



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 08:10 PM UTC

PDB ID : 7WTE / pdb_00007wte
EMDB ID : EMD-32780
Title : Cryo-EM structure of human pyruvate carboxylase with acetyl-CoA in the intermediate state 2
Authors : Chai, P.; Lan, P.; Wu, J.; Lei, M.
Deposited on : 2022-02-04
Resolution : 3.30 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 EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

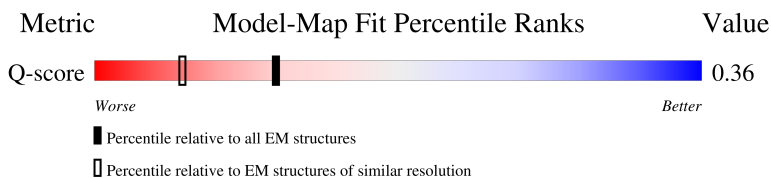
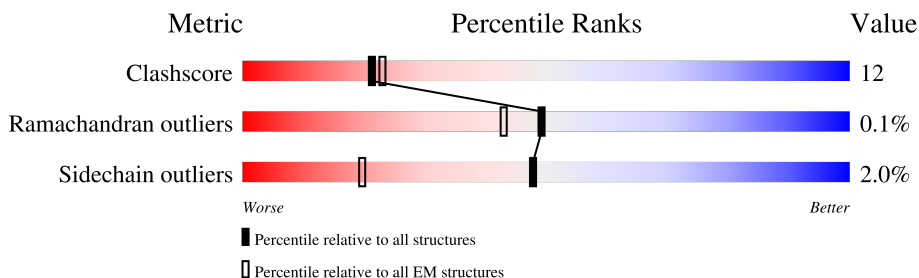
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1178	40% 11% 49%
1	B	1178	36% 15% 49%
1	C	1178	7% 71% 26% ..
1	D	1178	5% 72% 25% .

2 Entry composition [i](#)

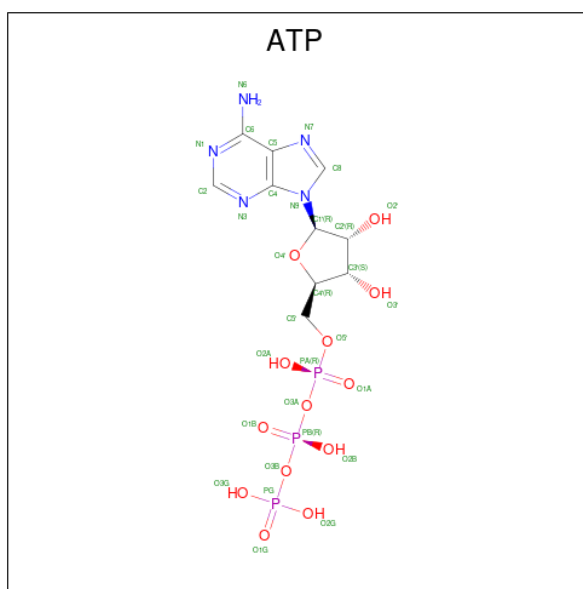
There are 3 unique types of molecules in this entry. The entry contains 27160 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Pyruvate carboxylase, mitochondrial.

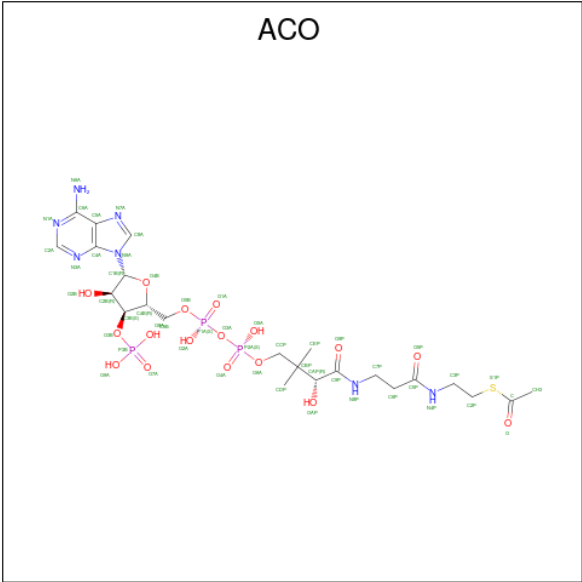
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	600	Total	C	N	O	S	0	0
			4625	2938	796	863	28		
1	B	600	Total	C	N	O	S	0	0
			4625	2938	796	863	28		
1	C	1146	Total	C	N	O	S	0	0
			8869	5612	1559	1651	47		
1	D	1147	Total	C	N	O	S	0	0
			8877	5618	1560	1652	47		

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

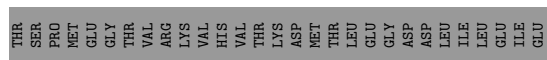


Mol	Chain	Residues	Atoms					AltConf
2	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
2	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 3 is ACETYL COENZYME *A (CCD ID: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$).



Mol	Chain	Residues	Atoms						AltConf
3	C	1	Total	C	N	O	P	S	0
			51	23	7	17	3	1	
3	D	1	Total	C	N	O	P	S	0
			51	23	7	17	3	1	



Chain B: 36% 15% 49%



MET
LYS
MET
GLU
PHE
THR
VAL
VAL
THR
THR
SER
PRO
GLY
MET
GLU
GLY
THR

• Molecule 1: Pyruvate carboxylase, mitochondrial

Chain C: 

MET	LEU	LYS	PHE	ARG	THR	VAL	VAL	HIS	GLY	SER	PRO	GLU	ARG	GLY	THR	VAL	THR	THR	THR	VAL	ALA	PRQ	ASP	ASP	ASP	LEU	TLE	LEU	GLU	TLE	GLU
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L121	S122	E123	R124	A125	D126	F127	R137	D151	E154	V164	T170	L174	T175	S176	H178	E179	E182	K194	A195	G199	G200	G201	R202	G203	P204	V207	Y210	L213	Y217	A224	F228	L233	E236	K237	K241	P242	H244	Q248
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D252	L260	D264	C265	S266	K273	V274	V275	E276	I277	A278	P279	A280	A281	R290	L298	E305	N306	T309	L313	V314	D315	R316	H320	N326	S327	V335	T336	E337	D343	L344	V345	H346	V351	S356	D359	I374	C376	R377	R385
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S386	F387	Q388	T391	G392	R393	I394	V396	M403	D408	Q414	P420	L425	H436	P437	M443	S444	R445	E449	R453	I459	A460	F461	N464	V465	T478	L490	Q494	N495	R496	K499	L500	L501	L504	M508	V509	T513	A520
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P524	R542	P550	R558	L564	L565	M566	D567	T568	R571	D572	A573	H574	A579	T580	V581	V582	R583	T584	T590	V593	V594	N597	E605	G608	R625	R626	L627	Q628	R631	F639	Q640	M641	L643	R644	G645	A646	N647	A648	V649	G650	Y651	D656
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V665	N669	D672	R675	V676	D678	S679	L680	M686	E701	S705	L720	M724	H736	K741	D742	M743	L746	L747	K748	P749	T750	T753	M754	L759	R760	D761	Q762	P767	L768	H771	S776	G777	A778	A787	A791	D792	V793	V794	D795	V796
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M804	P808	A812	L813	P827	R830	A818	Y837	L844	A847	T853	M854	N858	S859	D860	V861	Y862	E863	N864	E865	I866	Q870	Y871	T872	N873	L874	H875	F876	Q877	M881	G882	L883	K886	F887	K888	E889	K892	E896	Q899	M900	L901	G902	D903	L904
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V907	T908	P909	S910	S911	K912	T913	V914	G915	D916	L917	Q918	Q919	F920	M921	Q923	N924	L926	S927	R928	A929	E930	Q934	A935	E936	F937	F940	F947	L948	Q949	R964	S965	K966	V967	L968	K969	D970	L971	P972	R973	Y974	E975	L990	E993	R997	H998	M1012	Y1013	F1014	D1015
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V1016	K1021	D1031	M1034	T1035	R1036	L1037	F1038	L1039	Q1040	G1041	P1042	K1043	I1044	E1049	E1053	R1054	G1055	K1056	H1059	V1065	L1068	N1069	R1070	A1071	G1072	Q1073	V1076	L1080	N1081	S1086	L1087	L1088	V1089	M1095	M1099	F1100	H1101	P1102	K1103	A1104	L1105	K1106	D1107	V1108	K1109	G1110
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Q1111	I1112	G1113	A1114	P1115	M1116	P1117	G1118	K1119	V1120	I1121	D1122	I1123	K1124	V1125	V1126	A1127	G1128	A1129	K1130	V1131	A1132	K1133	G1134	Q1135	P1136	L1137	G1138	V1139	L1140	S1141	A1142	M1143	K1144	M1145	E1146	T1147	V1148	V1149	T1150	S1151	P1152	M1153	E1154	G1155	T1156	V1157	R1158	K1159	V1160	H1161	V1162	T1163	K1164	D1165	M1166	T1167	L1168	E1169	G1170
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D1171	D1172	L1173	I1174	L1175	E1176	I1177	E1178
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• Molecule 1: Pyruvate carboxylase, mitochondrial

Chain D: 

MET	LEU	LYS	PHE	ARG	THR	VAL	HIS	GLY	LEU	ARG	LEU	LEU	GLY	ILE	ARG	ARG	THR	SER	THR	ALA	PRO	ALA	ALA	SER	PRO	ASN	VAL	ARG	ARG	L32	K35	P36	I37	M41	V42	A43	N44	E47	I50	R51	V52	F53	E58	V64	A65	I66	H76	R77	K78	K79	A80
D81	E82	P242	I86	A91	Q94	Y254	H98	I99	F100	D101	D112	A113	V114	H115	P116	G117	L121	S122	E123	R124	F127	L283	R137	K152	V164	T170	P173	I174	K194	A195	A196	G201	R202	G203	M204	R205	V206	N216	L225	G231	A232	L233	F234	V235	E236						
K241	P242	R243	Q248	I249	Y254	Q375	C376	D382	R385	S386	F387	D390	T391	G392	R393	I394	A278	P279	A280	L283	L287	N306	T309	L313	V314	R316	Y422	D423	H421	Y422	D423	S424	M443	G444	R445	A446	L447	A448	E449	V452	R453	G454	H346	I349	H350	E353					
S356	L487	D359	Q489	L490	R491	Q494	N495	A496	A497	R499	L500	L501	H502	Y503	L504	M508	T513	T514	P515	I516	P517	S399	G400	E401	A410	Q414	G415	A416	P420	H421	Y422	D423	S424	M443	G444	R445	A446	L447	A448	E449	V452	R453	G454	H346	I349	H350	E353				
V476	D586	K589	I590	A591	H596	G608	Q608	E621	A497	R625	E629	L630	R631	L634	P635	N636	M641	R644	N647	V665	P522	S523	P524	P533	I534	G535	P536	P537	P538	D543	I544	E548	G549	P550	R558	L565	R571	A579	T580	R581	K456	V582	N464	V465	H585						
R760	D761	R762	P767	H771	D795	V796	D799	M804	A812	T820	M828	F832	D833	Y834	S835	E836	L844	Y845	S856	G857	N858	S859	D860	N864	E865	I866	T716	K717	Y722	Y723	M724	G725	L726	A727	E728	E729	L730	H736	L738	V739	K741	D742	M743	Q899	M900						
L901	Y907	T908	P909	M921	G925	R928	A929	E930	Q934	E937	R942	S943	F947	L948	R964	D970	L987	K992	E993	L994	Y995	D996	R997	P1004	E1005	D1006	V1007	L1008	M1012	D1015	H1019	F1020	K1021	D1031	S1032	L1033	A893	Y894	V895	R1036	L1037	F1038	L1039								
Q1040	G1041	P1042	K1043	F1048	E1049	L1052	E1053	R1054	G1055	K1056	T1057	L1058	H1059	T1060	M1069	R1070	A1071	L1080	L1084	R1085	S1086	D1091	T1092	Q1093	A1094	M1095	K1096	E1097	D996	R997	P1004	E1005	D1006	V1007	L1008	M1012	D1015	H1019	F1020	K1021	D1031	S1032	L1033	A893	Y894	V895	R1036	L1037	F1038	L1039	
G1128	A1129	K1130	V1131	A1132	K1133	G1134	Q1135	P1136	L1137	L1140	S1141	A1142	M1143	K1144	M1145	E1146	T1147	V1148	V1149	T1150	S1151	P1152	M1153	E1154	G1155	T1156	V1157	R1158	K1159	V1160	H1161	V1162	T1163	K1164	D1165	M1166	T1167	L1168	E1169	L1173	I1174	L1175	E1176	I1177	E1178						

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	139123	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.043	Depositor
Minimum map value	-0.023	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.006	Depositor
Map size ($\text{\AA}$)	343.2, 343.2, 343.2	wwPDB
Map dimensions	312, 312, 312	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0/4734	0.40	0/6425
1	B	0.15	0/4734	0.37	0/6425
1	C	0.27	0/9060	0.47	1/12277 (0.0%)
1	D	0.32	0/9068	0.48	0/12288
All	All	0.26	0/27596	0.44	1/37415 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	649	VAL	N-CA-C	-5.51	108.47	113.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4625	0	4573	88	0
1	B	4625	0	4573	127	0
1	C	8869	0	8831	215	0
1	D	8877	0	8842	215	0
2	C	31	0	12	8	0
2	D	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	51	0	34	13	0
3	D	51	0	34	5	0
All	All	27160	0	26911	637	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 12.

All (637) 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:C:524:PRO:CA	1:C:1036:ARG:HH22	1.10	1.64
1:C:583:ARG:NH2	1:C:1031:ASP:HA	1.39	1.33
1:B:1079:GLU:HG3	1:B:1084:LEU:CD2	1.71	1.21
1:C:524:PRO:HA	1:C:1036:ARG:NH2	0.88	1.19
1:D:514:THR:HG21	1:D:1038:PHE:CZ	1.81	1.16
1:C:494:GLN:HG2	3:C:2001:ACO:O5A	1.50	1.10
1:C:199:GLY:O	2:C:2000:ATP:PA	2.16	1.03
1:C:1080:LEU:HD21	3:C:2001:ACO:O2B	1.60	1.02
1:C:524:PRO:CA	1:C:1036:ARG:NH2	1.85	1.01
1:C:524:PRO:HA	1:C:1036:ARG:CZ	1.92	0.99
1:B:1063:LEU:HG	1:B:1079:GLU:OE1	1.25	0.99
1:D:112:ASP:OD1	1:D:137:ARG:NH1	1.96	0.98
1:D:194:LYS:HE3	1:D:236:GLU:OE2	1.63	0.97
1:D:621:GLU:OE2	1:D:1031:ASP:HB3	1.65	0.97
1:C:583:ARG:NH2	1:C:1031:ASP:CA	2.29	0.95
1:D:514:THR:HG21	1:D:1038:PHE:HZ	1.21	0.93
1:B:1079:GLU:HG3	1:B:1084:LEU:HD23	1.51	0.92
1:D:583:ARG:NH1	1:D:1031:ASP:HA	1.84	0.91
1:D:583:ARG:CZ	1:D:1031:ASP:HA	2.01	0.90
1:D:32:LEU:N	1:D:254:TYR:HH	1.69	0.90
1:C:583:ARG:HH22	1:C:1031:ASP:HA	1.36	0.85
1:D:497:ALA:HB2	3:D:2001:ACO:H4B	1.56	0.85
1:B:1063:LEU:CG	1:B:1079:GLU:OE1	2.13	0.84
1:C:1095:MET:H	1:C:1095:MET:HE2	1.43	0.83
1:C:199:GLY:O	2:C:2000:ATP:O3A	1.95	0.82
1:B:641:MET:HB3	1:B:671:MET:HE3	1.59	0.82
1:D:514:THR:CG2	1:D:1038:PHE:CZ	2.64	0.80
1:C:494:GLN:CG	3:C:2001:ACO:O5A	2.29	0.80
1:D:621:GLU:HG3	1:D:1031:ASP:OD2	1.82	0.80
1:C:199:GLY:O	2:C:2000:ATP:O1A	1.99	0.79
1:D:900:MET:HE2	1:D:928:ARG:HG3	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:844:LEU:HB3	1:C:1035:THR:HG21	1.63	0.79
1:D:864:ASN:HD21	1:D:891:LYS:HD3	1.46	0.78
1:D:524:PRO:HA	1:D:1036:ARG:HH21	1.49	0.78
1:D:241:LYS:HB2	1:D:316:ARG:HD2	1.64	0.78
1:A:783:MET:HE3	1:A:794:VAL:HB	1.66	0.77
1:C:844:LEU:HD13	1:C:1035:THR:OG1	1.85	0.77
1:B:875:HIS:CE1	1:B:879:HIS:HE1	2.03	0.76
1:C:584:THR:OG1	1:C:1031:ASP:OD2	2.02	0.76
1:A:948:LEU:HB3	1:A:968:LEU:HD21	1.66	0.76
1:B:600:LYS:NZ	1:B:825:GLU:OE1	2.18	0.76
1:B:1079:GLU:CG	1:B:1084:LEU:CD2	2.61	0.76
1:D:514:THR:CG2	1:D:1038:PHE:HZ	1.99	0.76
1:D:278:ALA:HB2	1:D:335:VAL:HG12	1.66	0.76
1:A:864:ASN:HD21	1:A:891:LYS:HB2	1.52	0.75
1:D:583:ARG:HH12	1:D:1031:ASP:H	1.35	0.75
1:A:920:PHE:O	1:A:924:ASN:HB2	1.86	0.74
1:B:1079:GLU:HG3	1:B:1084:LEU:HD21	1.68	0.74
1:C:583:ARG:HH21	1:C:1031:ASP:HA	1.45	0.74
1:D:558:ARG:O	1:D:558:ARG:NH1	2.21	0.74
1:D:571:ARG:HD3	1:D:608:GLY:HA3	1.70	0.73
1:D:35:LYS:CD	1:D:137:ARG:HH21	2.02	0.73
1:A:571:ARG:HD3	1:A:608:GLY:HA3	1.71	0.72
1:C:741:LYS:HE3	1:C:743:MET:HE3	1.71	0.72
1:D:51:ARG:NH2	1:D:343:ASP:OD1	2.23	0.71
1:B:571:ARG:HD3	1:B:608:GLY:HA3	1.72	0.70
1:B:743:MET:HE2	1:B:907:VAL:HG22	1.71	0.70
1:C:51:ARG:NH2	1:C:343:ASP:OD1	2.25	0.70
1:D:44:ASN:ND2	1:D:116:PRO:O	2.25	0.70
1:C:948:LEU:O	1:C:964:ARG:NH1	2.24	0.70
1:A:641:MET:HB3	1:A:671:MET:HE1	1.72	0.69
1:B:1063:LEU:HD11	1:B:1084:LEU:HD22	1.73	0.69
1:B:752:CYS:SG	1:B:786:CYS:N	2.66	0.69
1:B:1068:LEU:HD23	1:B:1072:GLY:HA2	1.74	0.69
3:C:2001:ACO:HH32	1:D:53:PHE:HB3	1.73	0.68
1:B:600:LYS:NZ	1:B:825:GLU:O	2.26	0.68
1:C:53:PHE:HB3	3:D:2001:ACO:HH32	1.76	0.68
1:D:1058:LEU:HD21	3:D:2001:ACO:H1B	1.75	0.68
1:A:1061:LYS:HB2	1:A:1079:GLU:HB3	1.76	0.68
1:C:590:ILE:HG22	1:C:594:VAL:HG23	1.76	0.67
1:C:900:MET:HE2	1:C:928:ARG:HG3	1.76	0.67
1:D:58:GLU:OE1	1:D:346:HIS:NE2	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:ARG:HG3	1:C:425:LEU:HD13	1.75	0.67
1:C:874:LEU:HG	1:C:887:PHE:HE1	1.60	0.67
1:D:1173:LEU:HD11	1:D:1176:GLU:HB2	1.75	0.67
1:D:516:ILE:HD11	1:D:1039:LEU:HD22	1.76	0.67
1:A:677:PHE:HE2	1:A:907:VAL:HG11	1.60	0.67
3:C:2001:ACO:N6A	1:D:80:ALA:O	2.27	0.67
1:D:864:ASN:HB3	1:D:866:ILE:HG13	1.77	0.67
1:B:760:ARG:HH21	1:B:768:LEU:HD23	1.60	0.66
1:C:241:LYS:HB3	1:C:316:ARG:HH11	1.60	0.66
1:D:641:MET:HB2	1:D:671:MET:HE3	1.77	0.66
1:C:1133:LYS:NZ	1:C:1152:PRO:O	2.28	0.66
1:C:542:ARG:NH1	1:C:672:ASP:OD2	2.28	0.66
1:D:907:VAL:HG12	1:D:908:THR:H	1.59	0.66
1:B:760:ARG:NH2	1:B:790:GLY:O	2.29	0.66
1:C:199:GLY:C	2:C:2000:ATP:O2B	2.39	0.66
1:C:771:HIS:ND1	1:C:795:ASP:OD2	2.29	0.66
1:D:248:GLN:HG2	1:D:260:LEU:HD12	1.77	0.66
1:B:1073:GLN:HE21	1:B:1088:LEU:HB3	1.61	0.65
1:D:900:MET:HE1	1:D:921:MET:HE1	1.78	0.65
1:B:787:ALA:HA	1:B:791:ALA:HB3	1.79	0.65
1:D:771:HIS:ND1	1:D:795:ASP:OD2	2.25	0.65
1:C:260:LEU:HD11	1:C:344:LEU:HD21	1.78	0.65
1:D:1156:THR:OG1	1:D:1158:ARG:NH1	2.30	0.65
1:B:883:LEU:HA	1:B:886:LYS:HE2	1.79	0.65
1:D:583:ARG:NH1	1:D:1031:ASP:CA	2.60	0.65
1:C:1073:GLN:HG2	1:C:1088:LEU:HD12	1.79	0.64
1:D:1128:GLY:H	1:D:1157:VAL:HG13	1.62	0.64
1:A:1090:LYS:NZ	1:A:1091:ASP:O	2.30	0.64
1:D:537:PRO:HB2	1:D:636:ASN:HD21	1.63	0.64
1:C:1128:GLY:H	1:C:1157:VAL:HG23	1.63	0.63
1:B:924:ASN:HB3	1:B:926:LEU:HD13	1.80	0.63
1:D:278:ALA:HB3	1:D:279:PRO:HD3	1.80	0.63
1:B:874:LEU:HG	1:B:887:PHE:HE1	1.63	0.63
1:A:995:VAL:HG23	1:A:1000:GLU:HA	1.80	0.63
1:C:35:LYS:HB2	1:C:137:ARG:HH22	1.64	0.63
1:B:1063:LEU:HD11	1:B:1079:GLU:CD	2.23	0.63
1:D:522:PRO:HD2	1:D:1040:GLN:HG3	1.81	0.62
1:D:1043:LYS:HE3	1:D:1043:LYS:HA	1.80	0.62
1:D:1053:GLU:HG2	1:D:1054:ARG:H	1.65	0.62
1:A:919:GLN:HB3	1:A:923:GLN:HE22	1.64	0.62
1:C:924:ASN:HB2	1:C:926:LEU:HD22	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:783:MET:HE2	1:B:794:VAL:HG13	1.82	0.62
1:B:1063:LEU:CD1	1:B:1079:GLU:CD	2.61	0.62
1:D:901:LEU:HD11	1:D:947:PHE:HE2	1.64	0.62
1:D:1125:VAL:HG13	1:D:1129:ALA:HB3	1.83	0.61
1:B:681:ASN:OD1	1:B:722:TYR:OH	2.17	0.61
1:D:583:ARG:HH12	1:D:1031:ASP:N	1.98	0.61
1:D:206:VAL:O	1:D:216:ASN:ND2	2.34	0.61
1:B:624:TRP:HZ2	1:B:1008:LEU:HD11	1.64	0.61
1:C:568:THR:HG22	1:C:605:GLU:HB3	1.82	0.61
1:C:583:ARG:HH22	1:C:1031:ASP:CA	2.03	0.61
1:A:1069:ASN:OD1	1:A:1070:ARG:N	2.34	0.61
1:C:80:ALA:O	3:D:2001:ACO:N6A	2.33	0.61
1:C:1056:LYS:NZ	3:C:2001:ACO:C8A	2.64	0.61
1:D:309:THR:HG21	1:D:330:GLN:HG3	1.82	0.61
1:D:382:ASP:OD2	1:D:385:ARG:NH1	2.33	0.61
1:D:522:PRO:HD2	1:D:1040:GLN:CG	2.31	0.61
1:C:625:ARG:NH1	1:C:628:GLN:OE1	2.33	0.61
1:A:1068:LEU:HD22	1:A:1072:GLY:HA2	1.81	0.60
1:C:571:ARG:HD3	1:C:608:GLY:HA3	1.82	0.60
1:D:874:LEU:HG	1:D:887:PHE:HZ	1.65	0.60
1:B:568:THR:OG1	1:B:807:GLN:OE1	2.14	0.60
1:D:194:LYS:CE	1:D:236:GLU:OE2	2.44	0.60
1:B:864:ASN:HD21	1:B:891:LYS:HB2	1.65	0.60
1:C:649:VAL:HB	1:C:1012:MET:HE1	1.83	0.60
1:C:243:ARG:NH1	1:C:264:ASP:OD2	2.35	0.60
1:C:1056:LYS:NZ	3:C:2001:ACO:N7A	2.48	0.60
1:C:199:GLY:O	2:C:2000:ATP:PB	2.60	0.60
1:D:91:ALA:HB3	1:D:94:GLN:HG2	1.83	0.60
1:B:853:THR:H	1:B:875:HIS:CE1	2.20	0.60
1:D:170:THR:HB	1:D:174:ILE:HD11	1.83	0.60
1:C:241:LYS:O	1:C:316:ARG:NH1	2.34	0.60
1:C:1049:GLU:OE1	1:C:1059:HIS:ND1	2.35	0.59
1:C:278:ALA:HB2	1:C:335:VAL:HB	1.84	0.59
1:D:583:ARG:NH2	1:D:1031:ASP:HA	2.17	0.59
1:D:625:ARG:NH2	1:D:629:GLU:OE2	2.35	0.59
1:A:817:THR:HG21	1:A:822:LEU:HD12	1.85	0.59
1:B:948:LEU:HD22	1:B:964:ARG:HB3	1.85	0.59
1:A:889:GLU:HA	1:A:892:LYS:NZ	2.17	0.59
1:C:170:THR:HG21	1:C:174:ILE:HG12	1.84	0.59
1:B:968:LEU:HG	1:B:971:LEU:HB2	1.85	0.58
1:C:164:VAL:HG11	1:C:298:LEU:HD12	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:ASP:OD1	1:C:316:ARG:N	2.35	0.58
1:D:262:GLU:OE2	1:D:280:ALA:N	2.35	0.58
1:D:677:PHE:HE2	1:D:907:VAL:HG11	1.69	0.58
1:C:787:ALA:HA	1:C:791:ALA:HB3	1.84	0.58
1:A:919:GLN:HA	1:A:922:VAL:HG22	1.86	0.58
1:B:1015:ASP:OD1	1:B:1016:VAL:N	2.35	0.58
1:D:498:GLN:O	1:D:502:HIS:ND1	2.33	0.58
1:C:746:LEU:HD11	1:C:865:GLU:HG2	1.86	0.58
1:C:1132:ALA:HB3	1:C:1135:GLN:HG2	1.85	0.57
1:A:721:GLN:HA	1:A:724:MET:HG2	1.86	0.57
1:D:385:ARG:HG3	1:D:386:SER:H	1.69	0.57
1:B:686:MET:HB3	1:B:690:MET:HE1	1.86	0.57
1:D:558:ARG:HE	1:D:760:ARG:HH22	1.51	0.57
1:C:126:ASP:OD1	1:C:127:PHE:N	2.37	0.57
1:C:385:ARG:HG3	1:C:386:SER:H	1.69	0.57
1:C:524:PRO:C	1:C:1036:ARG:NH2	2.58	0.57
1:A:804:MET:HE3	1:A:804:MET:HA	1.86	0.57
1:A:747:LEU:HD22	1:A:752:CYS:HB3	1.87	0.57
1:C:761:ASP:OD1	1:C:762:ARG:N	2.37	0.57
1:D:394:ILE:HG12	1:D:455:VAL:HG11	1.86	0.57
1:C:224:ALA:HA	1:C:228:PHE:HD2	1.70	0.57
1:C:864:ASN:HB3	1:C:866:ILE:HG12	1.86	0.57
1:D:423:ASP:OD1	1:D:424:SER:N	2.36	0.57
1:B:935:ALA:HB3	1:B:966:LYS:HE3	1.87	0.56
1:B:566:MET:HB3	1:B:602:PHE:HB3	1.87	0.56
1:B:576:SER:O	1:B:872:THR:HG21	2.05	0.56
1:B:853:THR:H	1:B:875:HIS:HE1	1.53	0.56
1:C:243:ARG:HH22	1:C:281:ALA:HB3	1.69	0.56
1:D:44:ASN:HD22	1:D:117:GLY:HA3	1.70	0.56
1:C:1143:MET:SD	1:C:1144:LYS:N	2.78	0.56
1:D:265:CYS:SG	1:D:273:LYS:HD3	2.45	0.56
1:D:921:MET:O	1:D:925:GLY:N	2.36	0.56
1:A:992:LYS:HA	1:A:995:VAL:HG12	1.88	0.56
1:B:1079:GLU:CG	1:B:1084:LEU:HD21	2.31	0.56
1:B:854:MET:H	1:B:875:HIS:CE1	2.24	0.56
1:D:558:ARG:HB2	1:D:767:PRO:HG3	1.87	0.56
1:D:50:ILE:HD11	1:D:76:HIS:HA	1.87	0.56
1:B:1000:GLU:HG2	1:B:1001:GLU:OE1	2.06	0.56
1:D:535:GLY:O	1:D:596:HIS:NE2	2.35	0.56
1:D:1070:ARG:NH1	1:D:1071:ALA:HB3	2.20	0.56
1:A:864:ASN:ND2	1:A:891:LYS:HB2	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:908:THR:HB	1:B:909:PRO:HD3	1.87	0.55
1:D:844:LEU:HD23	1:D:1035:THR:HB	1.87	0.55
1:B:799:ASP:OD2	1:C:859:SER:N	2.40	0.55
1:C:50:ILE:HD11	1:C:76:HIS:HA	1.88	0.55
1:C:908:THR:HB	1:C:909:PRO:HD3	1.87	0.55
1:C:520:ALA:HB3	1:C:847:ALA:HA	1.88	0.55
1:D:35:LYS:HD2	1:D:137:ARG:HH21	1.72	0.55
1:C:396:VAL:HB	1:C:453:ARG:HB2	1.89	0.55
1:D:35:LYS:HB3	1:D:137:ARG:NH2	2.22	0.55
1:D:393:ARG:HH22	1:D:1086:SER:HB3	1.72	0.55
1:C:1015:ASP:OD1	1:C:1016:VAL:N	2.40	0.55
1:D:761:ASP:OD1	1:D:762:ARG:N	2.40	0.55
1:C:199:GLY:C	2:C:2000:ATP:PB	2.90	0.55
1:A:722:TYR:CZ	1:A:726:LEU:HD11	2.42	0.54
1:A:888:LYS:HA	1:A:891:LYS:HD2	1.89	0.54
1:C:391:THR:HG21	1:C:420:PRO:HB3	1.90	0.54
1:B:854:MET:HG2	1:B:875:HIS:ND1	2.23	0.54
1:D:394:ILE:HD12	1:D:416:ALA:HB3	1.89	0.54
1:A:631:ARG:NH2	1:A:634:ILE:O	2.34	0.54
1:A:598:PHE:HB3	1:A:601:LEU:HD23	1.89	0.54
1:B:581:ARG:HA	1:B:619:LEU:HD11	1.88	0.54
1:D:1145:MET:SD	1:D:1146:GLU:N	2.81	0.54
1:A:778:ALA:HB2	1:D:812:ALA:HB1	1.90	0.54
1:B:558:ARG:HB2	1:B:767:PRO:HG3	1.90	0.54
1:C:178:HIS:NE2	1:C:182:GLU:OE2	2.40	0.54
1:C:1070:ARG:HA	1:C:1070:ARG:NH1	2.23	0.54
1:A:776:SER:HG	1:A:862:TYR:HH	1.55	0.54
1:B:906:LYS:HA	1:B:910:SER:OG	2.08	0.54
1:C:265:CYS:SG	1:C:276:GLU:HG3	2.48	0.54
1:C:930:GLU:HB2	1:C:934:GLN:NE2	2.23	0.54
1:D:390:ASP:OD2	1:D:456:LYS:HB2	2.07	0.54
1:D:1095:MET:O	1:D:1096:LYS:HD2	2.06	0.54
1:B:801:MET:HE1	1:B:838:TRP:CG	2.43	0.54
1:B:864:ASN:ND2	1:B:891:LYS:HB2	2.23	0.54
1:C:1056:LYS:HZ3	3:C:2001:ACO:C8A	2.19	0.54
1:D:121:LEU:HD23	1:D:124:ARG:HG3	1.89	0.54
1:D:621:GLU:HG3	1:D:1031:ASP:CG	2.32	0.54
1:C:1069:ASN:OD1	1:C:1070:ARG:N	2.39	0.53
1:C:37:ILE:HG23	1:C:112:ASP:HB3	1.90	0.53
1:D:35:LYS:HD3	1:D:137:ARG:NH2	2.22	0.53
1:D:942:ARG:NH2	1:D:943:SER:OG	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:642:LEU:HD13	1:B:675:ARG:HD2	1.91	0.53
1:C:641:MET:SD	1:C:643:LEU:HB2	2.49	0.53
1:C:854:MET:SD	1:C:875:HIS:ND1	2.81	0.53
1:D:47:GLU:HB3	1:D:410:ALA:HB2	1.89	0.53
1:C:645:GLY:N	1:C:677:PHE:O	2.41	0.53
1:C:873:ASN:OD1	1:C:874:LEU:N	2.41	0.53
1:D:1008:LEU:O	1:D:1012:MET:HG2	2.09	0.53
1:A:907:VAL:HG12	1:A:908:THR:H	1.74	0.53
1:A:1018:ALA:HA	1:A:1021:LYS:HE3	1.91	0.53
1:B:598:PHE:HB3	1:B:601:LEU:HD23	1.89	0.53
1:B:820:THR:HG22	1:B:822:LEU:H	1.74	0.53
1:C:524:PRO:N	1:C:1036:ARG:HH22	1.95	0.53
1:D:37:ILE:HG23	1:D:112:ASP:HB3	1.90	0.53
1:C:1068:LEU:HD11	1:C:1072:GLY:HA2	1.91	0.52
1:B:597:ASN:HB3	1:B:830:ARG:HD2	1.91	0.52
1:C:82:GLU:HG2	1:D:1055:GLY:HA3	1.91	0.52
1:D:399:SER:OG	1:D:401:GLU:OE1	2.20	0.52
1:D:524:PRO:HA	1:D:1036:ARG:NH2	2.22	0.52
1:B:677:PHE:CZ	1:B:907:VAL:HG21	2.42	0.52
1:C:1065:VAL:HG22	1:C:1076:VAL:HG23	1.92	0.52
1:C:1081:ASN:HD22	1:D:77:ARG:NH1	2.08	0.52
1:C:1119:LYS:NZ	1:C:1120:VAL:O	2.43	0.52
1:C:678:ASP:HB3	1:C:686:MET:HE2	1.92	0.52
1:B:775:THR:HG23	1:B:805:THR:HG22	1.90	0.52
1:C:51:ARG:NH2	1:C:337:GLU:OE2	2.42	0.52
1:C:583:ARG:HH22	1:C:1031:ASP:H	1.58	0.52
1:C:583:ARG:HH22	1:C:1031:ASP:N	2.07	0.52
1:C:919:GLN:HA	1:C:922:VAL:HG12	1.92	0.52
1:D:524:PRO:O	1:D:1036:ARG:NH2	2.42	0.52
1:D:591:ALA:HB1	1:D:634:ILE:HD11	1.91	0.52
1:C:1013:TYR:HB3	1:C:1016:VAL:HG22	1.91	0.52
2:C:2000:ATP:H5'1	2:C:2000:ATP:H8	1.75	0.52
1:B:816:CYS:O	1:C:748:LYS:NZ	2.43	0.52
1:A:576:SER:O	1:A:872:THR:HG21	2.10	0.52
1:A:711:ALA:HA	1:A:754:MET:HE1	1.92	0.52
1:C:1034:ASN:HB2	1:C:1037:LEU:HG	1.92	0.52
1:D:265:CYS:SG	1:D:273:LYS:HG2	2.50	0.52
1:D:538:PRO:O	1:D:636:ASN:ND2	2.32	0.52
1:C:558:ARG:HB2	1:C:767:PRO:HG3	1.92	0.51
1:D:987:LEU:H	1:D:987:LEU:HD23	1.75	0.51
1:B:631:ARG:NH2	1:B:634:ILE:O	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1145:MET:HE1	1:D:1147:THR:OG1	2.10	0.51
1:B:1079:GLU:HG3	1:B:1084:LEU:HD22	1.80	0.51
1:C:356:SER:OG	1:C:359:ASP:OD2	2.23	0.51
1:C:724:MET:HE1	1:C:759:LEU:HD22	1.92	0.51
1:D:908:THR:OG1	1:D:909:PRO:HD3	2.10	0.51
1:B:913:ILE:HD13	1:B:947:PHE:HB2	1.92	0.51
1:C:242:PRO:HD2	1:C:478:THR:HB	1.91	0.51
1:C:386:SER:OG	1:C:388:GLN:OE1	2.27	0.51
1:C:903:ASP:OD1	1:C:903:ASP:N	2.44	0.51
1:D:123:GLU:OE1	1:D:328:ARG:HD3	2.10	0.51
1:D:335:VAL:HG21	1:D:375:GLN:HB2	1.92	0.51
1:D:715:ARG:HE	1:D:717:LYS:H	1.58	0.51
1:D:741:LYS:HG2	1:D:743:MET:HE3	1.91	0.51
1:D:1162:VAL:HB	1:D:1174:ILE:HA	1.92	0.51
1:A:761:ASP:OD1	1:A:762:ARG:N	2.43	0.51
1:B:517:PRO:HG3	1:B:876:PHE:HE1	1.75	0.51
1:D:504:LEU:O	1:D:508:MET:HG2	2.10	0.51
1:C:265:CYS:SG	1:C:273:LYS:HD2	2.51	0.50
1:C:935:ALA:HB1	1:C:940:PHE:CZ	2.46	0.50
1:D:907:VAL:HG12	1:D:908:THR:N	2.26	0.50
1:D:704:ILE:HD11	1:D:738:LEU:HD11	1.93	0.50
1:A:1073:GLN:HG2	1:A:1088:LEU:HD12	1.93	0.50
1:B:677:PHE:HZ	1:B:907:VAL:HG21	1.77	0.50
1:C:290:ARG:HD3	1:C:320:HIS:CE1	2.47	0.50
1:C:859:SER:OG	1:C:860:ASP:N	2.43	0.50
1:B:644:ARG:HB2	1:B:647:ASN:O	2.11	0.50
1:B:858:ASN:ND2	1:B:871:TYR:OH	2.41	0.50
1:D:496:ARG:HG2	3:D:2001:ACO:O2A	2.11	0.50
1:C:459:ILE:HD12	1:C:459:ILE:H	1.77	0.50
1:D:314:VAL:HA	1:D:320:HIS:HA	1.93	0.50
1:B:849:ASP:OD1	1:B:850:CYS:N	2.45	0.50
1:D:508:MET:SD	1:D:1042:PRO:HD2	2.51	0.50
1:B:624:TRP:CZ2	1:B:1008:LEU:HD11	2.46	0.49
1:B:853:THR:HB	1:B:875:HIS:CE1	2.46	0.49
1:C:207:VAL:HG11	1:C:213:LEU:HD13	1.93	0.49
1:D:196:ALA:HB3	1:D:232:ALA:HB3	1.94	0.49
1:D:583:ARG:HH12	1:D:1031:ASP:CA	2.24	0.49
1:D:631:ARG:NH2	1:D:634:ILE:O	2.40	0.49
1:D:828:MET:HB3	1:D:832:PHE:CE2	2.47	0.49
1:A:575:GLN:HA	1:A:580:THR:HB	1.93	0.49
1:D:64:VAL:HA	1:D:82:GLU:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:606:ASN:OD1	1:A:607:TRP:N	2.45	0.49
1:B:853:THR:OG1	1:B:879:HIS:NE2	2.42	0.49
1:B:1063:LEU:HD12	1:B:1077:PHE:HB3	1.94	0.49
1:C:1157:VAL:HG11	1:C:1175:LEU:HD23	1.94	0.49
1:A:710:VAL:HG11	1:A:755:LEU:HD21	1.93	0.49
1:A:998:HIS:ND1	1:A:1021:LYS:HD2	2.27	0.49
1:B:903:ASP:N	1:B:903:ASP:OD1	2.43	0.49
1:C:210:TYR:HA	1:C:213:LEU:HB3	1.94	0.49
1:A:782:ALA:O	1:A:786:CYS:HB2	2.12	0.49
1:A:1030:LEU:HD13	1:A:1038:PHE:HE1	1.78	0.49
1:B:977:ARG:HG2	1:B:980:ALA:H	1.76	0.49
1:C:309:THR:HB	1:C:326:ASN:HB2	1.94	0.49
1:D:522:PRO:CD	1:D:1040:GLN:CG	2.91	0.49
1:A:583:ARG:NH1	1:A:1033:LEU:O	2.43	0.49
1:B:900:MET:SD	1:B:928:ARG:HD2	2.52	0.49
1:C:393:ARG:NH2	1:C:1086:SER:OG	2.43	0.49
1:D:397:PHE:N	1:D:414:GLN:OE1	2.41	0.49
1:B:824:THR:HG22	1:B:826:VAL:HG23	1.95	0.49
1:D:35:LYS:HD3	1:D:137:ARG:HH21	1.71	0.49
1:C:926:LEU:HB2	1:C:930:GLU:OE2	2.13	0.48
1:D:1033:LEU:HB3	1:D:1037:LEU:HD23	1.93	0.48
1:A:1042:PRO:HB3	1:A:1048:PHE:CE1	2.48	0.48
1:B:987:LEU:H	1:B:987:LEU:HD23	1.77	0.48
1:D:1052:LEU:HB3	1:D:1056:LYS:HB2	1.95	0.48
1:A:888:LYS:O	1:A:891:LYS:HG2	2.13	0.48
1:C:82:GLU:OE1	1:C:84:TYR:OH	2.25	0.48
1:C:1070:ARG:HA	1:C:1070:ARG:CZ	2.44	0.48
1:A:566:MET:SD	1:A:603:SER:OG	2.72	0.48
1:A:909:PRO:HA	1:A:912:LYS:HE3	1.94	0.48
1:B:632:GLU:N	1:B:632:GLU:OE1	2.47	0.48
1:A:593:TYR:O	1:A:597:ASN:ND2	2.43	0.48
1:A:817:THR:HG22	1:A:823:ASP:HA	1.96	0.48
1:B:586:ASP:OD2	1:B:1035:THR:OG1	2.32	0.48
1:B:591:ALA:HB1	1:B:633:LEU:HB3	1.94	0.48
1:C:177:LEU:HB2	1:C:217:TYR:CE2	2.48	0.48
1:C:656:ASP:OD1	1:C:656:ASP:N	2.45	0.48
1:D:265:CYS:SG	1:D:273:LYS:CD	3.01	0.48
1:D:677:PHE:CE2	1:D:907:VAL:HG11	2.48	0.48
1:D:725:GLY:O	1:D:729:GLU:OE1	2.32	0.48
1:D:993:GLU:O	1:D:997:ARG:HB2	2.14	0.48
1:A:570:PHE:HE1	1:A:838:TRP:HZ2	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:720:LEU:HD13	1:A:755:LEU:HD23	1.94	0.48
1:C:627:LEU:HD22	1:C:669:ASN:HB3	1.96	0.48
1:C:858:ASN:ND2	1:C:871:TYR:OH	2.45	0.48
1:C:1099:HIS:CE1	1:C:1101:HIS:HB2	2.49	0.48
1:A:907:VAL:O	1:A:911:SER:N	2.27	0.47
1:B:859:SER:OG	1:B:860:ASP:N	2.46	0.47
1:B:717:LYS:HE3	1:B:957:GLY:HA3	1.96	0.47
1:B:866:ILE:HD13	1:B:871:TYR:HD1	1.78	0.47
1:C:58:GLU:OE2	1:C:346:HIS:NE2	2.46	0.47
1:C:244:HIS:HB3	1:C:313:LEU:HD12	1.95	0.47
1:C:853:THR:HG22	1:C:854:MET:SD	2.54	0.47
1:C:1102:PRO:HB2	1:C:1173:LEU:HB3	1.95	0.47
1:B:741:LYS:HD2	1:B:771:HIS:HD1	1.78	0.47
1:B:920:PHE:O	1:B:923:GLN:HG3	2.14	0.47
1:B:710:VAL:HG22	1:B:720:LEU:HD13	1.96	0.47
1:B:1013:TYR:HB2	1:B:1016:VAL:HG22	1.96	0.47
1:C:990:LEU:O	1:C:993:GLU:HG3	2.15	0.47
1:C:566:MET:HE2	1:C:795:ASP:HB3	1.97	0.47
1:D:385:ARG:HG3	1:D:386:SER:N	2.28	0.47
1:A:1001:GLU:CD	1:A:1001:GLU:H	2.23	0.47
1:B:593:TYR:O	1:B:597:ASN:ND2	2.35	0.47
1:C:935:ALA:HB1	1:C:940:PHE:HZ	1.79	0.47
1:D:283:LEU:HD12	1:D:287:LEU:HD23	1.96	0.47
1:B:801:MET:HE1	1:B:838:TRP:CD2	2.49	0.47
1:C:395:GLU:O	1:C:414:GLN:NE2	2.34	0.47
1:C:936:GLU:HA	1:C:966:LYS:NZ	2.29	0.47
1:D:265:CYS:SG	1:D:273:LYS:CG	3.03	0.47
1:D:456:LYS:HD2	1:D:456:LYS:HA	1.67	0.47
1:D:522:PRO:CD	1:D:1040:GLN:HG2	2.44	0.47
1:D:585:HIS:O	1:D:589:LYS:HG2	2.15	0.47
1:C:385:ARG:HG3	1:C:386:SER:N	2.29	0.47
1:C:720:LEU:HD22	1:C:754:MET:HE1	1.97	0.47
1:D:514:THR:HG21	1:D:1038:PHE:CE2	2.45	0.47
1:D:1131:VAL:O	1:D:1154:GLU:HG2	2.14	0.47
1:A:741:LYS:HE2	1:A:743:MET:SD	2.55	0.47
1:A:832:PHE:O	1:A:836:GLU:OE1	2.33	0.47
1:B:621:GLU:HG2	1:B:1031:ASP:HB3	1.97	0.47
1:B:770:ILE:HG21	1:B:783:MET:HE1	1.96	0.47
1:D:464:ASN:HD21	1:D:489:GLN:HB2	1.79	0.47
1:D:243:ARG:O	1:D:314:VAL:HG12	2.14	0.46
1:A:1013:TYR:HB3	1:A:1016:VAL:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:641:MET:SD	1:B:643:LEU:HB2	2.55	0.46
1:C:248:GLN:HG2	1:C:260:LEU:HD12	1.98	0.46
1:D:376:CYS:SG	1:D:443:MET:HE3	2.55	0.46
1:C:176:SER:HB2	1:C:179:GLU:HG2	1.97	0.46
1:D:391:THR:HG21	1:D:420:PRO:HB3	1.96	0.46
1:D:550:PRO:HB2	1:D:736:HIS:NE2	2.31	0.46
1:B:499:LYS:HG2	1:B:1027:PHE:C	2.41	0.46
1:C:202:ARG:HB3	1:C:203:GLY:H	1.63	0.46
1:C:403:MET:HE3	1:D:337:GLU:HG2	1.97	0.46
1:C:909:PRO:O	1:C:912:LYS:HG2	2.16	0.46
1:D:225:LEU:HD22	1:D:231:GLY:HA3	1.98	0.46
1:C:88:ARG:HE	1:C:88:ARG:HB2	1.59	0.46
1:C:194:LYS:HD3	1:C:204:MET:HE1	1.97	0.46
1:C:1169:GLU:HG3	1:C:1172:ASP:OD2	2.16	0.46
1:A:737:ILE:HG12	1:A:767:PRO:HB2	1.98	0.46
1:B:827:PRO:HD2	1:B:830:ARG:NH2	2.30	0.46
1:B:853:THR:HB	1:B:875:HIS:HE1	1.81	0.46
1:C:571:ARG:NH1	1:C:572:ASP:OD1	2.48	0.46
1:C:644:ARG:HB2	1:C:647:ASN:O	2.16	0.46
1:D:335:VAL:CG2	1:D:375:GLN:HB2	2.45	0.46
1:D:533:PRO:HG2	1:D:596:HIS:CD2	2.51	0.46
1:C:344:LEU:HD23	1:C:344:LEU:HA	1.81	0.46
1:C:579:ALA:HB3	1:C:581:ARG:HD3	1.98	0.46
1:C:973:ARG:HG3	1:C:975:GLU:OE2	2.15	0.46
1:D:350:HIS:HA	1:D:353:GLU:OE2	2.16	0.46
1:A:974:VAL:HG11	1:A:978:PRO:HB3	1.96	0.45
1:B:1069:ASN:OD1	1:B:1070:ARG:HD3	2.16	0.45
1:D:900:MET:CE	1:D:921:MET:HE1	2.45	0.45
1:A:709:ASP:OD1	1:A:709:ASP:N	2.49	0.45
1:A:951:TYR:O	1:A:978:PRO:HG2	2.15	0.45
1:B:948:LEU:O	1:B:964:ARG:NH1	2.39	0.45
3:C:2001:ACO:HH33	1:D:79:LYS:HB3	1.97	0.45
1:D:99:ILE:HG12	1:D:127:PHE:HD1	1.81	0.45
1:D:1006:ASP:OD1	1:D:1007:VAL:N	2.49	0.45
1:C:899:GLN:OE1	1:C:928:ARG:NH2	2.50	0.45
1:D:35:LYS:CB	1:D:137:ARG:NH2	2.80	0.45
1:D:644:ARG:HB2	1:D:647:ASN:O	2.17	0.45
1:A:701:GLU:OE2	1:A:739:CYS:HB2	2.16	0.45
1:C:896:GLU:OE1	1:C:896:GLU:N	2.50	0.45
1:D:882:GLY:C	1:D:884:GLY:H	2.25	0.45
1:D:888:LYS:HD3	1:D:888:LYS:C	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:ALA:HA	1:C:233:LEU:HD23	1.99	0.45
1:C:705:SER:HA	1:C:741:LYS:HB3	1.98	0.45
1:C:883:LEU:HB3	1:C:886:LYS:HB2	1.98	0.45
1:D:280:ALA:HB1	1:D:283:LEU:HB2	1.98	0.45
1:A:683:LEU:HA	1:A:686:MET:HE2	1.97	0.45
1:B:597:ASN:O	1:B:830:ARG:NH1	2.50	0.45
1:D:543:ASP:OD1	1:D:544:ILE:N	2.50	0.45
1:A:594:VAL:HG13	1:A:598:PHE:HB2	1.99	0.45
1:B:565:LEU:HD22	1:B:796:VAL:HG21	1.99	0.45
1:B:739:CYS:SG	1:B:740:ILE:N	2.90	0.45
1:D:43:ALA:HA	1:D:66:ILE:HD11	1.99	0.45
1:A:889:GLU:HA	1:A:892:LYS:HZ2	1.79	0.45
1:B:565:LEU:HD23	1:B:794:VAL:HB	1.98	0.45
1:D:356:SER:OG	1:D:359:ASP:OD2	2.34	0.45
1:C:760:ARG:NH2	1:C:768:LEU:HD23	2.32	0.45
1:C:1049:GLU:CD	1:C:1059:HIS:HD1	2.26	0.44
1:D:893:ALA:HA	1:D:896:GLU:OE2	2.17	0.44
1:A:942:ARG:NH2	1:A:943:SER:OG	2.50	0.44
1:B:617:ARG:HH21	1:B:1016:VAL:HG11	1.81	0.44
1:B:728:GLU:OE1	1:B:762:ARG:NH1	2.51	0.44
1:A:909:PRO:O	1:A:912:LYS:HG2	2.18	0.44
1:C:590:ILE:HD11	1:C:837:TYR:CD2	2.52	0.44
1:A:680:LEU:O	1:A:682:TYR:N	2.51	0.44
1:C:827:PRO:HB2	1:C:830:ARG:HE	1.81	0.44
1:A:869:GLY:O	1:A:872:THR:OG1	2.34	0.44
1:A:907:VAL:HG12	1:A:908:THR:N	2.32	0.44
1:C:1081:ASN:HD22	1:D:77:ARG:HH12	1.66	0.44
1:B:888:LYS:HA	1:B:891:LYS:HZ3	1.82	0.44
1:C:496:ARG:HB2	3:C:2001:ACO:O2A	2.18	0.44
1:C:677:PHE:HZ	1:C:907:VAL:HG21	1.82	0.44
1:C:796:VAL:HG13	1:C:808:PRO:O	2.17	0.44
1:B:748:LYS:HD3	1:B:748:LYS:HA	1.73	0.44
1:C:631:ARG:HD2	1:C:639:PHE:HE2	1.83	0.44
1:D:66:ILE:HB	1:D:86:ILE:HG12	2.00	0.44
1:D:833:ASP:O	1:D:836:GLU:HG3	2.18	0.44
1:A:651:TYR:CD2	1:A:912:LYS:HE2	2.52	0.44
1:C:593:TYR:O	1:C:597:ASN:ND2	2.37	0.44
1:C:917:LEU:O	1:C:921:MET:HG3	2.17	0.44
1:A:1043:LYS:HE3	1:A:1046:GLU:HG2	1.99	0.43
1:C:997:ARG:HH11	1:C:998:HIS:HB3	1.83	0.43
1:C:1068:LEU:HD12	1:C:1068:LEU:HA	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:889:GLU:HA	1:C:892:LYS:HB2	2.01	0.43
1:A:908:THR:HB	1:A:909:PRO:HD3	2.00	0.43
1:B:683:LEU:HA	1:B:686:MET:HE2	1.99	0.43
1:D:260:LEU:HD11	1:D:344:LEU:HD11	2.00	0.43
1:B:812:ALA:HB1	1:C:778:ALA:HB2	1.99	0.43
1:B:1034:ASN:HB2	1:B:1037:LEU:HD23	2.00	0.43
1:D:858:ASN:OD1	1:D:860:ASP:N	2.44	0.43
1:A:641:MET:SD	1:A:643:LEU:HB2	2.58	0.43
1:D:267:ILE:HD13	1:D:476:VAL:HG11	1.99	0.43
1:D:636:ASN:N	1:D:636:ASN:OD1	2.51	0.43
1:A:624:TRP:CD2	1:A:1005:GLU:HB2	2.53	0.43
1:D:280:ALA:HB1	1:D:283:LEU:HD23	1.99	0.43
1:D:349:ILE:O	1:D:353:GLU:HG3	2.18	0.43
1:D:422:TYR:O	1:D:1143:MET:HG2	2.18	0.43
1:D:895:VAL:O	1:D:899:GLN:HG2	2.18	0.43
1:D:992:LYS:HA	1:D:995:VAL:HG12	1.99	0.43
1:B:1065:VAL:HG22	1:B:1076:VAL:HG22	2.01	0.43
1:C:877:GLN:HB3	1:C:881:MET:HE1	2.01	0.43
1:C:1039:LEU:HD12	1:C:1040:GLN:N	2.33	0.43
1:D:260:LEU:O	1:D:261:TYR:CG	2.72	0.43
1:A:968:LEU:O	1:A:971:LEU:HD23	2.19	0.43
1:B:503:TYR:HB2	1:B:1027:PHE:HB3	2.01	0.43
1:B:1061:LYS:HB3	1:B:1079:GLU:HB2	1.99	0.43
1:D:194:LYS:HB3	1:D:234:PHE:HB2	2.00	0.43
1:D:1012:MET:HE3	1:D:1012:MET:HA	2.00	0.43
1:D:1036:ARG:HG3	1:D:1037:LEU:N	2.33	0.43
1:A:661:LYS:O	1:A:664:GLU:HG2	2.18	0.43
1:A:1068:LEU:HD23	1:A:1074:ARG:HG3	2.00	0.43
1:B:872:THR:O	1:B:875:HIS:HB3	2.19	0.43
1:C:237:LYS:H	1:C:237:LYS:HG2	1.45	0.43
1:D:558:ARG:HA	1:D:558:ARG:HD2	1.82	0.43
1:D:726:LEU:O	1:D:730:LEU:HD23	2.19	0.43
1:B:594:VAL:HG23	1:B:598:PHE:HD2	1.84	0.43
1:C:436:HIS:HB3	1:C:437:PRO:HD3	2.01	0.43
1:D:269:ARG:NH2	1:D:270:ARG:HE	2.16	0.43
1:D:930:GLU:O	1:D:934:GLN:HG2	2.19	0.43
1:B:701:GLU:HG2	1:B:737:ILE:HB	2.02	0.42
1:C:504:LEU:HD23	1:C:1042:PRO:HG3	2.00	0.42
1:C:680:LEU:HD11	1:C:904:LEU:HD11	2.00	0.42
1:C:870:GLN:NE2	1:C:874:LEU:HB2	2.33	0.42
1:D:937:GLU:OE1	1:D:937:GLU:N	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:701:GLU:HG2	1:A:737:ILE:HB	2.01	0.42
1:B:778:ALA:HB2	1:C:812:ALA:HB1	2.01	0.42
1:C:464:ASN:ND2	1:C:490:LEU:O	2.52	0.42
1:C:597:ASN:OD1	1:C:830:ARG:HG2	2.19	0.42
1:D:1004:PRO:O	1:D:1008:LEU:HD13	2.18	0.42
1:A:1043:LYS:HG3	1:A:1046:GLU:HG2	2.02	0.42
1:B:1068:LEU:HD12	1:B:1068:LEU:H	1.82	0.42
1:C:376:CYS:SG	1:C:443:MET:HE3	2.59	0.42
1:C:1080:LEU:HG	1:C:1081:ASN:OD1	2.19	0.42
1:C:1116:MET:SD	1:C:1117:PRO:HD2	2.59	0.42
1:D:878:ALA:HB1	1:D:884:GLY:HA3	2.02	0.42
1:A:679:SER:HB2	1:A:909:PRO:HD2	2.02	0.42
1:B:574:HIS:CD2	1:B:582:VAL:HB	2.55	0.42
1:C:252:ASP:HA	1:C:351:VAL:HG21	2.02	0.42
1:C:278:ALA:HB3	1:C:279:PRO:HD3	2.02	0.42
1:C:574:HIS:HB3	1:C:580:THR:HA	2.01	0.42
1:D:35:LYS:CD	1:D:137:ARG:NH2	2.75	0.42
1:D:279:PRO:HG2	1:D:372:CYS:SG	2.59	0.42
1:D:313:LEU:O	1:D:321:TYR:N	2.49	0.42
1:B:590:ILE:HD11	1:B:837:TYR:CG	2.55	0.42
1:B:828:MET:HE2	1:B:832:PHE:HZ	1.83	0.42
1:C:200:GLY:HA2	2:C:2000:ATP:O2B	2.19	0.42
1:C:461:PHE:O	1:C:465:VAL:HG23	2.20	0.42
1:C:1053:GLU:CD	1:C:1055:GLY:H	2.27	0.42
1:A:1015:ASP:OD1	1:A:1015:ASP:N	2.49	0.42
1:D:558:ARG:HH21	1:D:760:ARG:NH2	2.17	0.42
1:C:1056:LYS:HD3	3:C:2001:ACO:C4A	2.50	0.42
1:B:590:ILE:HG21	1:B:834:TYR:HE1	1.85	0.42
1:B:731:VAL:HG11	1:B:763:PHE:CE1	2.55	0.42
1:C:374:ILE:HD11	1:C:436:HIS:CE1	2.55	0.42
1:C:804:MET:HA	1:C:804:MET:HE3	2.01	0.42
1:C:1080:LEU:HG	1:C:1081:ASN:H	1.84	0.42
1:D:269:ARG:HD2	1:D:387:PHE:CE2	2.54	0.42
1:C:53:PHE:CE2	1:C:80:ALA:HB2	2.54	0.42
1:C:509:VAL:HG21	1:C:1089:VAL:HG21	2.01	0.42
1:C:796:VAL:HG21	1:C:813:LEU:HG	2.01	0.42
1:D:194:LYS:O	1:D:234:PHE:N	2.52	0.42
1:C:916:ASP:O	1:C:919:GLN:HG3	2.20	0.41
1:C:971:LEU:O	1:C:972:PRO:C	2.63	0.41
1:D:173:PRO:HB3	1:D:232:ALA:HB1	2.01	0.41
1:D:544:ILE:O	1:D:548:GLU:N	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:722:TYR:CZ	1:D:726:LEU:HD11	2.56	0.41
1:D:804:MET:HE1	1:D:856:SER:C	2.44	0.41
1:D:948:LEU:HD22	1:D:964:ARG:HG3	2.02	0.41
1:D:1049:GLU:OE2	1:D:1057:THR:HG23	2.20	0.41
1:A:921:MET:HE3	1:A:921:MET:HB3	1.79	0.41
1:C:445:ARG:NH1	1:C:449:GLU:OE1	2.51	0.41
1:C:665:VAL:O	1:C:669:ASN:ND2	2.47	0.41
1:D:396:VAL:HA	1:D:414:GLN:HE22	1.85	0.41
1:D:565:LEU:HD22	1:D:796:VAL:HG21	2.01	0.41
1:C:151:ASP:HB3	1:C:154:GLU:OE1	2.20	0.41
1:C:496:ARG:CB	3:C:2001:ACO:O2A	2.69	0.41
1:C:508:MET:HE1	1:C:1044:ILE:HD11	2.02	0.41
1:C:564:LEU:HB2	1:C:793:VAL:HG22	2.03	0.41
1:D:647:ASN:OD1	1:D:647:ASN:N	2.54	0.41
1:D:1053:GLU:HG2	1:D:1054:ARG:N	2.33	0.41
1:D:1101:HIS:CD2	1:D:1168:LEU:HD11	2.55	0.41
1:A:560:HIS:HA	1:A:561:PRO:HD3	1.89	0.41
1:A:1056:LYS:NZ	1:A:1058:LEU:HD23	2.35	0.41
1:B:796:VAL:HG11	1:B:810:MET:HG3	2.02	0.41
1:C:675:ARG:HG3	1:C:701:GLU:OE2	2.19	0.41
1:D:500:LEU:HD23	1:D:500:LEU:HA	1.89	0.41
1:C:750:THR:HA	1:C:753:THR:HG22	2.02	0.41
1:D:464:ASN:ND2	1:D:489:GLN:HB2	2.35	0.41
1:D:586:ASP:OD2	1:D:845:TYR:OH	2.17	0.41
1:B:1075:GLN:OE1	1:B:1086:SER:HB3	2.21	0.41
1:A:853:THR:HG21	1:A:876:PHE:HB3	2.03	0.41
1:A:1030:LEU:HD23	1:A:1030:LEU:HA	1.88	0.41
1:B:706:TYR:HE1	1:B:710:VAL:HB	1.85	0.41
1:C:565:LEU:HD12	1:C:796:VAL:HB	2.02	0.41
1:C:746:LEU:HD22	1:C:862:TYR:HA	2.03	0.41
1:C:949:GLN:NE2	1:C:968:LEU:HD22	2.35	0.41
1:C:1122:ASP:HA	1:C:1164:LYS:NZ	2.36	0.41
1:D:970:ASP:OD1	1:D:970:ASP:N	2.49	0.41
1:D:1069:ASN:OD1	1:D:1070:ARG:N	2.49	0.41
1:C:550:PRO:HB2	1:C:736:HIS:NE2	2.36	0.41
1:D:98:HIS:ND1	1:D:101:ASP:HB2	2.35	0.41
1:D:522:PRO:HG3	1:D:1036:ARG:HA	2.03	0.41
1:D:579:ALA:O	1:D:581:ARG:HD2	2.20	0.41
1:D:665:VAL:O	1:D:668:GLU:HG2	2.21	0.41
1:D:724:MET:HE3	1:D:724:MET:HA	2.02	0.41
1:D:1091:ASP:OD1	1:D:1092:THR:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:PHE:O	1:A:557:VAL:HG23	2.21	0.41
1:A:721:GLN:HA	1:A:724:MET:HE3	2.02	0.41
1:A:853:THR:HB	1:A:879:HIS:CD2	2.56	0.41
1:A:934:GLN:O	1:A:934:GLN:HG2	2.21	0.41
1:B:613:ASP:OD1	1:B:614:VAL:N	2.52	0.41
1:B:656:ASP:OD1	1:B:657:ASN:N	2.53	0.41
3:C:2001:ACO:HH33	1:D:79:LYS:O	2.21	0.41
1:D:365:GLU:H	1:D:365:GLU:CD	2.28	0.41
1:D:725:GLY:O	1:D:728:GLU:HB2	2.20	0.41
1:D:799:ASP:HB3	1:D:835:SER:OG	2.21	0.41
1:C:584:THR:HG22	1:C:626:ARG:NE	2.36	0.41
1:C:910:SER:O	1:C:914:VAL:HG22	2.20	0.41
1:D:269:ARG:HH22	1:D:270:ARG:NE	2.18	0.41
1:A:889:GLU:HA	1:A:892:LYS:HZ1	1.84	0.40
1:B:550:PRO:HB3	1:B:699:VAL:HG22	2.03	0.40
1:B:1036:ARG:HG3	1:B:1037:LEU:HD22	2.03	0.40
1:C:248:GLN:HB3	1:C:260:LEU:HB2	2.02	0.40
1:D:447:LEU:HD23	1:D:447:LEU:HA	1.95	0.40
1:D:1048:PHE:CZ	1:D:1060:ILE:HB	2.56	0.40
1:B:709:ASP:OD2	1:B:712:ASP:N	2.54	0.40
1:C:267:ILE:HG22	1:C:274:VAL:HB	2.03	0.40
1:C:647:ASN:HD22	1:C:651:TYR:HA	1.85	0.40
1:C:776:SER:OG	1:C:862:TYR:OH	2.38	0.40
1:C:901:LEU:HD23	1:C:947:PHE:CE2	2.56	0.40
1:D:41:MET:HE2	1:D:114:VAL:HG12	2.02	0.40
1:B:677:PHE:CE1	1:B:705:SER:HB3	2.56	0.40
1:C:1021:LYS:HD2	1:C:1021:LYS:HA	1.75	0.40
1:B:810:MET:HE3	1:B:810:MET:HB2	1.88	0.40
1:D:249:ILE:HD13	1:D:249:ILE:HA	1.97	0.40
1:C:910:SER:HA	1:C:913:ILE:HD12	2.03	0.40
1:C:921:MET:HE2	1:C:921:MET:HB3	1.81	0.40
1:D:465:VAL:HG22	1:D:487:LEU:HD21	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	598/1178 (51%)	563 (94%)	35 (6%)	0	100	100
1	B	598/1178 (51%)	547 (92%)	51 (8%)	0	100	100
1	C	1144/1178 (97%)	1064 (93%)	79 (7%)	1 (0%)	48	75
1	D	1145/1178 (97%)	1081 (94%)	63 (6%)	1 (0%)	48	75
All	All	3485/4712 (74%)	3255 (93%)	228 (6%)	2 (0%)	49	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	517	PRO
1	C	972	PRO

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	493/968 (51%)	490 (99%)	3 (1%)	78	81
1	B	493/968 (51%)	492 (100%)	1 (0%)	87	88
1	C	942/968 (97%)	921 (98%)	21 (2%)	45	66
1	D	943/968 (97%)	912 (97%)	31 (3%)	33	59
All	All	2871/3872 (74%)	2815 (98%)	56 (2%)	48	68

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	870	GLN
1	A	874	LEU
1	A	875	HIS
1	B	923	GLN

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Mol	Chain	Res	Type
1	C	85	LEU
1	C	86	ILE
1	C	88	ARG
1	C	120	PHE
1	C	121	LEU
1	C	122	SER
1	C	124	ARG
1	C	202	ARG
1	C	204	MET
1	C	236	GLU
1	C	237	LYS
1	C	305	GLU
1	C	306	ASN
1	C	494	GLN
1	C	496	ARG
1	C	499	LYS
1	C	500	LEU
1	C	501	LEU
1	C	513	THR
1	C	969	LYS
1	C	1021	LYS
1	D	86	ILE
1	D	152	LYS
1	D	164	VAL
1	D	202	ARG
1	D	204	MET
1	D	306	ASN
1	D	309	THR
1	D	330	GLN
1	D	445	ARG
1	D	449	GLU
1	D	452	VAL
1	D	453	ARG
1	D	456	LYS
1	D	490	LEU
1	D	491	ARG
1	D	494	GLN
1	D	495	ASN
1	D	496	ARG
1	D	513	THR
1	D	518	VAL
1	D	820	THR

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Mol	Chain	Res	Type
1	D	1015	ASP
1	D	1019	HIS
1	D	1020	PHE
1	D	1021	LYS
1	D	1080	LEU
1	D	1084	LEU
1	D	1085	ARG
1	D	1093	GLN
1	D	1098	MET
1	D	1100	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	510	ASN
1	A	585	HIS
1	A	681	ASN
1	A	864	ASN
1	A	873	ASN
1	A	923	GLN
1	A	988	GLN
1	A	1073	GLN
1	B	506	HIS
1	B	510	ASN
1	B	574	HIS
1	B	721	GLN
1	B	864	ASN
1	B	875	HIS
1	B	923	GLN
1	B	1073	GLN
1	C	208	HIS
1	C	348	GLN
1	C	436	HIS
1	C	484	ASN
1	C	495	ASN
1	C	510	ASN
1	C	773	HIS
1	C	807	GLN
1	C	870	GLN
1	C	879	HIS
1	C	924	ASN
1	C	934	GLN

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Mol	Chain	Res	Type
1	D	244	HIS
1	D	248	GLN
1	D	259	HIS
1	D	268	GLN
1	D	364	GLN
1	D	470	GLN
1	D	489	GLN
1	D	494	GLN
1	D	510	ASN
1	D	640	GLN
1	D	653	ASN
1	D	721	GLN
1	D	864	ASN
1	D	870	GLN
1	D	924	ASN
1	D	1019	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ATP	D	2002	-	32,33,33	0.28	0	48,52,52	0.28	0
2	ATP	C	2000	-	32,33,33	0.56	0	48,52,52	0.54	0
3	ACO	C	2001	-	51,53,53	0.49	0	73,79,79	0.77	1 (1%)
3	ACO	D	2001	-	51,53,53	0.48	0	73,79,79	0.76	1 (1%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	D	2002	-	-	6/22/38/38	0/3/3/3
2	ATP	C	2000	-	-	8/22/38/38	0/3/3/3
3	ACO	C	2001	-	-	20/51/67/67	0/3/3/3
3	ACO	D	2001	-	-	20/51/67/67	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2001	ACO	P3B-O3B-C3B	-5.03	110.00	123.43
3	D	2001	ACO	P3B-O3B-C3B	-5.01	110.04	123.43

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2000	ATP	PB-O3B-PG-O3G
2	C	2000	ATP	C5'-O5'-PA-O1A
2	C	2000	ATP	C5'-O5'-PA-O2A
2	C	2000	ATP	C5'-O5'-PA-O3A
2	D	2002	ATP	C5'-O5'-PA-O1A
2	D	2002	ATP	C5'-O5'-PA-O2A
2	D	2002	ATP	C5'-O5'-PA-O3A
3	C	2001	ACO	CCP-O6A-P2A-O3A
3	C	2001	ACO	CCP-O6A-P2A-O4A
3	C	2001	ACO	CCP-O6A-P2A-O5A
3	C	2001	ACO	CDP-CBP-CCP-O6A
3	C	2001	ACO	CEP-CBP-CCP-O6A
3	C	2001	ACO	CAP-CBP-CCP-O6A

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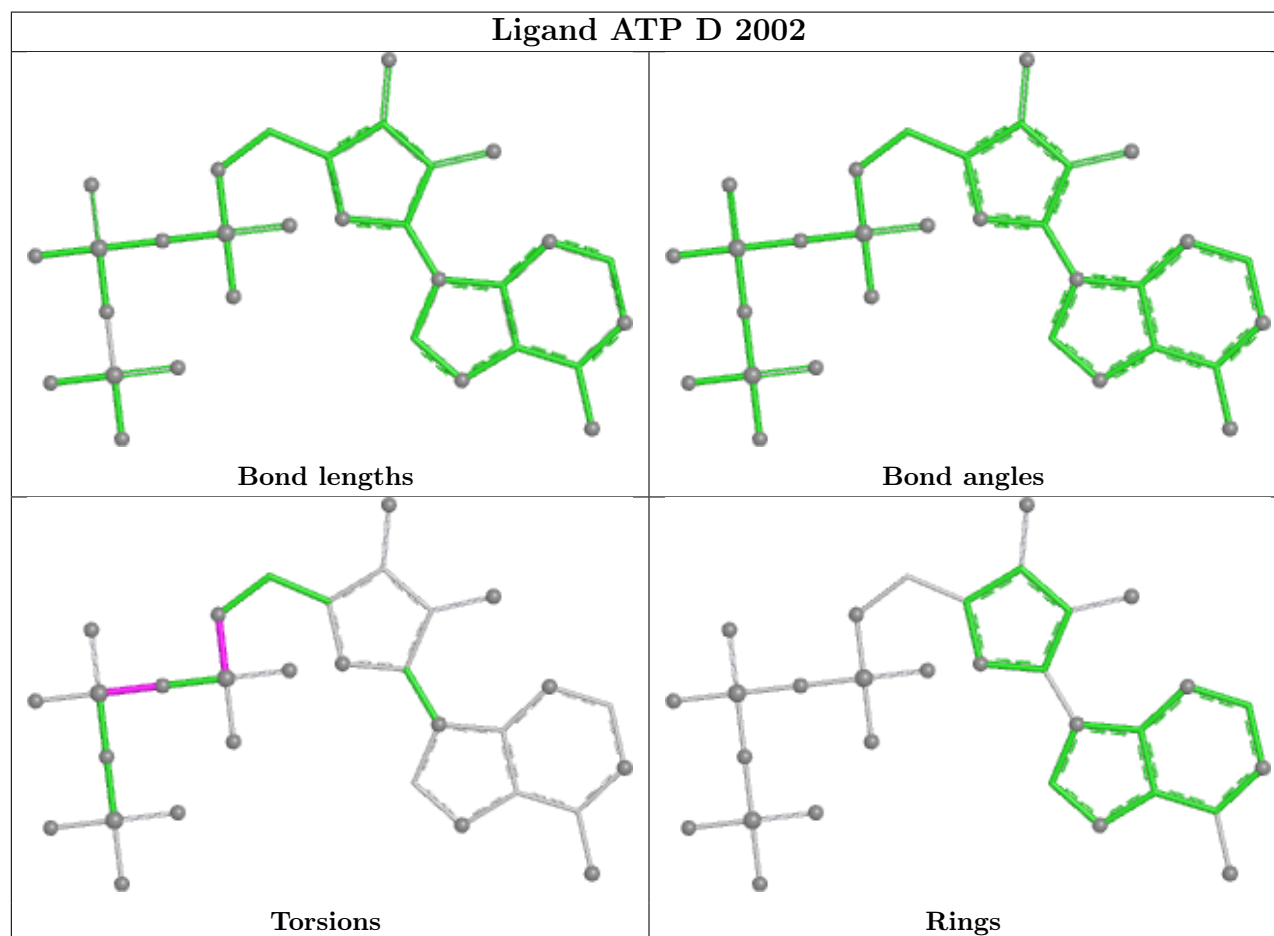
Mol	Chain	Res	Type	Atoms
3	C	2001	ACO	C9P-CAP-CBP-CCP
3	C	2001	ACO	C9P-CAP-CBP-CDP
3	C	2001	ACO	C9P-CAP-CBP-CEP
3	C	2001	ACO	N8P-C9P-CAP-OAP
3	C	2001	ACO	O-C-S1P-C2P
3	C	2001	ACO	CH3-C-S1P-C2P
3	D	2001	ACO	CCP-O6A-P2A-O3A
3	D	2001	ACO	CCP-O6A-P2A-O4A
3	D	2001	ACO	CCP-O6A-P2A-O5A
3	D	2001	ACO	CDP-CBP-CCP-O6A
3	D	2001	ACO	CEP-CBP-CCP-O6A
3	D	2001	ACO	CAP-CBP-CCP-O6A
3	D	2001	ACO	C9P-CAP-CBP-CCP
3	D	2001	ACO	C9P-CAP-CBP-CDP
3	D	2001	ACO	C9P-CAP-CBP-CEP
3	D	2001	ACO	N8P-C9P-CAP-OAP
3	D	2001	ACO	O-C-S1P-C2P
3	D	2001	ACO	CH3-C-S1P-C2P
3	C	2001	ACO	OAP-CAP-CBP-CDP
3	C	2001	ACO	OAP-CAP-CBP-CEP
3	D	2001	ACO	OAP-CAP-CBP-CDP
3	D	2001	ACO	OAP-CAP-CBP-CEP
3	C	2001	ACO	O9P-C9P-CAP-OAP
3	D	2001	ACO	O9P-C9P-CAP-OAP
3	C	2001	ACO	C5B-O5B-P1A-O1A
3	C	2001	ACO	OAP-CAP-CBP-CCP
3	D	2001	ACO	C5B-O5B-P1A-O1A
3	D	2001	ACO	OAP-CAP-CBP-CCP
2	C	2000	ATP	PB-O3B-PG-O1G
2	C	2000	ATP	PB-O3A-PA-O2A
2	D	2002	ATP	PA-O3A-PB-O3B
3	C	2001	ACO	C3B-O3B-P3B-O7A
3	D	2001	ACO	C3B-O3B-P3B-O7A
3	C	2001	ACO	C5P-C6P-C7P-N8P
3	D	2001	ACO	C5P-C6P-C7P-N8P
2	D	2002	ATP	PA-O3A-PB-O1B
3	C	2001	ACO	C2P-C3P-N4P-C5P
3	D	2001	ACO	C2P-C3P-N4P-C5P
2	C	2000	ATP	PG-O3B-PB-O2B
2	C	2000	ATP	PA-O3A-PB-O2B
2	D	2002	ATP	PA-O3A-PB-O2B

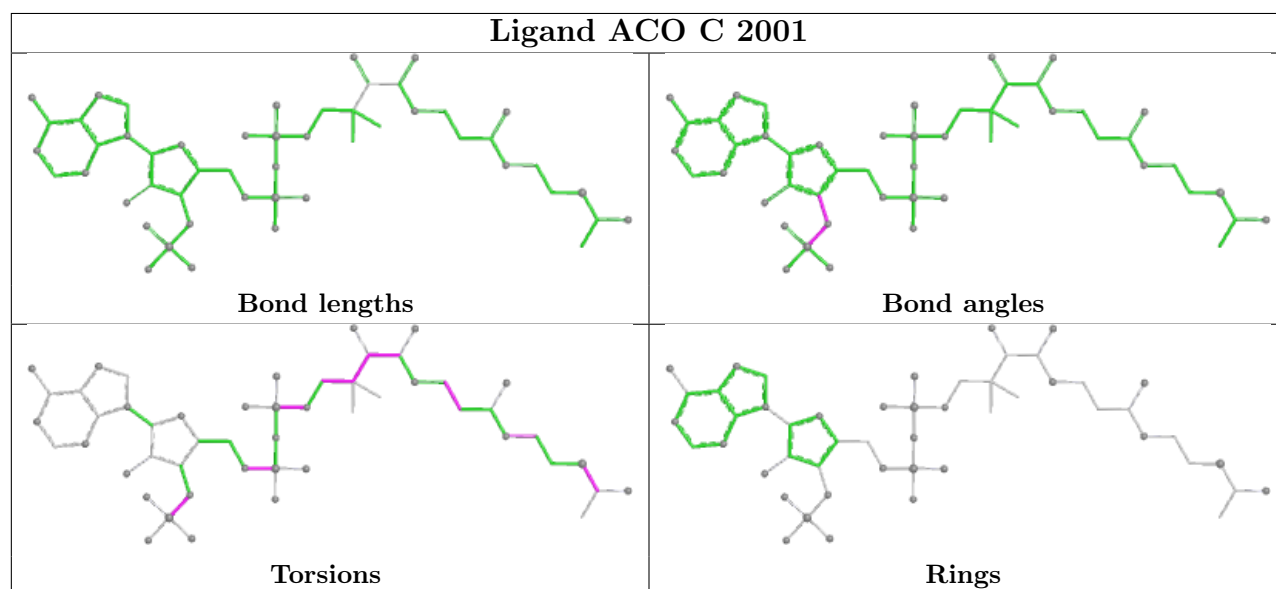
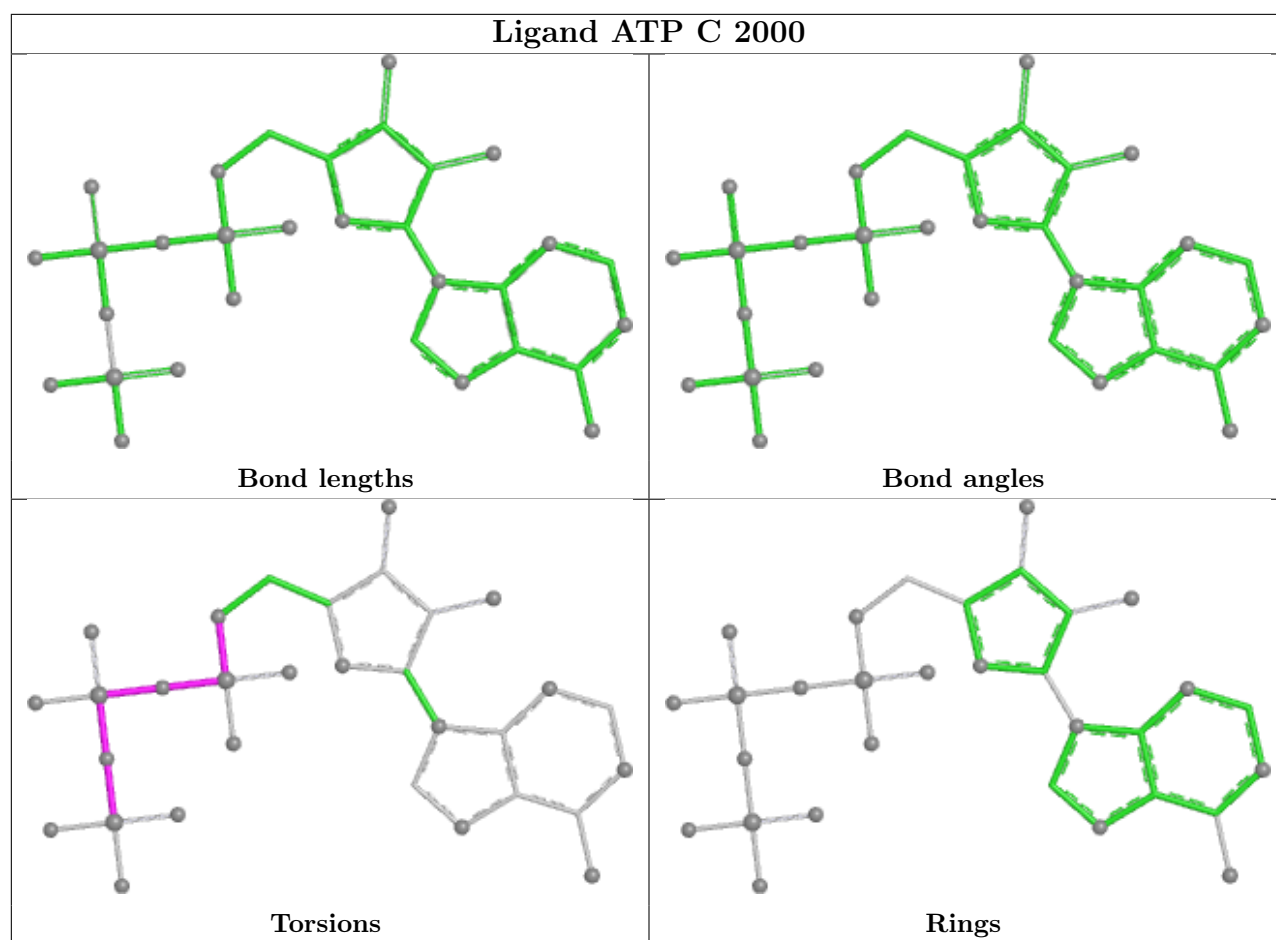
There are no ring outliers.

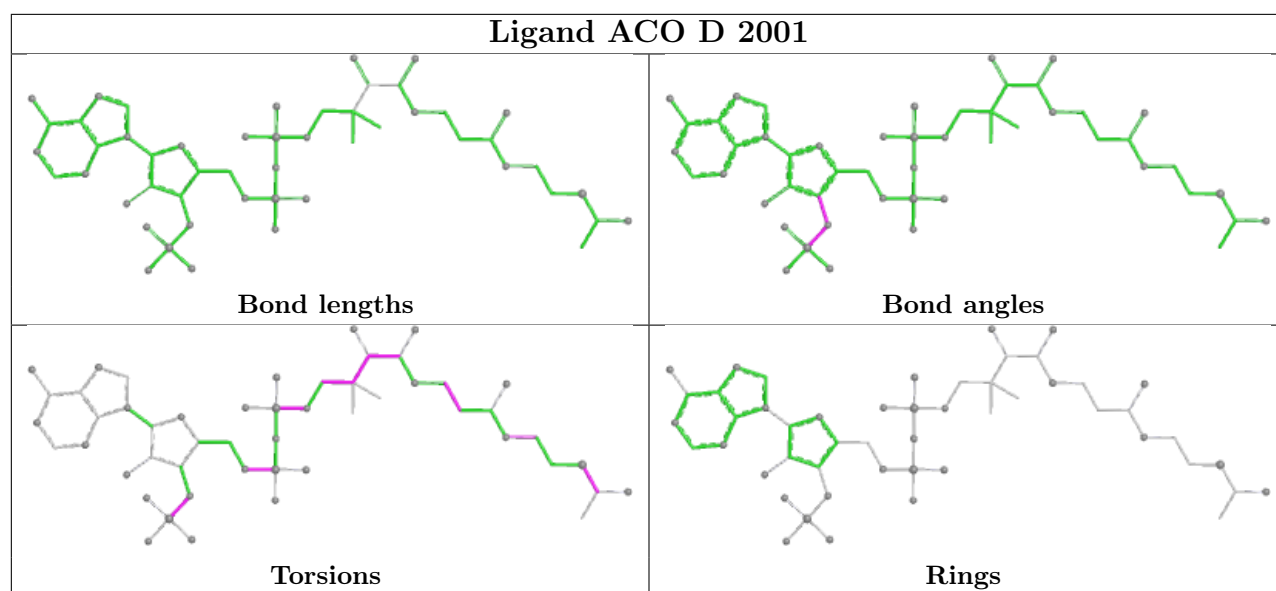
3 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2000	ATP	8	0
3	C	2001	ACO	13	0
3	D	2001	ACO	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

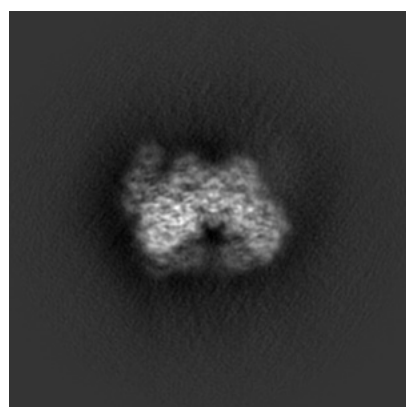
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32780. These allow visual inspection of the internal detail of the map and identification of artifacts.

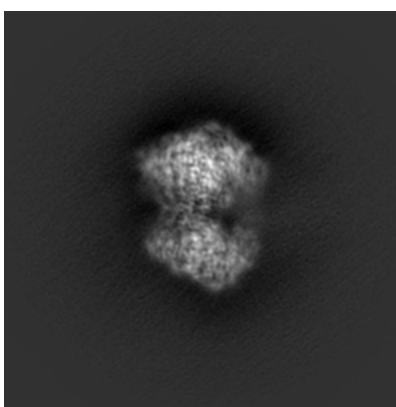
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

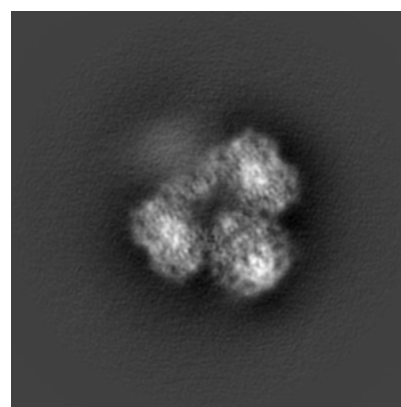
6.1.1 Primary map



X



Y

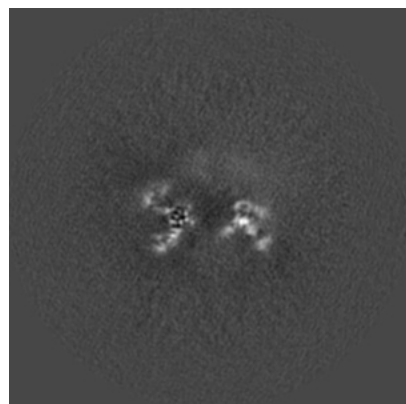


Z

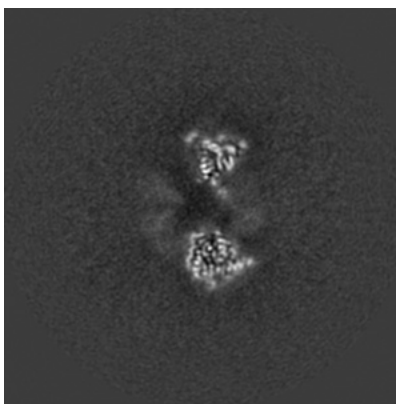
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

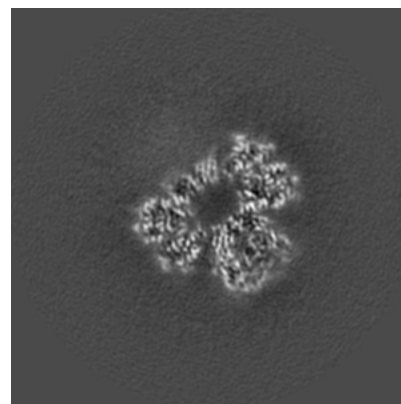
6.2.1 Primary map



X Index: 156



Y Index: 156

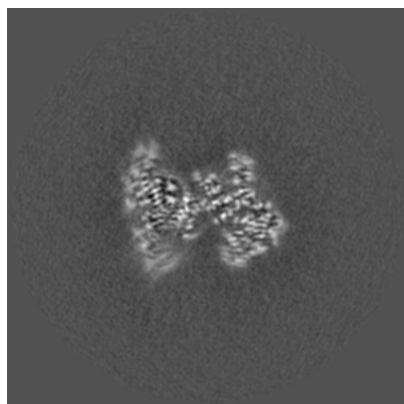


Z Index: 156

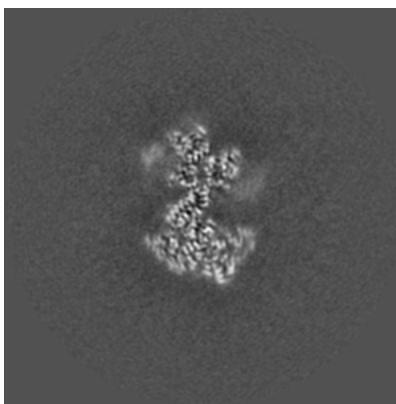
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

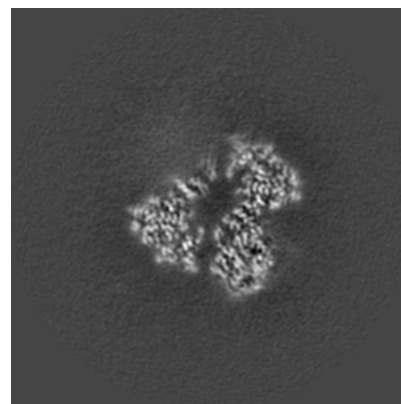
6.3.1 Primary map



X Index: 193



Y Index: 129



Z Index: 160

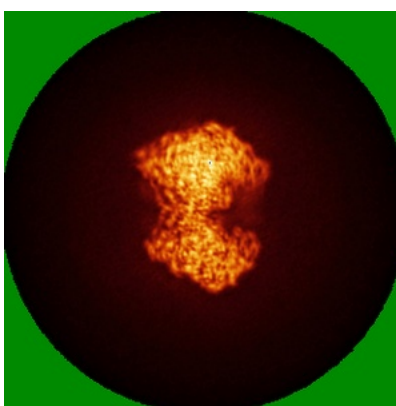
The images above show the largest variance slices of the map in three orthogonal directions.

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

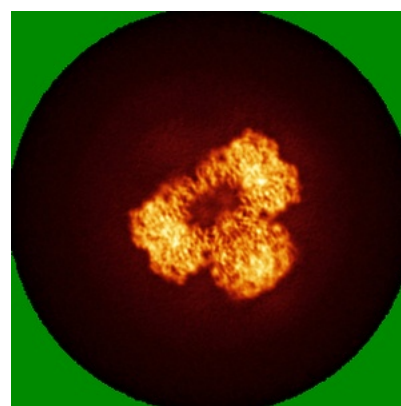
6.4.1 Primary map



X



Y

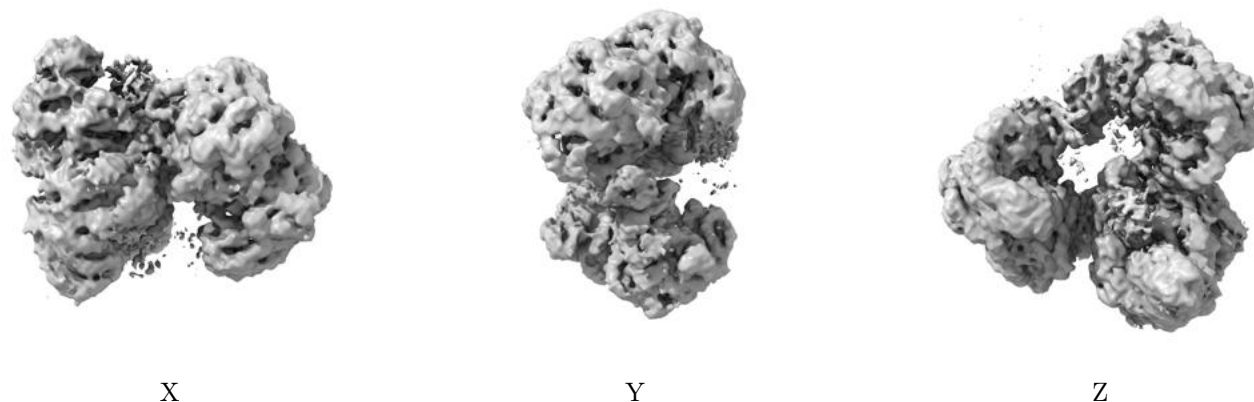


Z

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 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

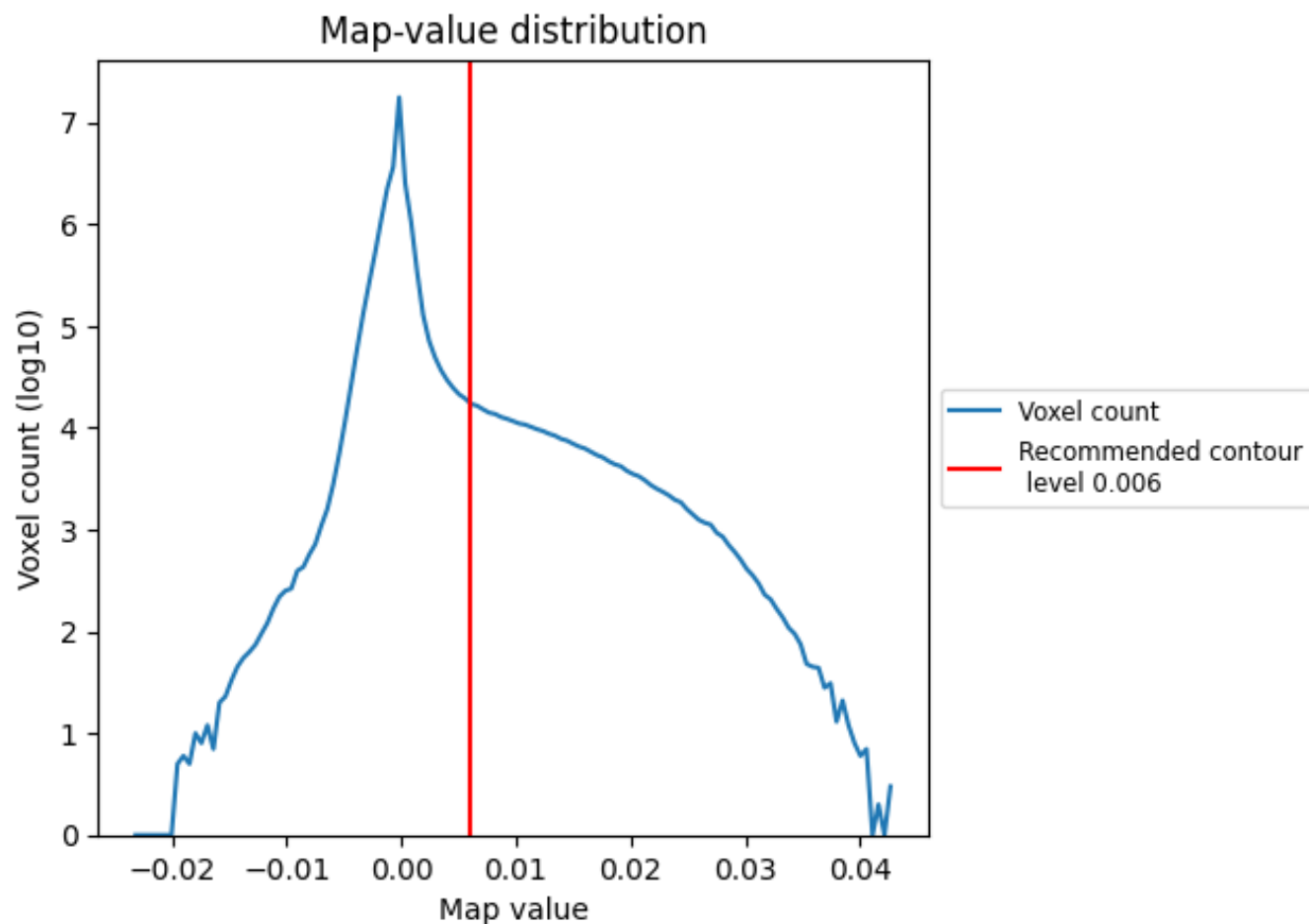
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

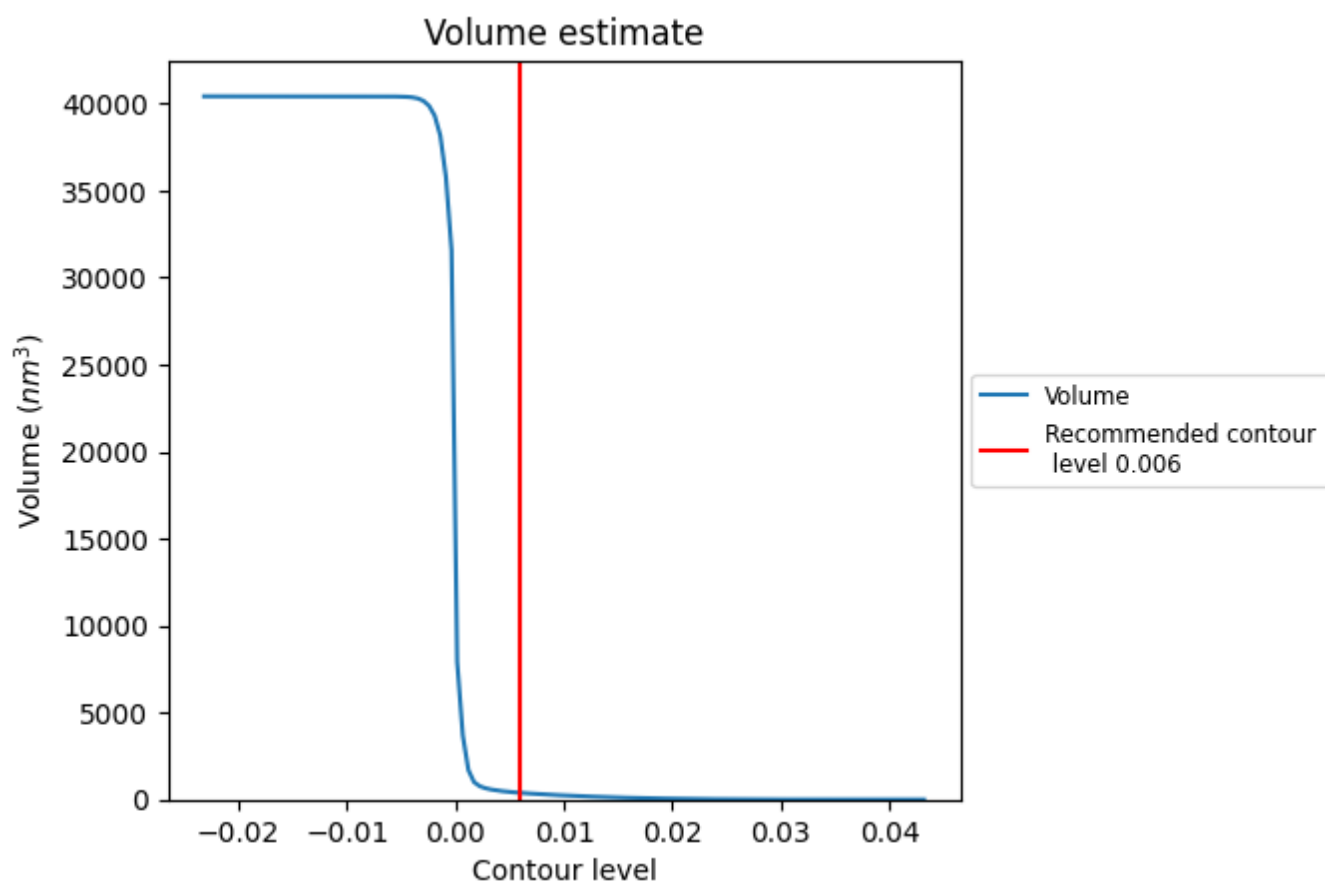
This section contains the results of statistical analysis of the map.

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.

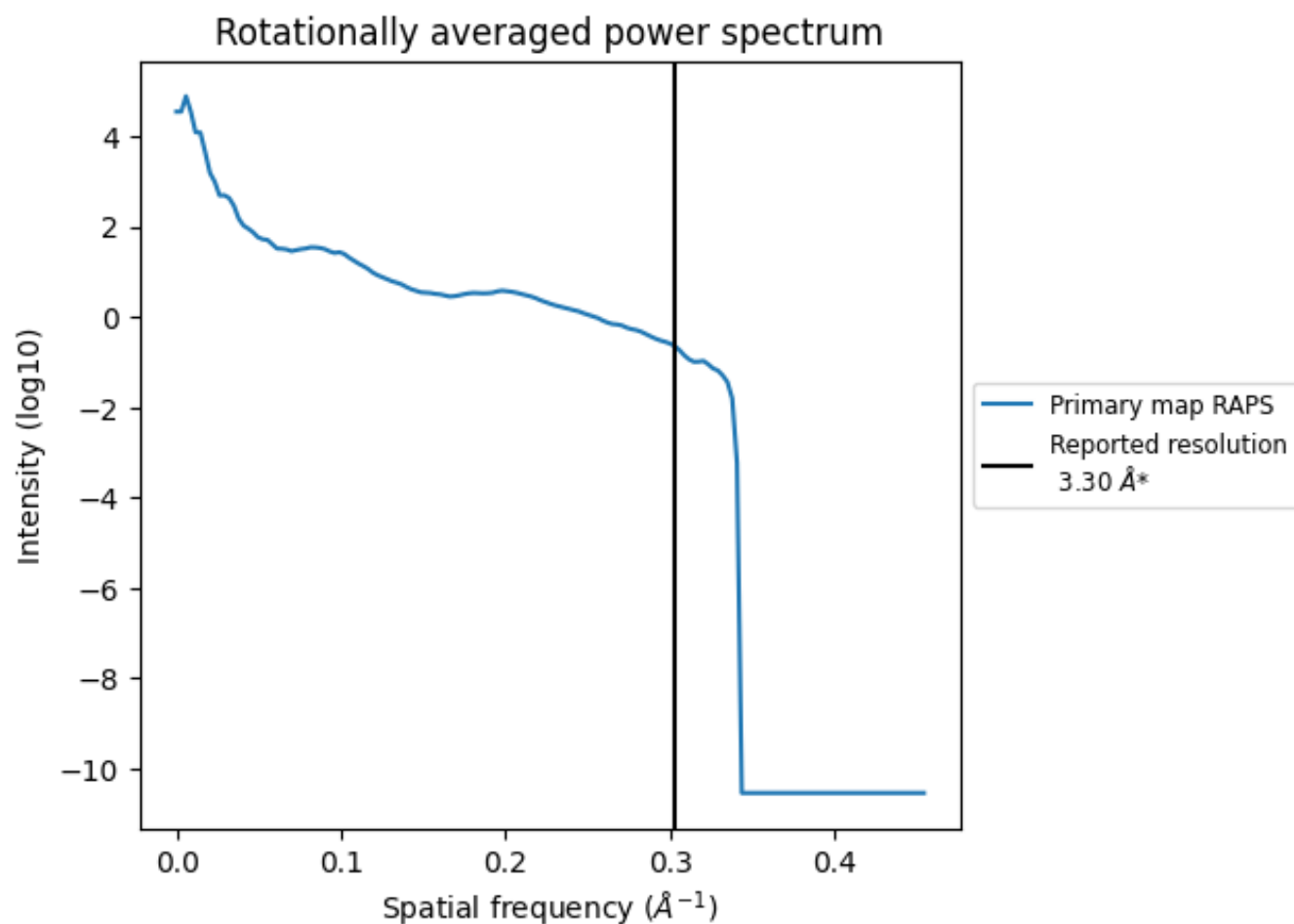
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 386 nm³; this corresponds to an approximate mass of 348 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

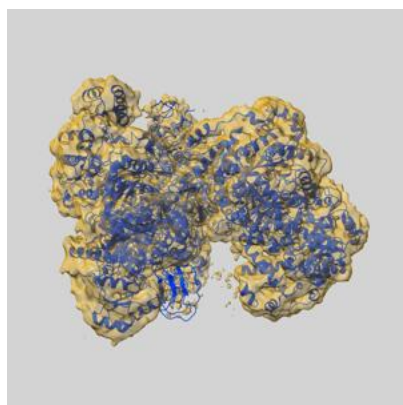
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

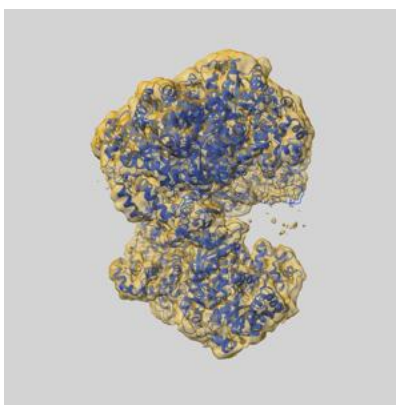
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32780 and PDB model 7WTE. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

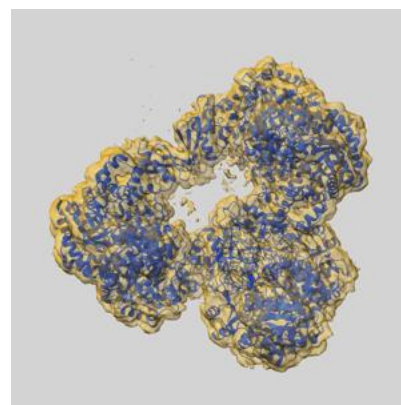
9.1 Map-model overlay [i](#)



X



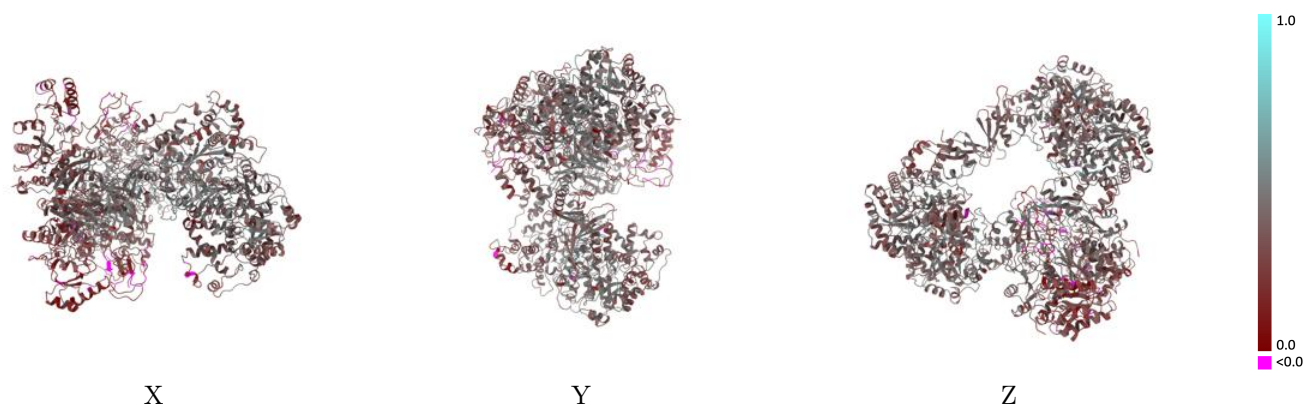
Y



Z

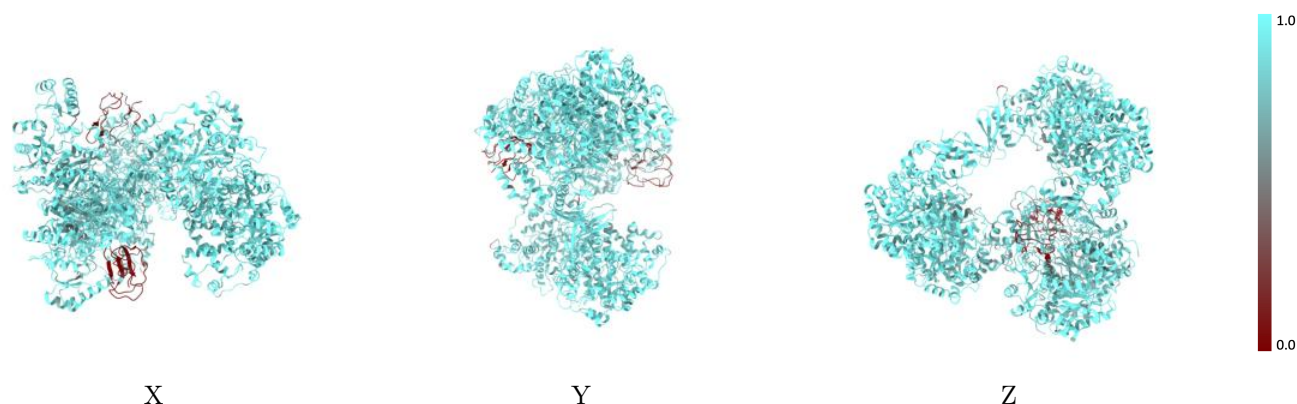
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



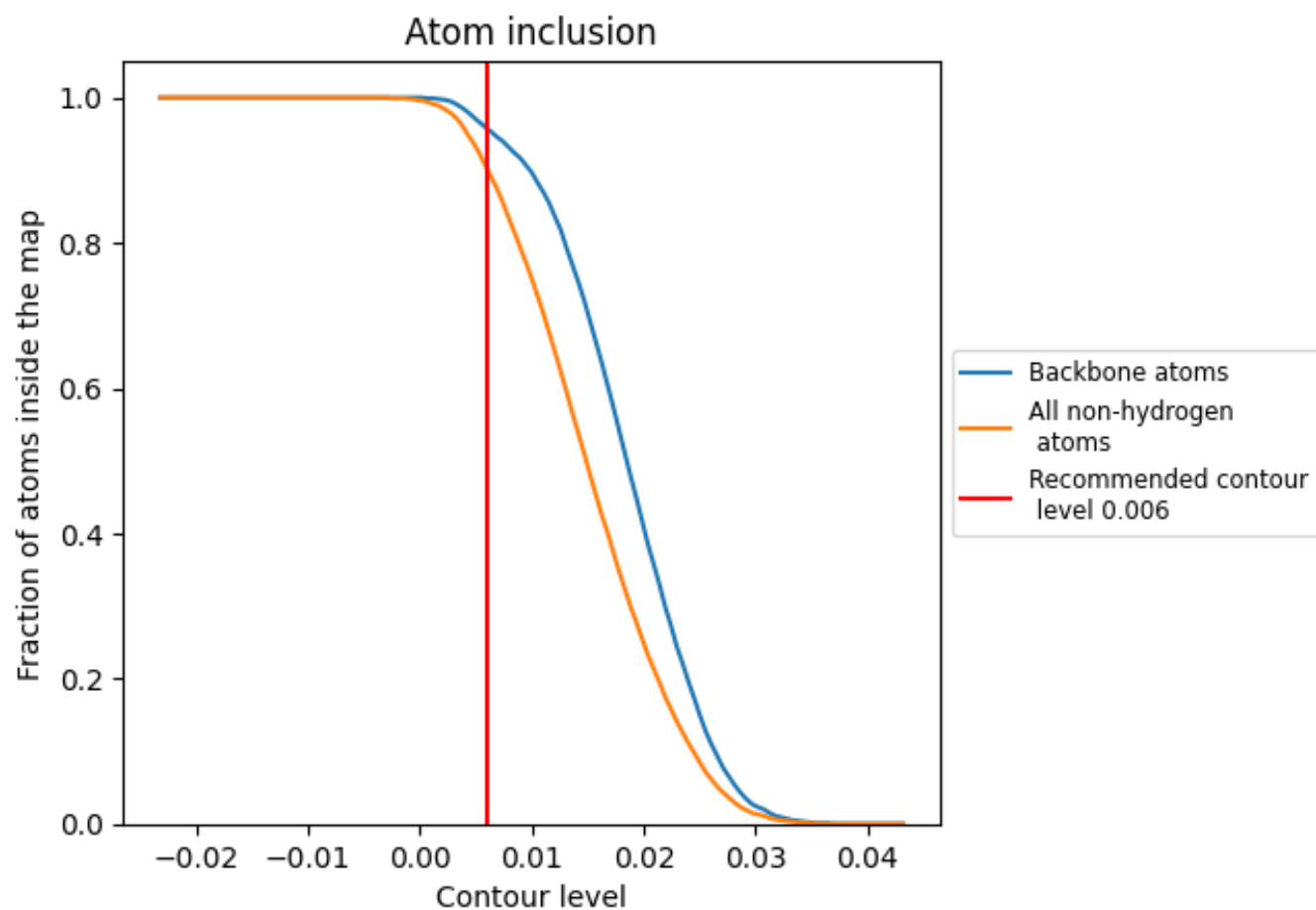
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.006).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 90% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9030	0.3600
A	0.9530	0.3810
B	0.9540	0.3920
C	0.8670	0.3370
D	0.8880	0.3550

