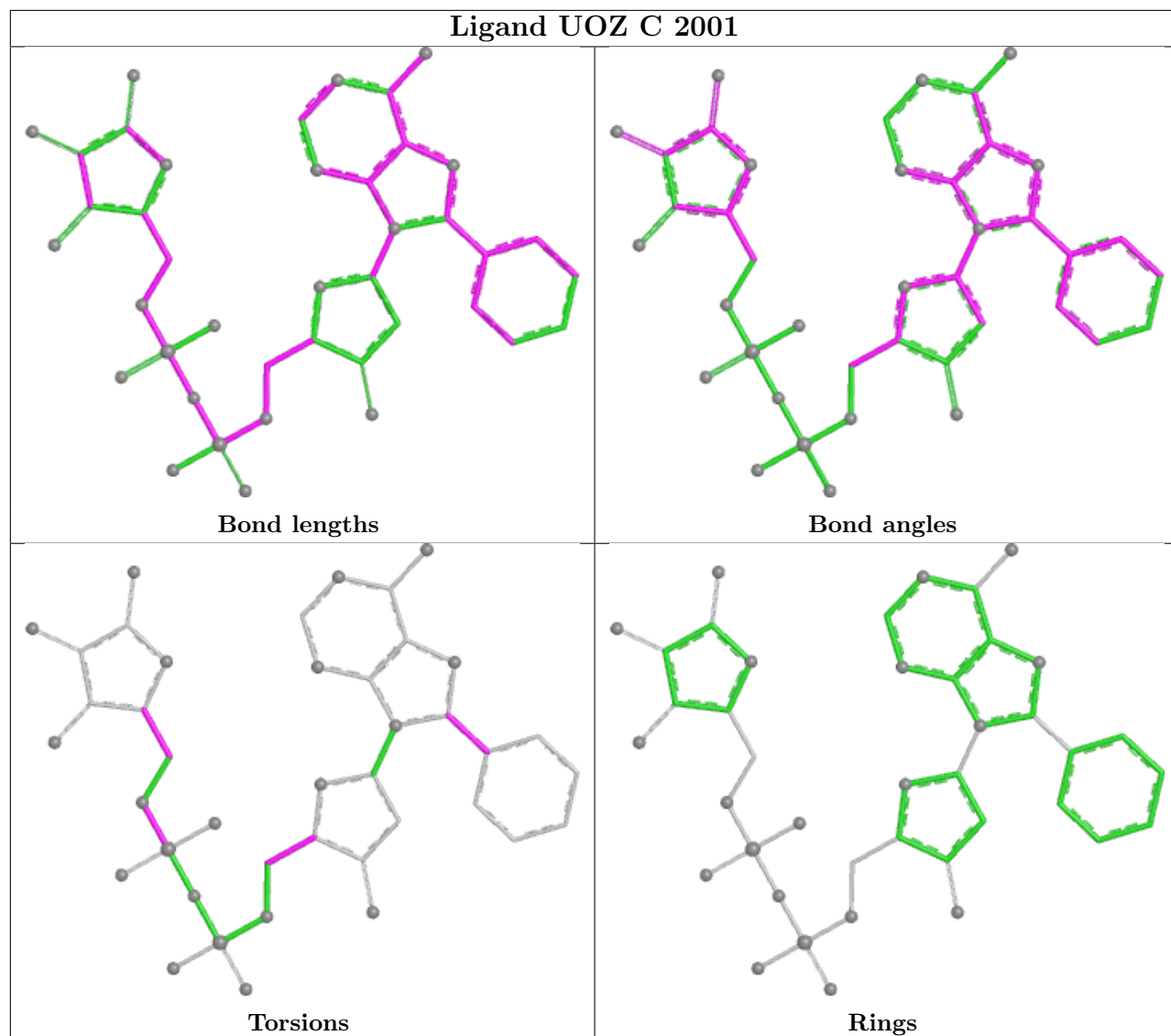


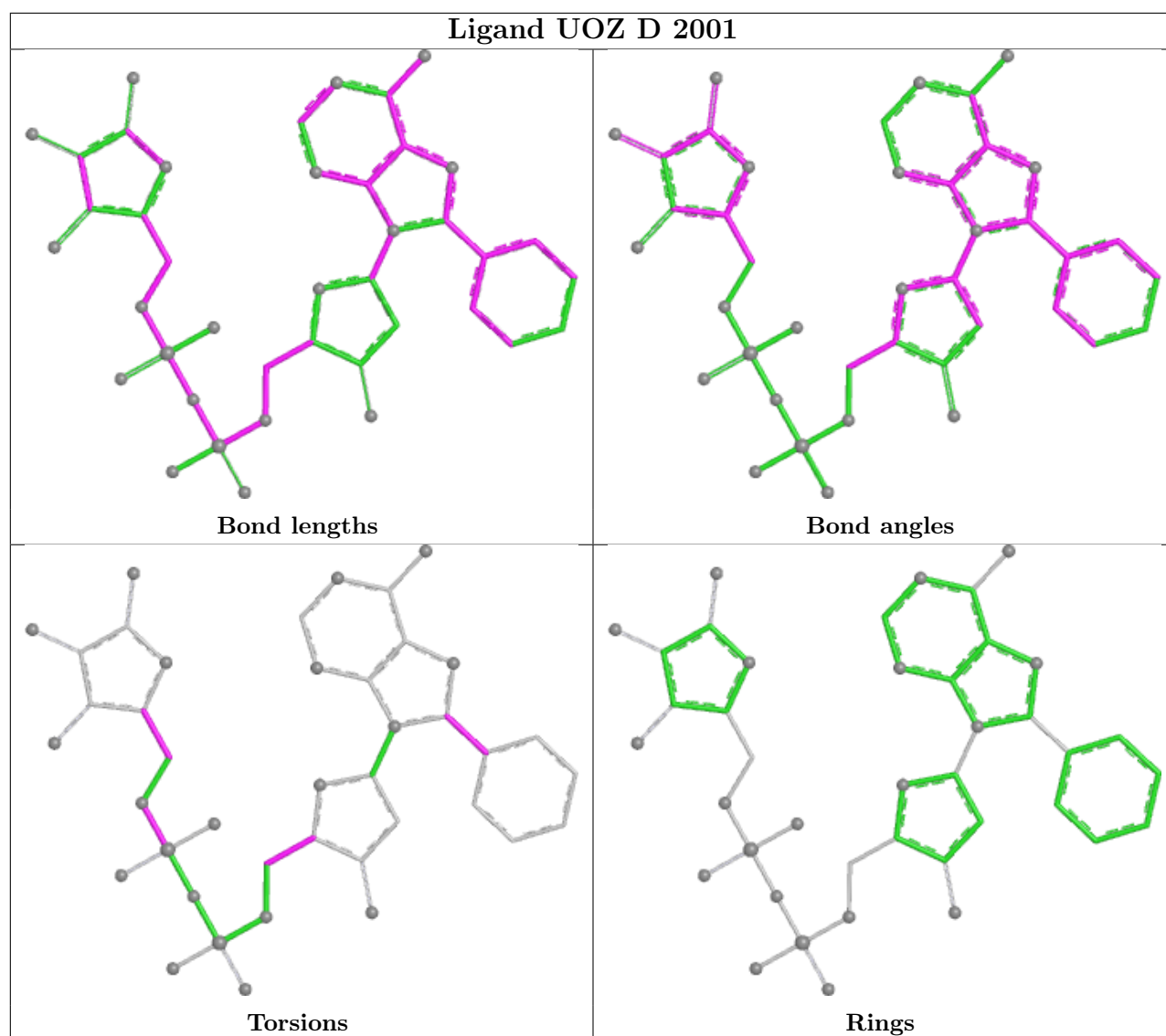












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

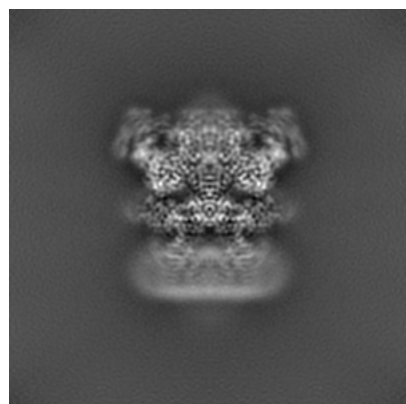
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27926. These allow visual inspection of the internal detail of the map and identification of artifacts.

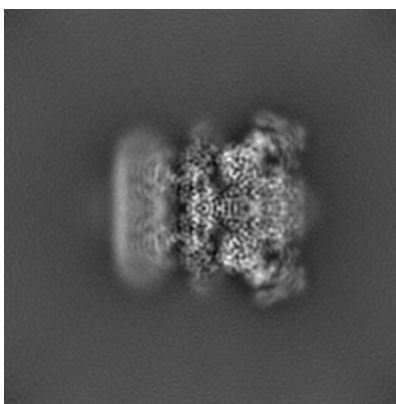
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

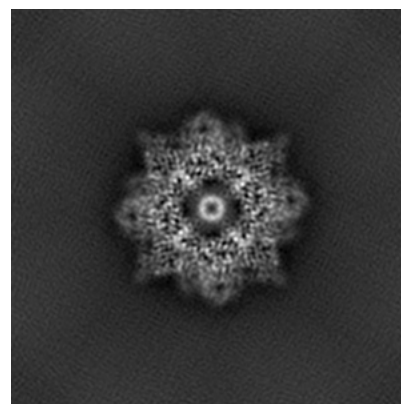
6.1.1 Primary map



X

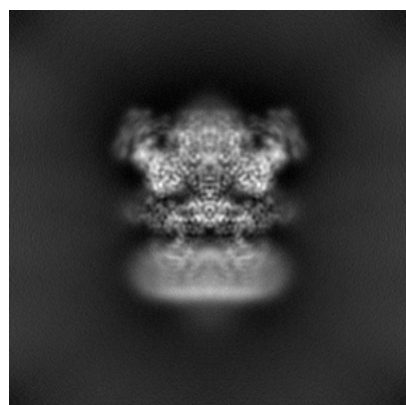


Y

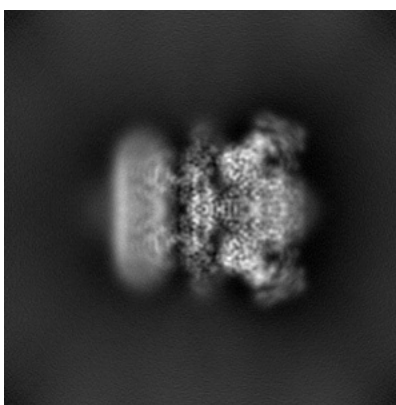


Z

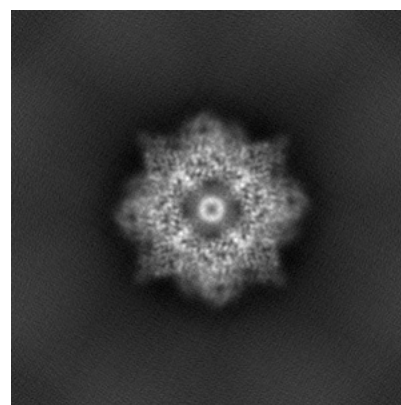
6.1.2 Raw map



X



Y

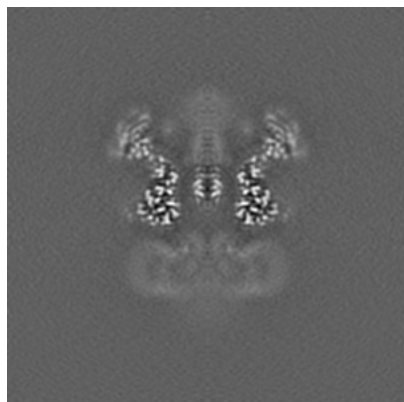


Z

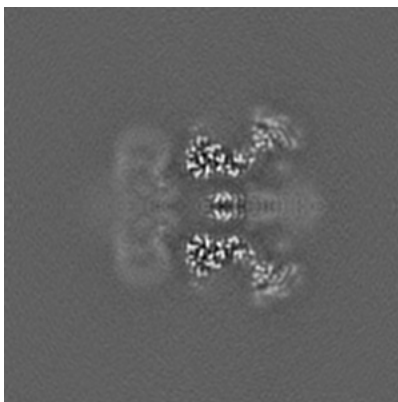
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

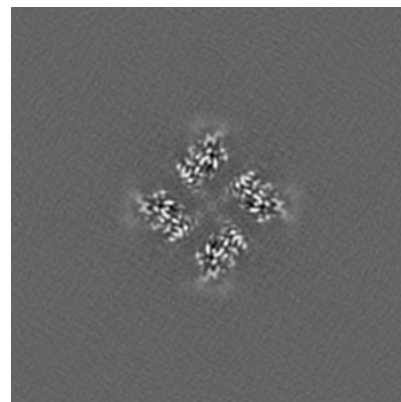
6.2.1 Primary map



X Index: 150

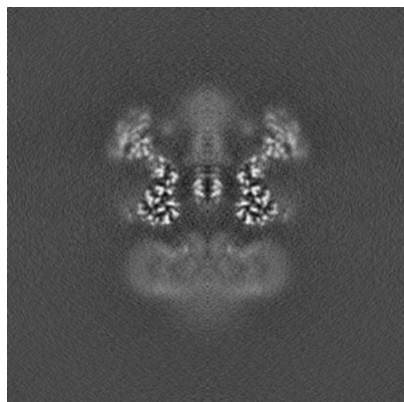


Y Index: 150

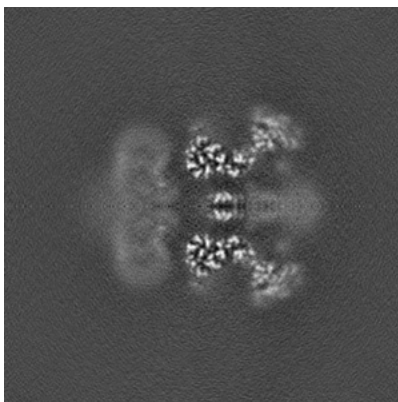


Z Index: 150

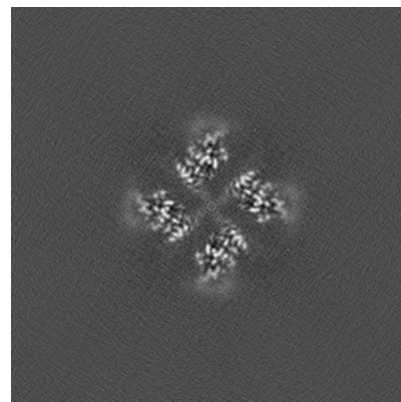
6.2.2 Raw map



X Index: 150



Y Index: 150

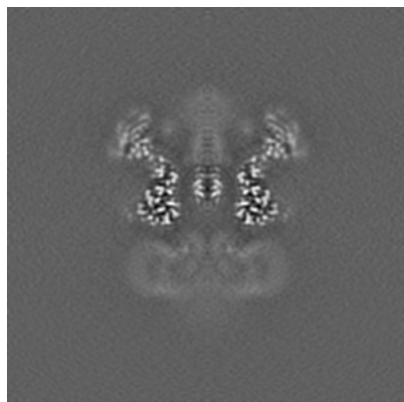


Z Index: 150

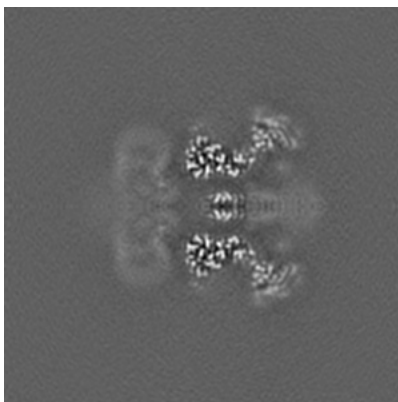
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

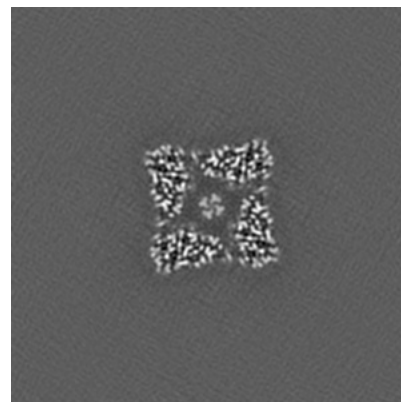
6.3.1 Primary map



X Index: 150

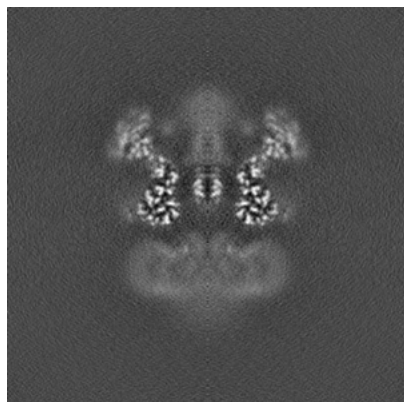


Y Index: 150

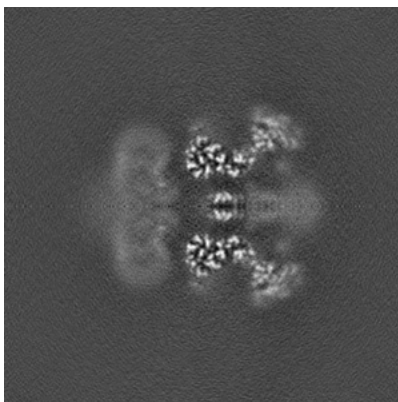


Z Index: 173

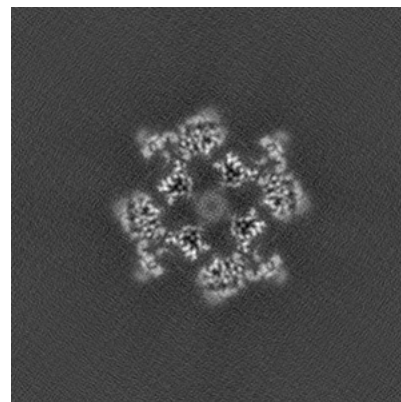
6.3.2 Raw map



X Index: 150



Y Index: 150

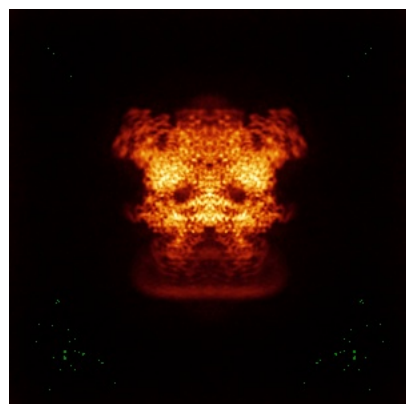


Z Index: 191

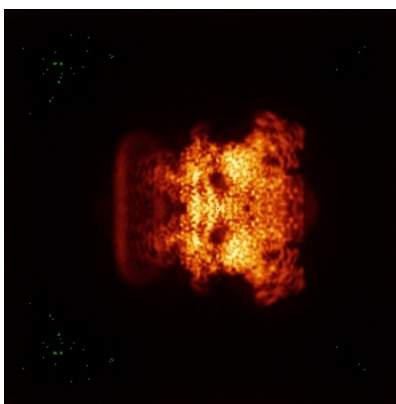
The images above show the largest variance slices of the map in three orthogonal directions.

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

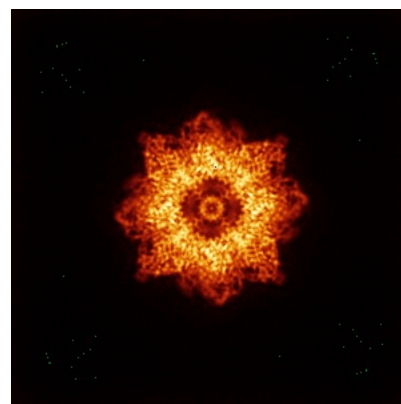
6.4.1 Primary map



X

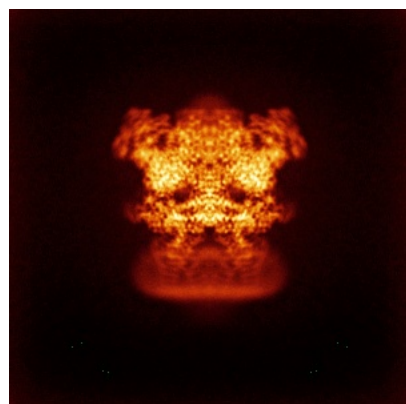


Y

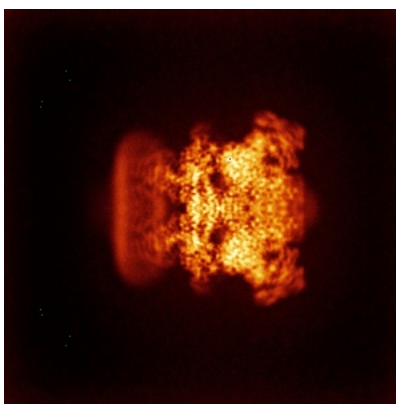


Z

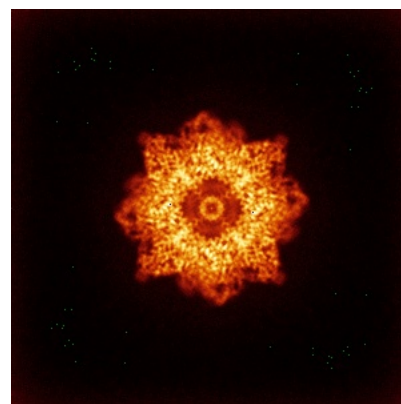
6.4.2 Raw map



X



Y

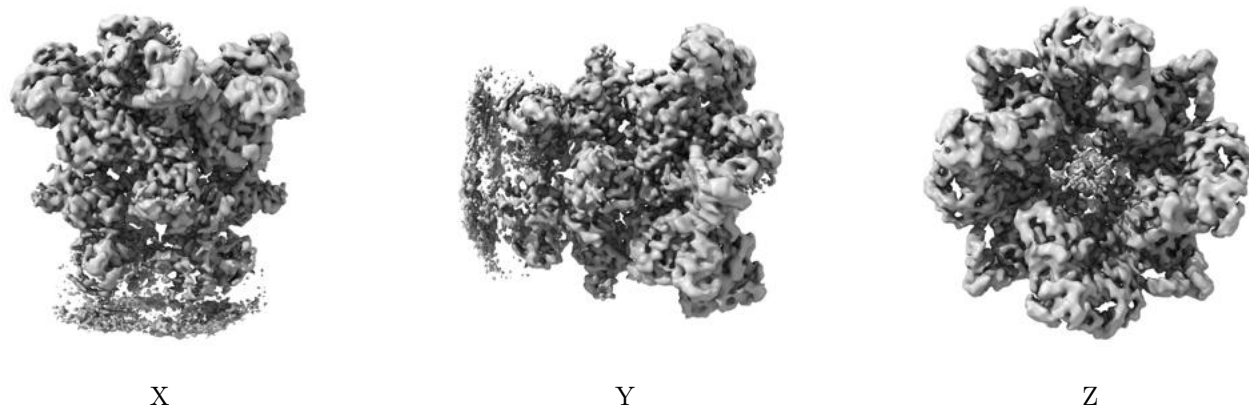


Z

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.

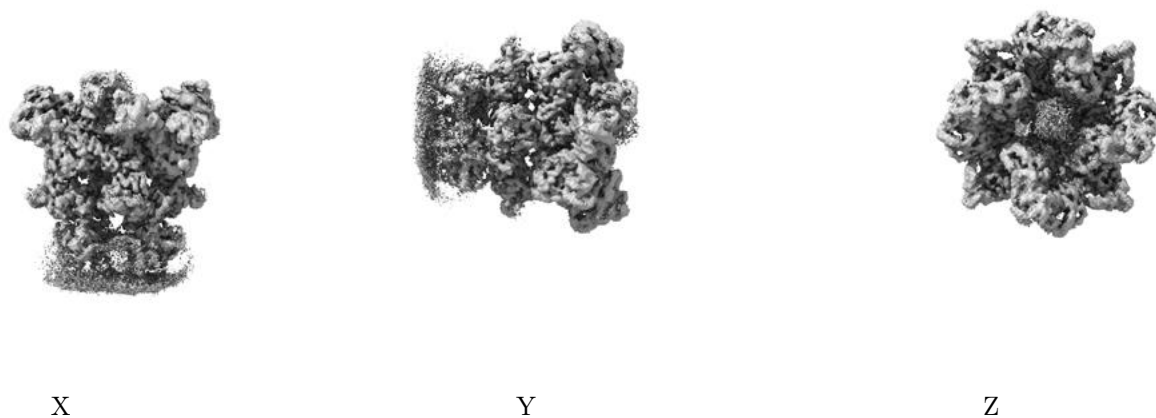
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.234. 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.

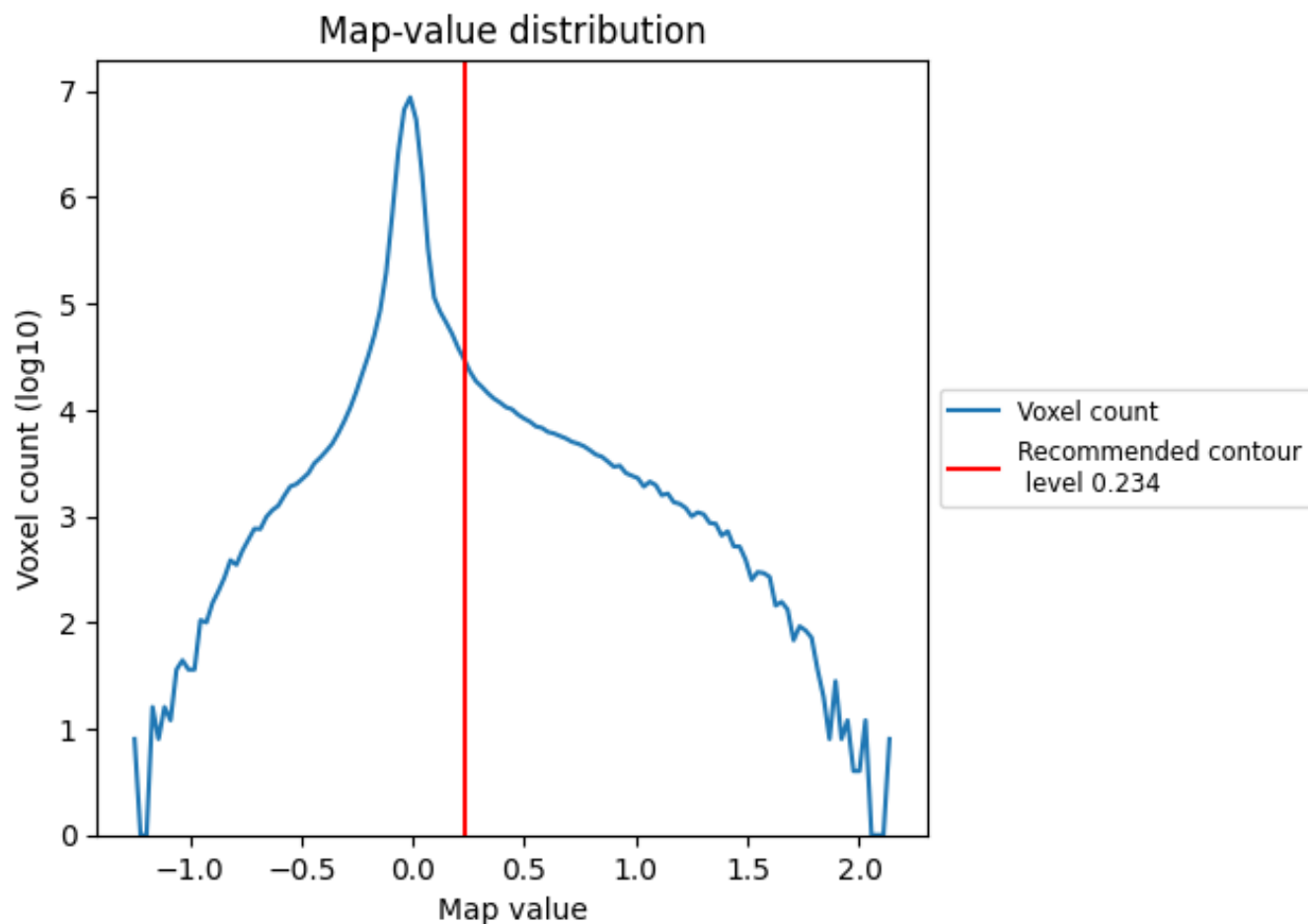
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

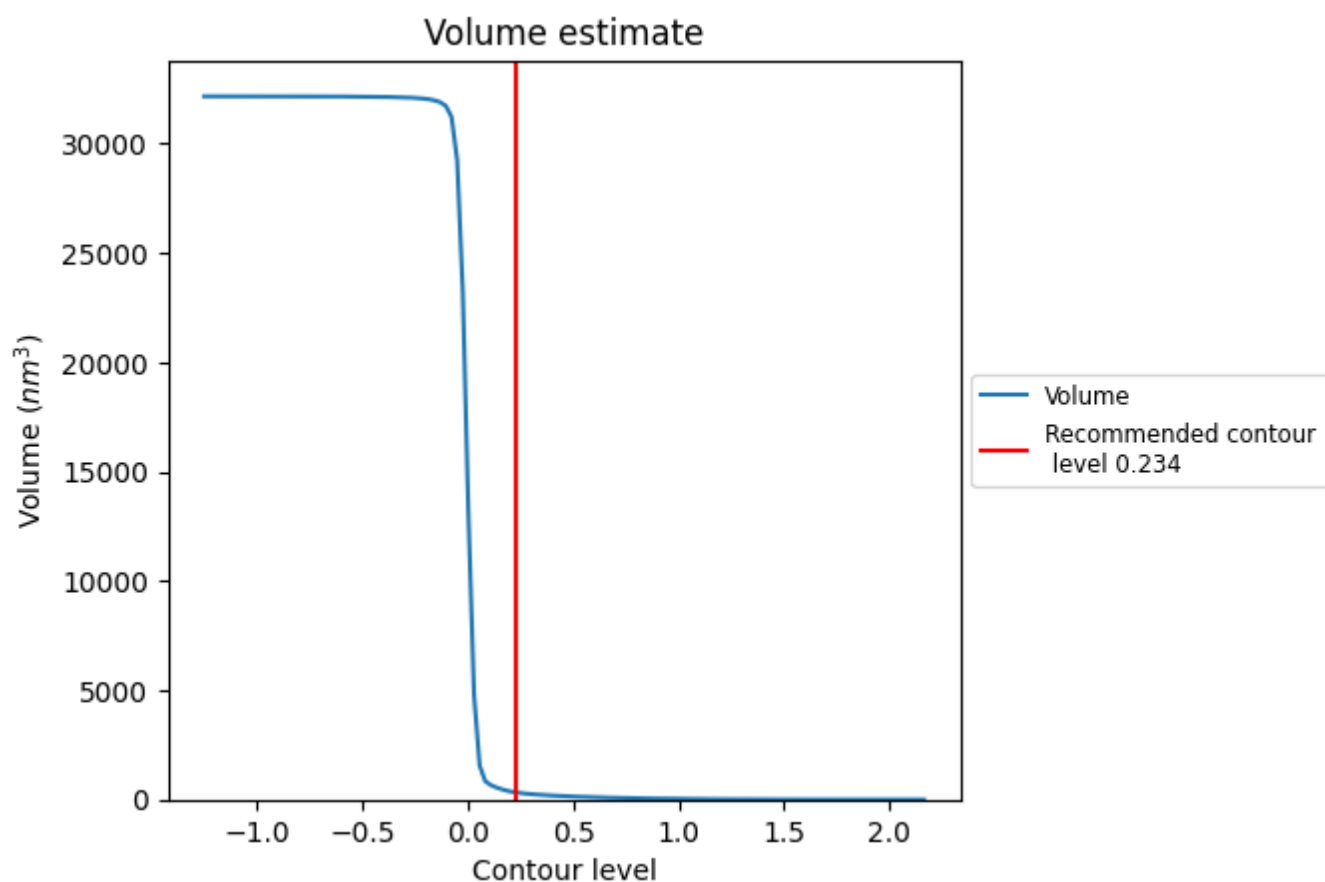
This section contains the results of statistical analysis of the map.

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.

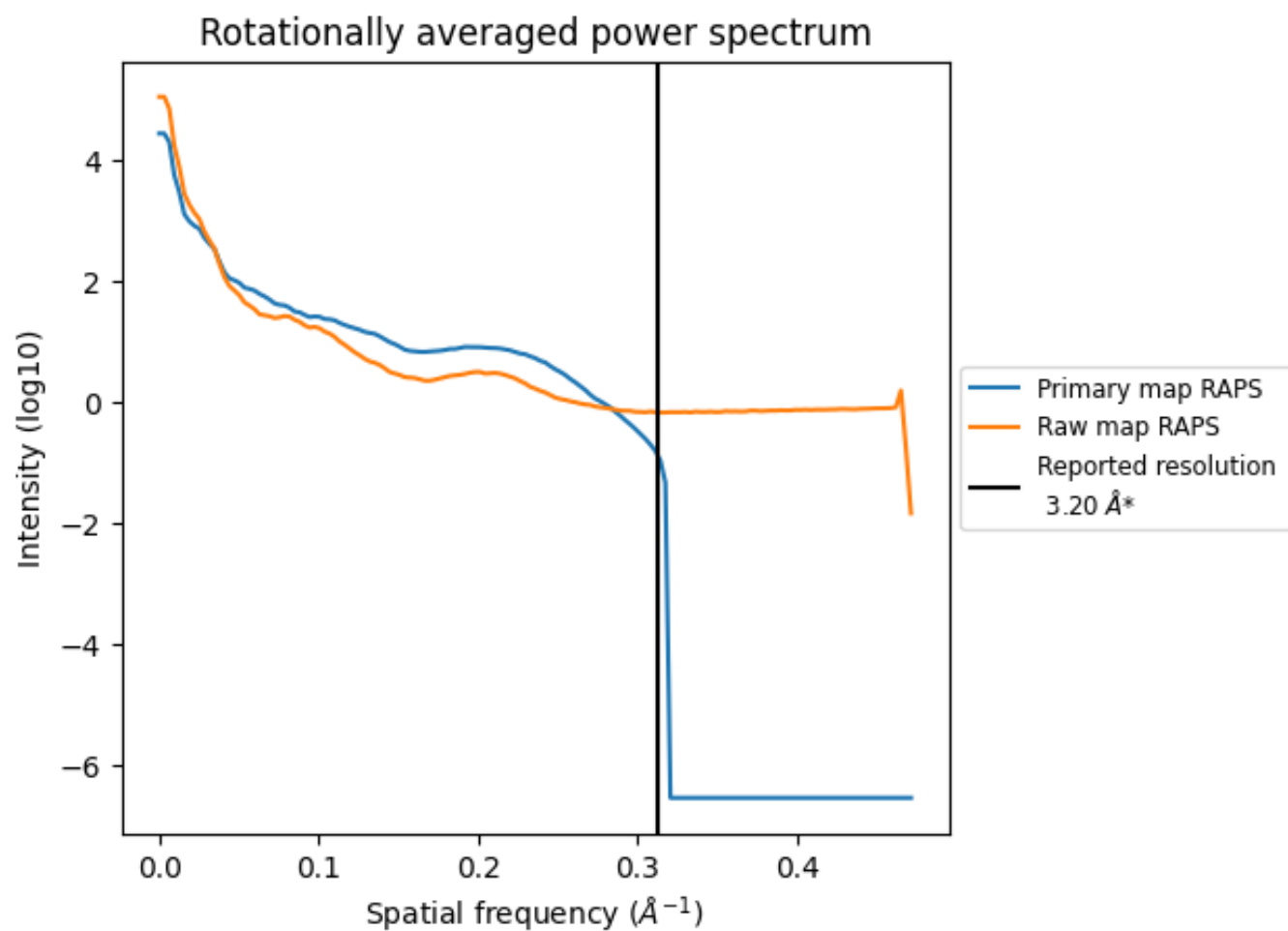
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 321 nm³; this corresponds to an approximate mass of 290 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 ⓘ

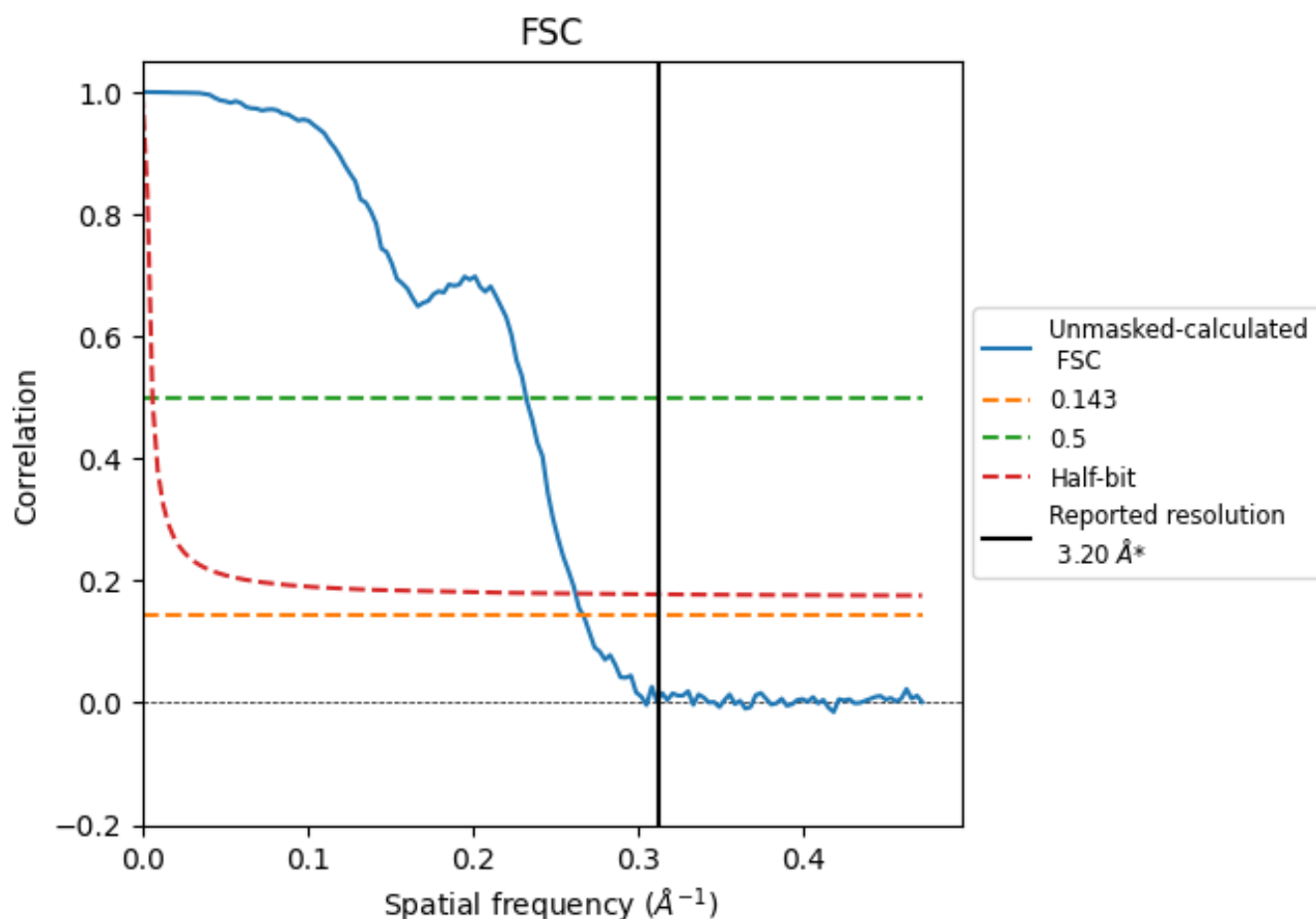


*Reported resolution corresponds to spatial frequency of $0.312 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

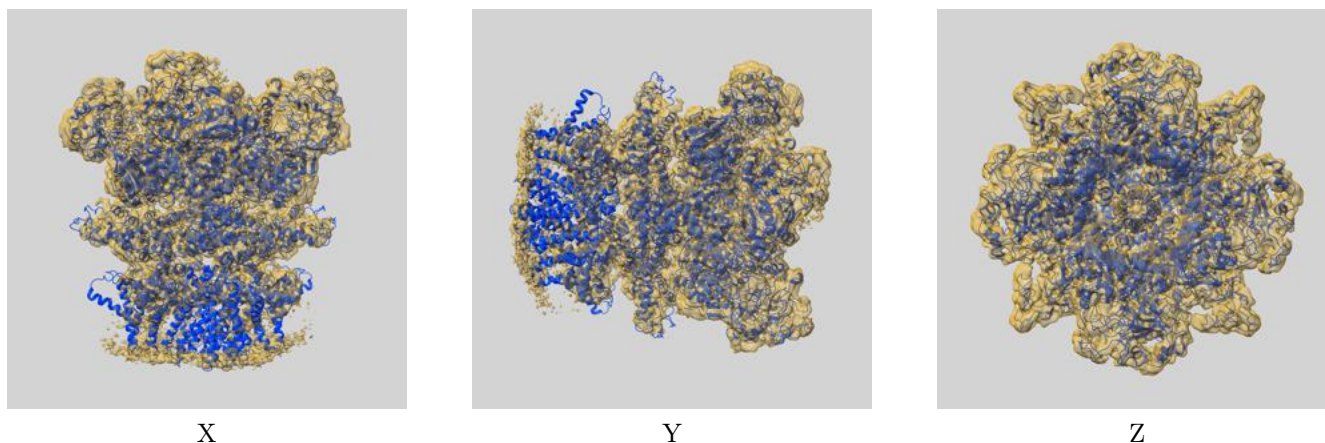
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.75	4.31	3.82

*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 3.75 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

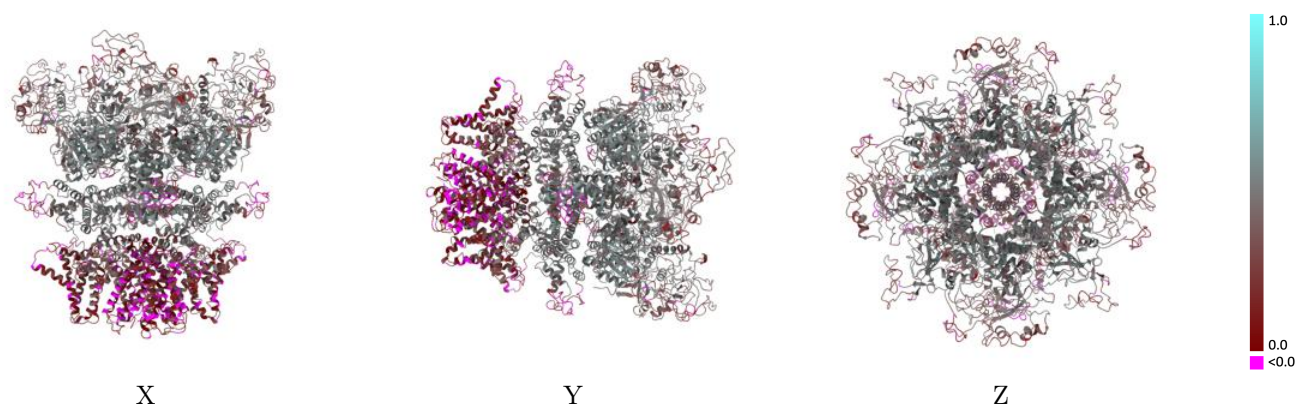
This section contains information regarding the fit between EMDB map EMD-27926 and PDB model 8E6U. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



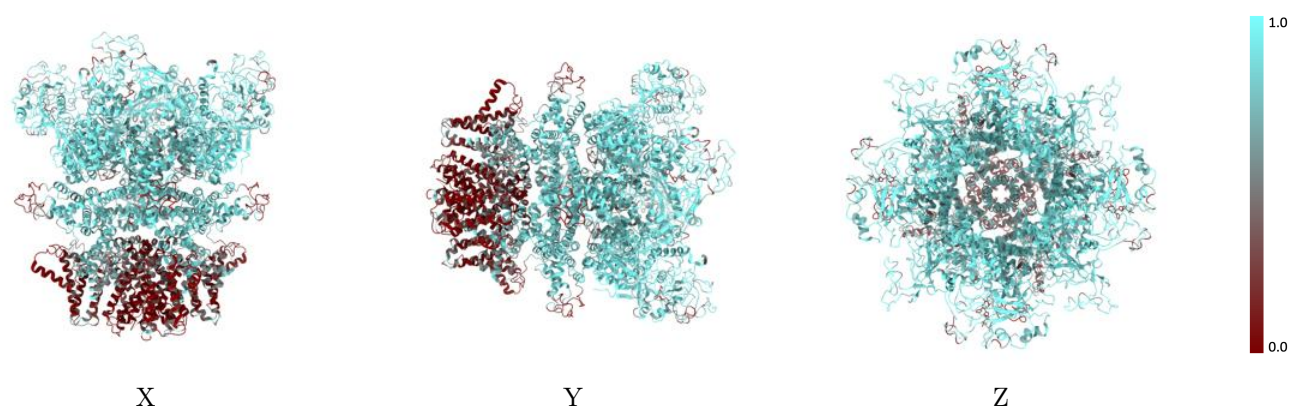
The images above show the 3D surface view of the map at the recommended contour level 0.234 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



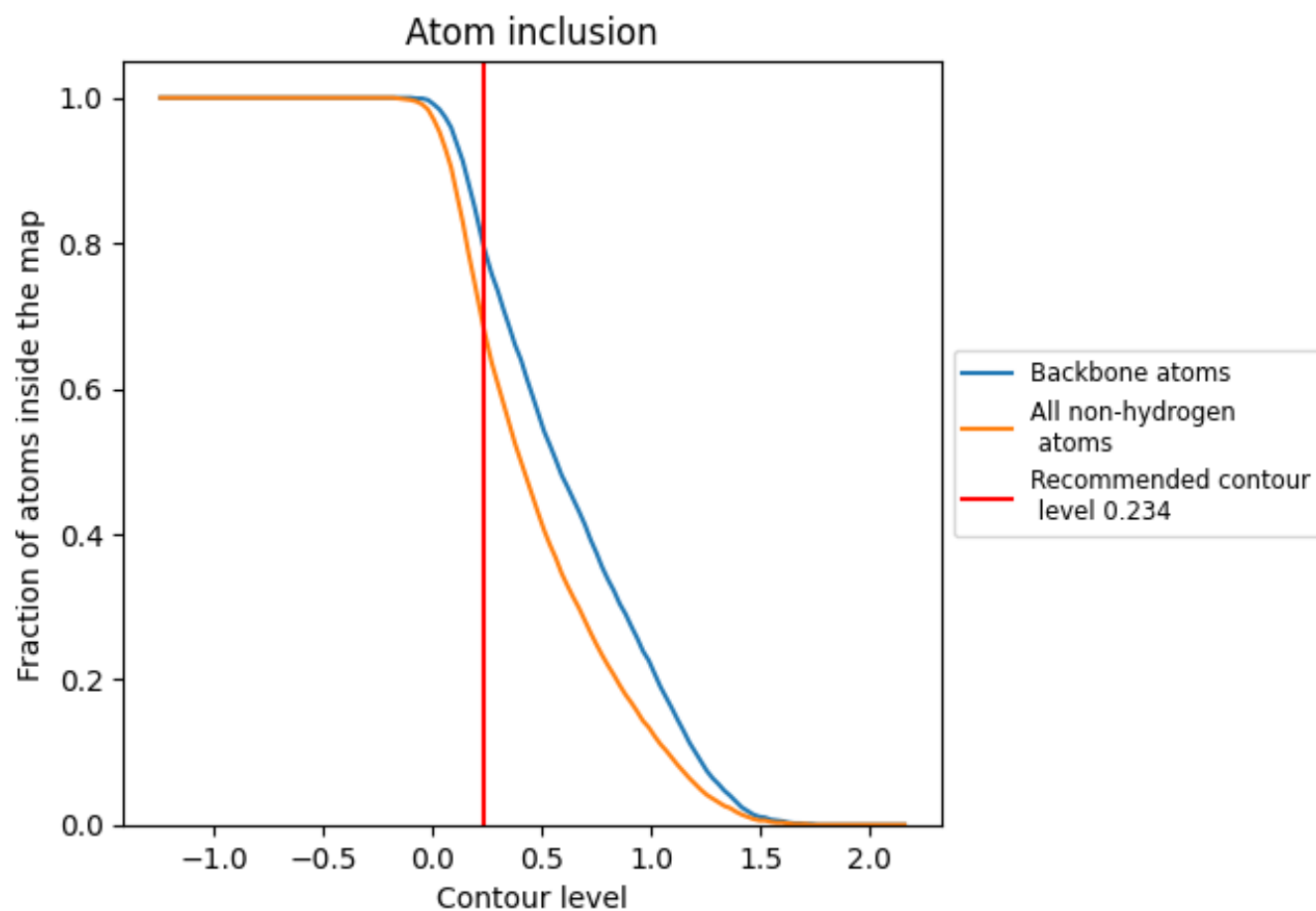
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.234).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 68% 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 (0.234) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6830	0.3530
A	0.6830	0.3530
B	0.6830	0.3540
C	0.6830	0.3530
D	0.6840	0.3530

