



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:00 AM UTC

PDB ID : 1L9U / pdb_0000119u
Title : THERMUS AQUATICUS RNA POLYMERASE HOLOENZYME AT 4 Å
RESOLUTION
Authors : Murakami, K.S.; Masuda, S.; Darst, S.A.
Deposited on : 2002-03-26
Resolution : 4.00 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

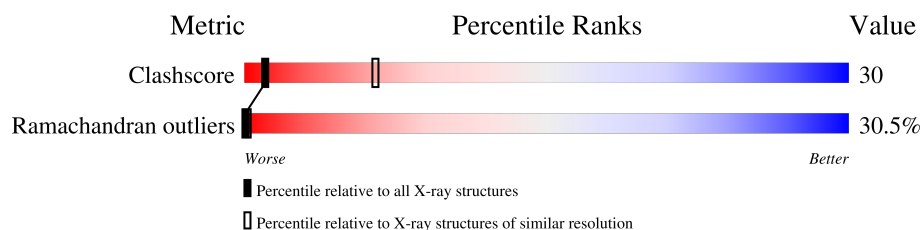
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	314	40% 29% . 29%
1	B	314	42% 25% . 30%
1	J	314	40% 29% . 29%
1	K	314	42% 25% . 30%
2	C	1118	51% 39% 6% .
2	L	1118	51% 39% 7% .
3	D	1524	35% 37% 6% 22%
3	M	1524	35% 37% 6% 22%
4	E	99	43% 44% 5% 7%

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Mol	Chain	Length	Quality of chain
4	N	99	43% 45% • 7%
5	H	332	73% 22% • •
5	Q	332	73% 22% • •

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18756 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 RNA POLYMERASE, ALPHA SUBUNIT.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	0	0	0
			672	448	224			
1	B	220	Total	C	N	0	0	0
			660	440	220			
1	J	224	Total	C	N	0	0	0
			672	448	224			
1	K	220	Total	C	N	0	0	0
			660	440	220			

- Molecule 2 is a protein called RNA POLYMERASE, BETA SUBUNIT.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	1084	Total	C	N	0	0	0
			3252	2168	1084			
2	L	1084	Total	C	N	0	0	0
			3252	2168	1084			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	GLU	deletion	UNP Q9KWU7
L	?	-	GLU	deletion	UNP Q9KWU7

- Molecule 3 is a protein called RNA POLYMERASE, BETA-PRIME SUBUNIT.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	D	1183	Total	C	N	0	0	0
			3549	2366	1183			
3	M	1183	Total	C	N	0	0	0
			3549	2366	1183			

- Molecule 4 is a protein called RNA POLYMERASE, OMEGA SUBUNIT.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	E	92	Total	C	N	0	0	0
			276	184	92			
4	N	92	Total	C	N	0	0	0
			276	184	92			

- Molecule 5 is a protein called SIGMA FACTOR SIGA.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
5	H	322	Total	C	N	0	0	0
			966	644	322			
5	Q	322	Total	C	N	0	0	0
			966	644	322			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	?	-	ILE	deletion	UNP Q9EZJ8
H	?	-	GLN	deletion	UNP Q9EZJ8
H	?	-	LYS	deletion	UNP Q9EZJ8
H	?	-	ILE	deletion	UNP Q9EZJ8
H	?	-	PRO	deletion	UNP Q9EZJ8
H	?	-	GLY	deletion	UNP Q9EZJ8
H	?	-	LEU	deletion	UNP Q9EZJ8
H	?	-	LYS	deletion	UNP Q9EZJ8
H	?	-	GLU	deletion	UNP Q9EZJ8
H	?	-	LYS	deletion	UNP Q9EZJ8
H	?	-	PRO	deletion	UNP Q9EZJ8
H	?	-	ASP	deletion	UNP Q9EZJ8
H	?	-	PRO	deletion	UNP Q9EZJ8
H	?	-	LYS	deletion	UNP Q9EZJ8
H	?	-	THR	deletion	UNP Q9EZJ8
Q	?	-	ILE	deletion	UNP Q9EZJ8
Q	?	-	GLN	deletion	UNP Q9EZJ8
Q	?	-	LYS	deletion	UNP Q9EZJ8
Q	?	-	ILE	deletion	UNP Q9EZJ8
Q	?	-	PRO	deletion	UNP Q9EZJ8
Q	?	-	GLY	deletion	UNP Q9EZJ8
Q	?	-	LEU	deletion	UNP Q9EZJ8
Q	?	-	LYS	deletion	UNP Q9EZJ8
Q	?	-	GLU	deletion	UNP Q9EZJ8
Q	?	-	LYS	deletion	UNP Q9EZJ8
Q	?	-	PRO	deletion	UNP Q9EZJ8
Q	?	-	ASP	deletion	UNP Q9EZJ8

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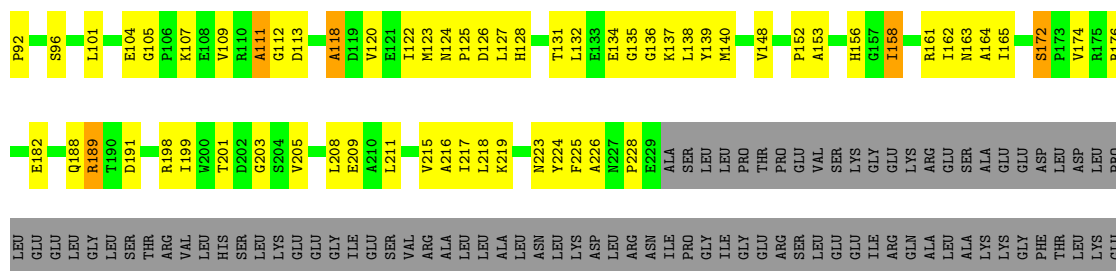
Chain	Residue	Modelled	Actual	Comment	Reference
Q	?	-	PRO	deletion	UNP Q9EZJ8
Q	?	-	LYS	deletion	UNP Q9EZJ8
Q	?	-	THR	deletion	UNP Q9EZJ8

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

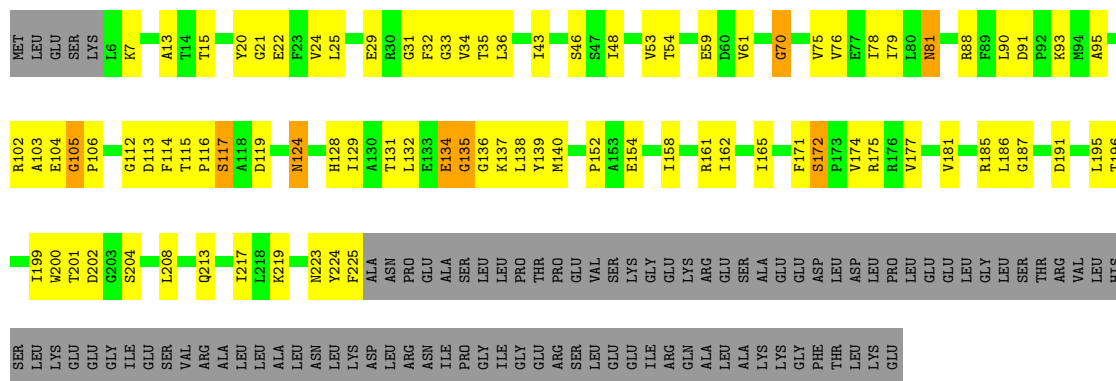
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Mg	0	0
			1	1		
6	M	1	Total	Mg	0	0
			1	1		

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

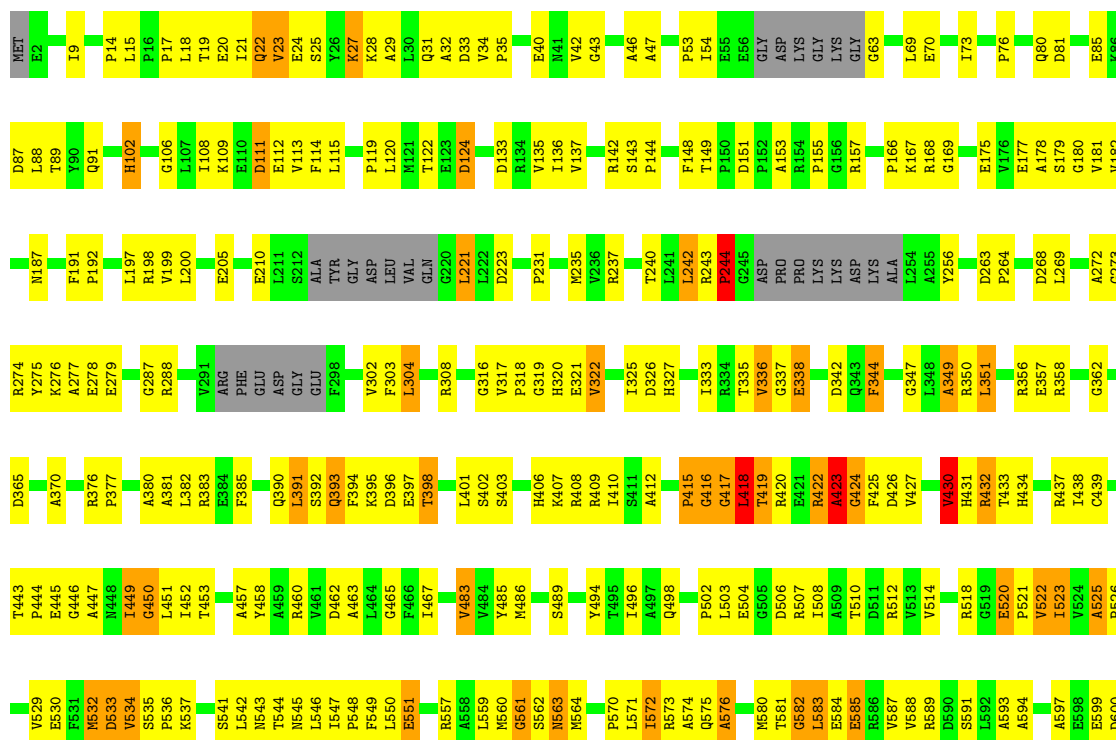
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	2	Total	Zn	0	0
			2	2		
7	M	2	Total	Zn	0	0
			2	2		

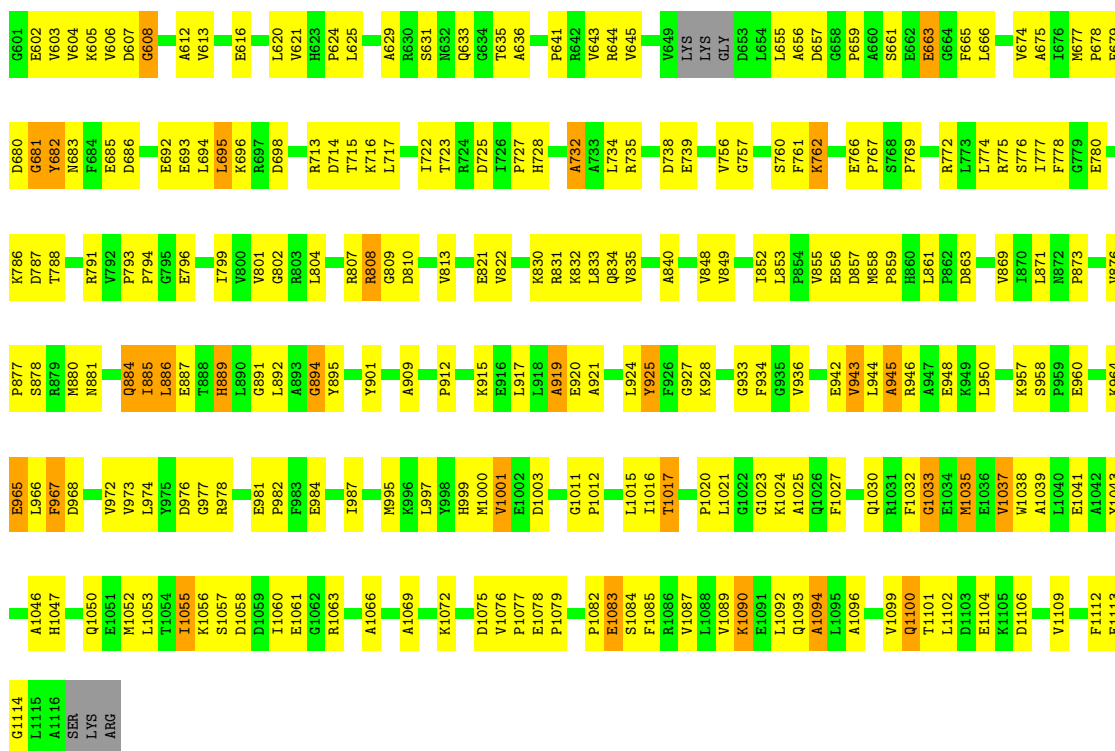


• Molecule 1: RNA POLYMERASE, ALPHA SUBUNIT



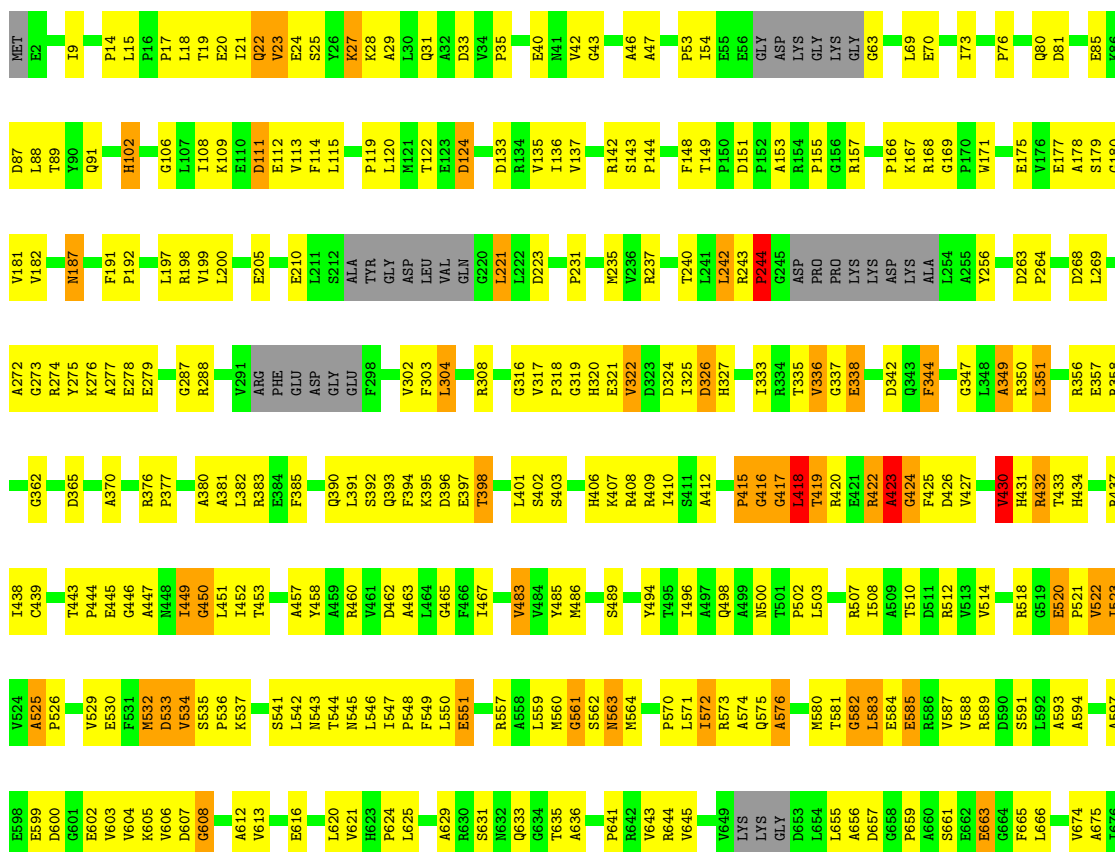
• Molecule 2: RNA POLYMERASE, BETA SUBUNIT





• Molecule 2: RNA POLYMERASE, BETA SUBUNIT

Chain L: 51% 39% 7% •



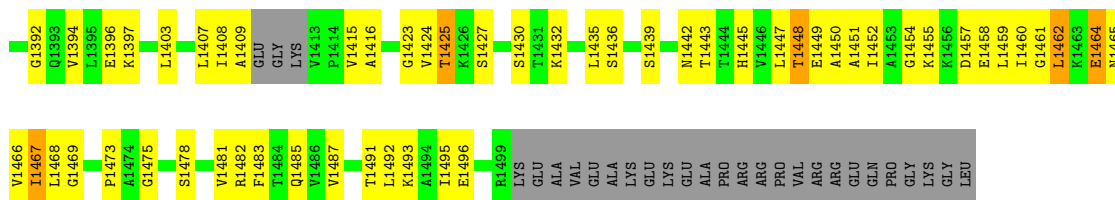
G1469	E1396	HIS	F1173	G1081	T999	L930	P846	A766	K684
P1473	K1397	THR	L1174	T1084	T1000	L931	D847	L770	D685
A1474	L1403	GLY	K1175	A1085	E1001	D932	E848	S771	E686
G1475	L1407	VAL	A1177	L1086	A1006	L934	A849		R801
S1478	L1408	ALA	A1178	L1087	V1007	K935	H855	S774	S602
	L1409	VAL	A1179	T1088	F1008	Y936	G856	G775	L603
V1481	A1409	GLY	A1180	T1089	K1009	Y937	G857	E776	T604
R1482	GLU	THR	V1188	D1090	F1010	G938	L857	G775	A690
F1483	GLY	ASP	G1092	S1091	F1011	F939	L858	S782	L607
T1484	LYS	ILE	R1189	G1093	E1012	T940	D862	R782	S608
Q1485	P1414	THR	S1190	V1093	P1016	L941	V663	R783	G609
V1486	V1414	GLN	P1191	L1094		S942	V664	D784	V694
V1487	V1415	GLY	L1192	T1095	P1019	T943	T865	I785	G609
	A1416	LEU	T1193	R1096	T944	T944	R872		L619
			Q1194	K1097	L1020	S945	T793	I792	G620
	G1423	A1343	C1195	L1098	T1021	G946	Q794		K821
	V1424	V1344	Q1195	V1099	Y1022	T947	V795	Q794	R622
	T1425	R1345	T1196	D1100	M1023	T948	R796	V795	V623
	K1426	E1261	R1197	V1101	A1024	T949	S876	K797	D624
	S1427	F1263	G1198	A1102		G950	E798	E798	L711
			V1200	H1103		G950	R879	E798	G712
			C1201	E1104	A1028	D952	R879	K799	S626
	S1430	E1351	Q1202	I1105	G1030	D953	F882		V630
	K1431	K1352	A1270	V1106	N1031	A954	A883	G803	A715
	V1432	V1353	A1271	R1107	P1032	R884	A807		V632
	L1435	K1354	K1271	Q1108	Q1033	V956	T808		V633
	A1436	Q1355	A1272	E1109	Q1034	P957	P809		
	L1437	Q1359	I1273	A1110	I1035	E958	E810		L637
	A1438	G1360	I1274	T1115	G1040	L964	E810		K638
	V1439	V1361	S1275	N1116	R1042	E965	E811		L639
	L1440	H1364	E1276			E966			H640
	A1441	H1365	I1277						Q641
	T1443	K1366	P1214						G843
	Q1441	K1367	V1215						S725
	L1442	L1368	S1216						L644
	A1443	E1369	E1219	Q1124	M1045				P645
	V1444	I1370	A1220	V1128	K1046				K646
	L1445	T1288	V1221	T1129	K1047				R647
	A1446	R1289	G1222	R1130	P1048				M648
	E1449	L1290	V1223	T1131	S1049				A649
	A1450	S1291	V1224	L1132	F1053				L650
	A1451	Q1374	A1225	R1133	E1054				
	L1452	L1375	A1226	L1134	P1055				P655
	A1453	K1376	E1227	K1135	V1086				
	G1454	K1377	S1228	K1136					E662
	K1455	V1381	L1229	E1141	S1059				A665
	V1456	P1306	G1230	F1061	S1060				F666
	D1457	E1231	P1232	G1143	R1062				A667
	E1458	V1313	T1237	G1146					P668
	L1459	G1385	T1238						
	T1460	K1314	T1239						A672
	G1461	D1386	Q1235						A673
	L1462	S1387	L1236						
	K1463	R1388	L1237						
	L1389	L1317	V1318						
	G1392	D1318	T1237						
	Q1393	V1319	T1237						
	V1466	E1320	R1239						
	L1467	A1321	T1240						
	T1468	L1395	THR						

• Molecule 3: RNA POLYMERASE, BETA-PRIME SUBUNIT

Chain M: 35% 37% 6% 22%

R86	R87	Y88	R89	G90	G91	H92	I93	E94	T97	P98	A99	A100	H101	I102	W103	F104	V108	P109	S110	G113	T114	L115	D117	L118	S119	A120	T121	E122	V126	L127	Y128	F129	R130	K131	Y132	I133	V134	L135	D136	P137	K138	G139	A140	V141	L142	D143	G144	V145	P146	V147	E148	K149	R150	Q151
MET	LYS	K3	E4	V5	R6	K7	I10	A11	L12	A13	S14	I18	W21	S22	V23	Q24	E25	V26	E27	K28	T31	I32	N33	R34	S35	T36	L37	K38	R41	D42	G43	L44	F45	E47	P52	I53	P56	C58	K64	R67	F68	V72	R82	S83	I84	Q151								

Y1318	T1237	L1072	L1073	W996	D847	L770	D685	G595	P521	I1E	SER	HIS	LEU	ARG	L152
V1319	M1238	S1073	S1073	T997	E848	L770	E686	G601	P522	D453	ILE	THR	ARG	VAL	L153
A1320	R1239	K1079	K1079	E998	A849	S771	W688	R602	P523	A454	LEU	THR	GLU	ASP	T154
A1321	T1240	H1172	H1172	T999	A850	S774	W689	R603	P524	R455	VAL	THR	GLU	TYR	D155
G1322	PHE	G1080	G1080	E1000	W853	G775	A690	T604	P525	W456	VAL	PHE	LEU	ARG	E156
Q1323	HIS	G1081	G1081	E1001	A854	G776	A691	D605	P526	G457	LYS	THR	GLU	ARG	E157
P1324	THR	G1084	G1084	E1006	H855	E776	L691	D606	P527		ALA	TRP	VAL	LYS	TYR
	GLY	T1084	T1084	A1006	G856		E692	L606	Q529	A460	ARG	THR	VAL	GLY	ARG
G1328	GLY	A1085	A1085	V1007	G857	S782	E693	L607	Q530	I461	VAL	THR	ALA	ARG	GLU
A1329	VAL	L1086	L1086	F1008	L857	R783	W694	S608	W530	Q462	THR	GLU	ARG	ALA	GLU
I1330	ALA	R1087	R1087	G938	L858	D784	L695	G609	P531	E463	PRO	GLU	ALA	ARG	LEU
D1331	VAL	T1088	T1088	N1010	D862	I785	H696		Q532	I464	PHE	LYS	PHE	LEU	ARG
P1332	GLY	A1089	A1089	N1010	W863		G697	L619	Q533	L465	ASP	THR	LEU	ARG	GLY
H1333	THR	D1090	D1090	E1012	V864	I792	W698	G620	Q534	K466	ASP	THR	PRO	LYS	LYS
Q1334	ASP	S1091	S1091	E1016	T865	I793	W698	G621	Q535	K467	ASP	THR	ALA	ARG	GLN
	ILE	R1189	R1189	P1016	T866	Q794	L702	R622	Q536	E467	VAL	VAL	PRO	GLU	GLU
K1339	THR	L1093	L1093	P1019	R872	W795	R710	W623	Q537	L468	VAL	ALA	GLU	THR	THR
G1340	GLN	L1094	L1094	P1020	T875	R796	R711	W624	Q538	D469	VAL	ALA	GLU	GLY	GLY
P1341	GLY	T1095	T1095	L1020	T876	K797	L712	W625	Q539	L470	PRO	ALA	GLU	VAL	PRO
E1342	LEU	R1096	R1096	Y1021	S877	E798	G713	W626	Q540	E471	THR	PRO	LEU	VAL	LEU
A1343	P1257	C1194	C1194	Y1022	P877	K799	W713		Q541	K472	THR	PRO	VAL	GLU	PRO
R1258	P1258	Q1195	Q1195	M1023	R878	E799	Q714	W630	Q542	L473	GLY	ASN	VAL	LYS	PRO
E1344	V1259	L1098	L1098	A1024	R879	G803	A715	W631	Q543	R474	ARG	ILE	VAL	GLY	ALA
E1345	T1196	V1099	V1099		R879	G803	A715	W632	Q544	R475	VAL	VAL	GLY	GLY	GLY
R1346	R1197	D1100	D1100		R879	G803	A715	W633	Q545	R476	VAL	VAL	GLY	VAL	VAL
Y1347	E1261	L1101	L1101	A1028	F882	A807	Q716	W633	Q546	L477	ALA	PRO	GLY	ASP	ASP
	E1262	A1102	A1102	R1029	A883	T808	P718	W633	Q547	L478	PRO	GLU	ILE	ARG	ALA
D1350	F1263	H1103	H1103	G1030	R884	P809	W719	L637	Q548	E479	GLY	GLU	VAL	PRO	LEU
E1351		L1104	L1104	N1031	R885	E810	L720	K638	Q549	E480	ASP	ALA	GLU	GLY	VAL
P1268	P1268	E1104	E1104	P1032	R886	E811	W721	L639	Q550	M481	VAL	LYS	GLU	GLY	VAL
K1269	K1269	L1105	L1105	P1033	W886	E811	W721	L640	Q551	K482	VAL	VAL	GLY	VAL	ASP
Q1353	P1270	V1106	V1106	Q1033	G887		G723	W641	Q552	R483	ALA	GLN	GLY	GLY	GLY
K1354	A1270	L1107	L1107	G1034	F889	A815	Q724	W642	Q553	P484	ASP	ALA	PRO	GLU	GLU
V1355	E1271	R1108	R1108	I1035	D892	Y816	Q724	W643	Q554	S485	GLY	GLY	ALA	GLU	GLU
	K1272	E1109	E1109	R1036	E893	E817	S725	Q643	Q555	R486	GLY	GLY	ALA	LEU	VAL
V1273	V1273	A1110	A1110	Q1037	R894	R818	W726	L644	Q556	A487	LYS	LYS	GLU	SER	VAL
K1360	I1274	D1111	D1111			G819	Q727	W645	Q557	R488	VAL	ILE	GLY	GLY	LYS
V1361	M1211	C1112	C1112	G1040	Q897	E820	P730	W646	Q558	R489	LYS	LYS	GLY	PRO	GLY
	S1275	G1113	G1113	M1041	E898	W821	L731	W647	Q559	A490	ALA	ALA	GLY	TYR	GLN
E1276	E1276	T1114	T1114	R1042	R899	A822	W732	W648	Q560	K491	SER	GLY	LEU	LEU	GLU
I1277	I1277	L1115	L1115		Q901	A825	C733	W649	Q561	A492	ILE	ILE	PHE	LEU	LEU
	P1214	M1116	M1116	M1045	N902	P826	E734	L650	Q562	R493	TYR	GLY	ARG	ALA	ALA
V1280	V1280	Q1124	Q1124	Q1046	Q903	R827	A735	P655	Q563	L496	ARG	GLY	PRO	GLY	GLY
V1281	V1281			K1047	N904	W828	W736	P656	Q564	E497	VAL	VAL	ARG	VAL	VAL
	S1216			P1048	Q905	W829	F736	E662	Q565	V498	VAL	GLY	GLY	VAL	VAL
	E1219			S1049	Q906	W829	D739	W662	Q566		VAL	GLY	GLY	VAL	VAL
E1287	E1287	V1128	V1128	F1053	E907	G831	D740	W665	Q567	F502	VAL	VAL	THR	SER	SER
D1288	D1288	T1129	T1129	E1054	Q908	R832	W741	F666	Q568	L503	ILE	ILE	THR	GLY	GLY
R1289	R1289	R1130	R1130	F1055	N909	R833	G742	W667	Q569	D504	ALA	ALA	VAL	VAL	ARG
L1290	L1290	L1131	L1131	V1056	Q912	W834	D743	W668	Q570	S505	VAL	VAL	LYS	GLY	GLY
S1291	S1291	R1132	R1132	P1056	D913	S835			Q571	G506	ASN	ASN	GLY	VAL	VAL
Q1374	Q1374	L1133	L1133	L1056	A918	R838	A757	W672	Q572	R507	VAL	VAL	GLY	ASP	ALA
M1375	S1296	R1134	R1134	P1056	F919	L839	A759	W673	Q573	R508	VAL	VAL	THR	ALA	ALA
L1376	L1376	L1134	L1134	P1056	L920	K840	W760	W678	Q574	P509	ARG	ARG	VAL	TYR	LEU
K1377	K1377	L1135	L1135	S1059	Q912	W842	D762	W679	Q575	E510	VAL	VAL	GLY	GLY	ARG
	F1299	R1136	R1136	S1060	D913	S835			Q576	W511	VAL	VAL	GLY	PHE	ARG
S1300	S1300	K1136	K1136	S1060	A918	R838	A757	W672	Q577	W512	VAL	VAL	GLY	GLY	PRO
	P1306	E1141	E1141	S1060	F919	L839	A759	W673	Q578	W513	VAL	VAL	GLY	HIS	PRO
P1385	P1385	S1142	S1142	R1062	L920	K840	W760	W679	Q579	W514	VAL	VAL	GLY	GLY	ARG
V1313	V1313	G1143	G1143	P1067	Q924	W842	D762	W680	Q580	W515	VAL	VAL	GLY	GLY	ARG
K1314	K1314	G1143	G1143	L1068	E925	F843	W763	W681	Q581	W516	VAL	VAL	GLY	GLY	ARG
D1386	D1386	G1146	G1146	L1068	E926	F844	W764	W682	Q582	W517	VAL	VAL	GLY	GLY	ARG
S1387	S1387	Q1235	Q1235	E1070	K926	N845	S765	W683	Q583	W518	VAL	VAL	GLY	GLY	ARG
R1388	R1388	L1236	L1236	Y1070	T927	N845	S765	W684	Q584	W519	VAL	VAL	GLY	GLY	ARG
L1389	L1389	L1149	L1149	F1071	A928	P846	A766	W684	Q585	W520	VAL	VAL	GLY	GLY	ARG



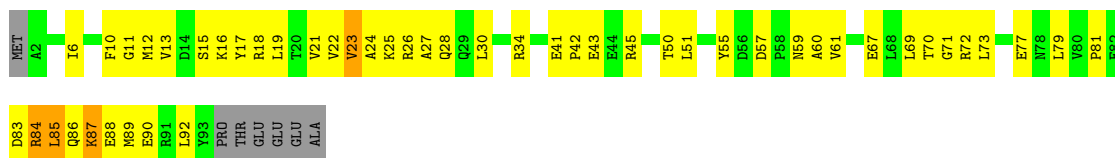
• Molecule 4: RNA POLYMERASE, OMEGA SUBUNIT

Chain E: 43% 44% 5% 7%



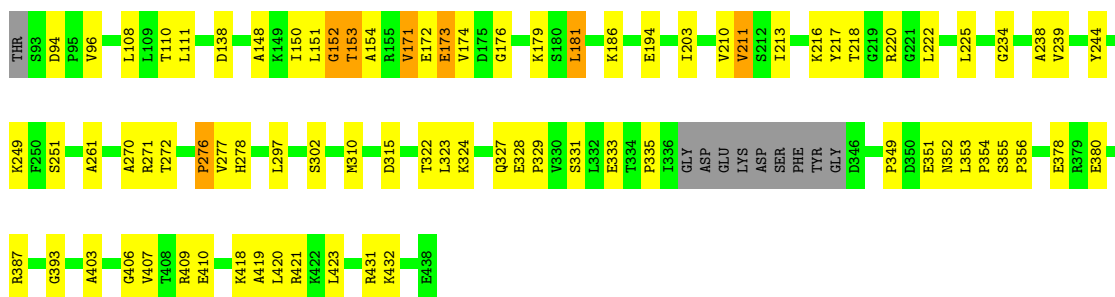
• Molecule 4: RNA POLYMERASE, OMEGA SUBUNIT

Chain N: 43% 45% 7%



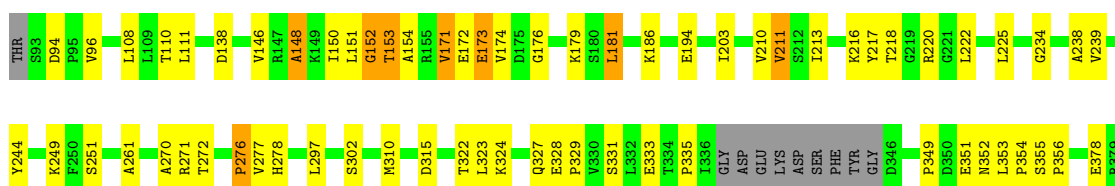
• Molecule 5: SIGMA FACTOR SIGA

Chain H: 73% 22%



• Molecule 5: SIGMA FACTOR SIGA

Chain Q: 73% 22%



E380	
R387	
G393	
A403	
G406	
V407	
T408	
R409	
E410	
K418	
A419	
L420	
R421	
K422	
L423	
K431	
K432	
E438	

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	155.00Å 271.20Å 155.30Å 90.00° 91.40° 90.00°	Depositor
Resolution (Å)	(Not available) – 4.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-4.00)	Depositor
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
Refinement program		Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18756	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.57	0/671	1.81	25/670 (3.7%)
1	B	0.54	0/659	1.88	21/658 (3.2%)
1	J	0.57	0/671	1.81	26/670 (3.9%)
1	K	0.54	0/659	1.88	21/658 (3.2%)
2	C	1.29	11/3246 (0.3%)	2.20	94/3240 (2.9%)
2	L	1.29	11/3246 (0.3%)	2.21	94/3240 (2.9%)
3	D	1.47	32/3545 (0.9%)	2.23	126/3541 (3.6%)
3	M	1.47	32/3545 (0.9%)	2.23	126/3541 (3.6%)
4	E	0.52	0/275	1.65	5/274 (1.8%)
4	N	0.52	0/275	1.65	5/274 (1.8%)
5	H	0.96	4/964 (0.4%)	1.60	11/962 (1.1%)
5	Q	0.95	4/964 (0.4%)	1.60	11/962 (1.1%)
All	All	1.24	94/18720 (0.5%)	2.10	565/18690 (3.0%)

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
2	C	0	8
2	L	0	8
3	D	0	7
3	M	0	7
All	All	0	30

All (94) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	91	GLY	C-N	-30.07	0.92	1.33
3	M	91	GLY	C-N	-30.07	0.92	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	244	PRO	C-N	-28.93	0.92	1.33
2	L	244	PRO	C-N	-28.90	0.92	1.33
2	C	417	GLY	C-N	-27.09	0.95	1.33
2	L	417	GLY	C-N	-27.03	0.95	1.33
3	D	44	LEU	C-N	26.16	1.70	1.33
3	M	44	LEU	C-N	26.10	1.70	1.33
2	L	418	LEU	C-N	-25.56	1.01	1.33
2	C	418	LEU	C-N	-25.52	1.01	1.33
2	L	422	ARG	C-N	-23.19	1.01	1.33
2	C	419	THR	C-N	-23.18	1.01	1.33
2	C	422	ARG	C-N	-23.14	1.01	1.33
2	L	419	THR	C-N	-23.14	1.01	1.33
3	D	521	PRO	C-N	-22.66	1.08	1.34
3	M	521	PRO	C-N	-22.59	1.09	1.34
3	D	531	ASP	C-N	-22.44	1.00	1.33
3	M	531	ASP	C-N	-22.41	1.00	1.33
2	L	240	THR	C-N	-21.67	0.98	1.33
2	C	240	THR	C-N	-21.62	0.99	1.33
5	H	239	VAL	C-N	-21.58	1.05	1.33
5	Q	239	VAL	C-N	-21.52	1.05	1.33
3	M	532	GLY	C-N	21.46	1.61	1.33
3	D	532	GLY	C-N	21.41	1.61	1.33
3	D	529	GLN	C-N	-19.84	1.06	1.33
3	M	529	GLN	C-N	-19.82	1.06	1.33
3	M	526	PRO	C-N	-17.70	1.09	1.33
3	D	526	PRO	C-N	-17.66	1.09	1.33
3	D	533	GLY	C-N	16.99	1.57	1.33
3	M	533	GLY	C-N	16.99	1.57	1.33
2	L	423	ALA	C-N	-16.58	1.13	1.33
2	C	423	ALA	C-N	-16.53	1.13	1.33
3	D	1087	ARG	C-N	-16.41	1.11	1.33
3	M	1087	ARG	C-N	-16.37	1.11	1.33
3	D	113	GLY	C-N	-15.07	1.12	1.33
3	M	113	GLY	C-N	-15.03	1.12	1.33
3	D	1080	GLY	C-N	13.64	1.50	1.33
3	M	1080	GLY	C-N	13.61	1.50	1.33
3	D	538	SER	C-N	12.68	1.51	1.33
3	D	115	LEU	C-N	-12.67	1.16	1.33
3	M	115	LEU	C-N	-12.66	1.16	1.33
3	M	538	SER	C-N	12.66	1.51	1.33
3	M	93	ILE	C-N	-11.41	1.17	1.33
3	D	93	ILE	C-N	-11.40	1.17	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	238	ALA	N-CA	10.84	1.59	1.46
5	Q	238	ALA	N-CA	10.83	1.59	1.46
3	M	528	VAL	C-N	10.05	1.50	1.33
3	D	528	VAL	C-N	10.04	1.50	1.33
3	D	523	ASP	C-N	-9.23	1.20	1.33
3	M	523	ASP	C-N	-9.21	1.20	1.33
3	D	534	ARG	C-N	-9.14	1.20	1.33
3	D	1096	ARG	C-N	-9.12	1.22	1.33
3	M	1096	ARG	C-N	-9.10	1.22	1.33
3	M	534	ARG	C-N	-9.08	1.21	1.33
3	M	88	TYR	C-N	8.82	1.46	1.33
3	D	88	TYR	C-N	8.81	1.46	1.33
3	D	1086	LEU	C-N	8.59	1.44	1.33
3	M	1086	LEU	C-N	8.57	1.44	1.33
3	M	113	GLY	N-CA	-8.37	1.34	1.45
3	M	527	MET	C-N	8.36	1.43	1.33
2	L	415	PRO	C-N	8.36	1.44	1.33
3	D	113	GLY	N-CA	-8.35	1.34	1.45
2	C	415	PRO	C-N	8.32	1.44	1.33
3	D	527	MET	C-N	8.31	1.43	1.33
2	C	416	GLY	C-N	-7.86	1.19	1.33
2	L	416	GLY	C-N	-7.83	1.19	1.33
3	M	1089	ALA	C-N	-7.79	1.21	1.33
3	D	1089	ALA	C-N	-7.79	1.21	1.33
2	C	424	GLY	C-N	-7.46	1.23	1.33
2	L	424	GLY	C-N	-7.45	1.23	1.33
3	M	537	THR	C-N	7.20	1.43	1.33
3	D	537	THR	C-N	7.17	1.43	1.33
3	M	522	PRO	C-N	7.06	1.43	1.33
3	D	522	PRO	C-N	7.04	1.43	1.33
5	Q	234	GLY	CA-C	-6.96	1.43	1.51
5	H	234	GLY	CA-C	-6.92	1.43	1.51
3	D	1088	THR	C-N	-6.72	1.24	1.33
3	M	1088	THR	C-N	-6.71	1.24	1.33
3	D	94	GLU	C-N	-6.61	1.24	1.33
3	M	94	GLU	C-N	-6.54	1.24	1.33
3	D	536	ALA	CA-C	6.54	1.60	1.52
3	M	1084	THR	C-N	6.53	1.43	1.33
3	D	1084	THR	C-N	6.51	1.43	1.33
3	M	536	ALA	CA-C	6.50	1.60	1.52
5	H	234	GLY	N-CA	5.78	1.52	1.45
5	Q	234	GLY	N-CA	5.77	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	1081	GLY	C-N	5.72	1.41	1.33
3	D	1081	GLY	C-N	5.70	1.41	1.33
3	M	1079	LYS	C-N	-5.54	1.26	1.33
3	D	1079	LYS	C-N	-5.53	1.26	1.33
3	M	92	HIS	N-CA	5.44	1.53	1.46
3	D	92	HIS	N-CA	5.44	1.53	1.46
2	L	416	GLY	CA-C	5.14	1.57	1.52
2	C	416	GLY	CA-C	5.12	1.57	1.52

All (565) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	417	GLY	CA-C-N	27.12	173.35	121.54
2	L	417	GLY	C-N-CA	27.12	173.35	121.54
2	C	417	GLY	CA-C-N	27.12	173.34	121.54
2	C	417	GLY	C-N-CA	27.12	173.34	121.54
2	C	419	THR	CA-C-N	25.46	170.16	121.54
2	C	419	THR	C-N-CA	25.46	170.16	121.54
2	L	419	THR	CA-C-N	25.45	170.14	121.54
2	L	419	THR	C-N-CA	25.45	170.14	121.54
3	M	534	ARG	CA-C-N	24.52	168.37	121.54
3	M	534	ARG	C-N-CA	24.52	168.37	121.54
3	D	534	ARG	CA-C-N	24.51	168.35	121.54
3	D	534	ARG	C-N-CA	24.51	168.35	121.54
3	D	529	GLN	CA-C-N	21.18	160.09	121.97
3	D	529	GLN	C-N-CA	21.18	160.09	121.97
2	C	244	PRO	CA-C-N	21.17	159.81	121.70
2	C	244	PRO	C-N-CA	21.17	159.81	121.70
3	M	529	GLN	CA-C-N	21.16	160.05	121.97
3	M	529	GLN	C-N-CA	21.16	160.05	121.97
2	L	244	PRO	CA-C-N	21.15	159.78	121.70
2	L	244	PRO	C-N-CA	21.15	159.78	121.70
3	M	526	PRO	CA-C-N	21.15	150.64	120.82
3	M	526	PRO	C-N-CA	21.15	150.64	120.82
3	D	526	PRO	CA-C-N	21.15	150.64	120.82
3	D	526	PRO	C-N-CA	21.15	150.64	120.82
2	C	422	ARG	CA-C-N	18.74	157.32	121.54
2	C	422	ARG	C-N-CA	18.74	157.32	121.54
2	L	422	ARG	CA-C-N	18.73	157.32	121.54
2	L	422	ARG	C-N-CA	18.73	157.32	121.54
3	D	91	GLY	CA-C-N	18.13	148.32	121.31
3	D	91	GLY	C-N-CA	18.13	148.32	121.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	91	GLY	CA-C-N	18.13	148.32	121.31
3	M	91	GLY	C-N-CA	18.13	148.32	121.31
3	D	88	TYR	CA-C-N	-17.61	96.02	122.09
3	D	88	TYR	C-N-CA	-17.61	96.02	122.09
3	M	88	TYR	CA-C-N	-17.59	96.06	122.09
3	M	88	TYR	C-N-CA	-17.59	96.06	122.09
2	L	418	LEU	CA-C-N	15.76	148.75	121.80
2	L	418	LEU	C-N-CA	15.76	148.75	121.80
2	C	418	LEU	CA-C-N	15.74	148.71	121.80
2	C	418	LEU	C-N-CA	15.74	148.71	121.80
3	M	694	VAL	N-CA-C	-15.33	99.48	111.90
3	D	694	VAL	N-CA-C	-15.31	99.50	111.90
3	D	531	ASP	CA-C-N	15.05	150.90	121.41
3	D	531	ASP	C-N-CA	15.05	150.90	121.41
3	M	531	ASP	CA-C-N	15.05	150.90	121.41
3	M	531	ASP	C-N-CA	15.05	150.90	121.41
2	C	242	LEU	CA-C-N	14.92	158.21	121.80
2	C	242	LEU	C-N-CA	14.92	158.21	121.80
2	L	242	LEU	CA-C-N	14.92	158.22	121.80
2	L	242	LEU	C-N-CA	14.92	158.22	121.80
2	L	423	ALA	CA-C-N	13.79	131.69	122.18
2	L	423	ALA	C-N-CA	13.79	131.69	122.18
2	C	423	ALA	CA-C-N	13.77	131.68	122.18
2	C	423	ALA	C-N-CA	13.77	131.68	122.18
3	M	521	PRO	CA-C-N	12.32	132.68	119.87
3	M	521	PRO	C-N-CA	12.32	132.68	119.87
3	D	521	PRO	CA-C-N	12.32	132.68	119.87
3	D	521	PRO	C-N-CA	12.32	132.68	119.87
3	D	93	ILE	CA-C-N	11.36	136.85	120.95
3	D	93	ILE	C-N-CA	11.36	136.85	120.95
3	M	93	ILE	CA-C-N	11.34	136.83	120.95
3	M	93	ILE	C-N-CA	11.34	136.83	120.95
3	D	846	PRO	N-CA-C	-11.10	100.88	114.20
3	M	846	PRO	N-CA-C	-11.09	100.89	114.20
3	D	1088	THR	CA-C-N	10.95	141.20	122.36
3	D	1088	THR	C-N-CA	10.95	141.20	122.36
3	M	1088	THR	CA-C-N	10.93	141.17	122.36
3	M	1088	THR	C-N-CA	10.93	141.17	122.36
3	D	1481	VAL	N-CA-C	10.72	121.64	106.53
3	M	1481	VAL	N-CA-C	10.71	121.64	106.53
3	D	1062	ARG	N-CA-C	-10.46	99.99	113.17
3	M	1062	ARG	N-CA-C	-10.45	100.00	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	536	ALA	N-CA-C	10.10	125.84	108.76
3	M	536	ALA	N-CA-C	10.10	125.83	108.76
2	C	349	ALA	N-CA-C	-10.01	103.22	114.62
2	L	349	ALA	N-CA-C	-9.99	103.23	114.62
2	C	606	VAL	N-CA-C	-9.89	104.32	113.71
2	L	606	VAL	N-CA-C	-9.85	104.36	113.71
3	D	933	ALA	N-CA-C	-9.83	101.04	113.43
3	M	933	ALA	N-CA-C	-9.82	101.05	113.43
1	A	63	HIS	N-CA-C	9.66	124.15	108.99
1	J	63	HIS	N-CA-C	9.65	124.14	108.99
3	D	1060	SER	N-CA-C	-9.56	98.14	111.52
3	M	1060	SER	N-CA-C	-9.53	98.18	111.52
4	E	85	LEU	N-CA-C	-9.42	101.71	113.01
4	N	85	LEU	N-CA-C	-9.42	101.71	113.01
1	A	37	GLY	N-CA-C	9.36	123.95	112.73
1	J	37	GLY	N-CA-C	9.32	123.91	112.73
1	J	81	ASN	N-CA-C	-9.19	102.64	114.04
1	A	81	ASN	N-CA-C	-9.14	102.71	114.04
2	C	191	PHE	N-CA-C	9.13	116.44	108.22
2	L	191	PHE	N-CA-C	9.12	116.42	108.22
2	C	881	ASN	N-CA-C	8.91	122.47	110.35
2	L	881	ASN	N-CA-C	8.91	122.47	110.35
2	L	365	ASP	N-CA-C	-8.82	100.65	111.33
2	C	365	ASP	N-CA-C	-8.79	100.69	111.33
3	M	1482	ARG	N-CA-C	-8.69	102.04	114.12
3	D	1482	ARG	N-CA-C	-8.68	102.05	114.12
5	H	225	LEU	CA-C-N	8.63	135.36	120.68
5	H	225	LEU	C-N-CA	8.63	135.36	120.68
5	Q	225	LEU	CA-C-N	8.63	135.36	120.68
5	Q	225	LEU	C-N-CA	8.63	135.36	120.68
3	D	1037	GLN	N-CA-C	-8.60	100.90	111.40
3	M	1037	GLN	N-CA-C	-8.59	100.92	111.40
2	L	780	GLU	N-CA-C	-8.43	101.46	112.41
2	C	780	GLU	N-CA-C	-8.42	101.46	112.41
3	M	711	LEU	N-CA-C	-8.35	101.07	111.75
3	D	711	LEU	N-CA-C	-8.34	101.07	111.75
3	M	466	LYS	N-CA-C	-8.31	103.26	113.15
4	E	28	GLN	N-CA-C	-8.31	101.91	110.97
4	N	28	GLN	N-CA-C	-8.31	101.92	110.97
3	D	120	ALA	N-CA-C	-8.28	103.07	113.01
3	D	466	LYS	N-CA-C	-8.27	103.31	113.15
3	M	473	LEU	N-CA-C	-8.25	103.22	113.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	120	ALA	N-CA-C	-8.24	103.12	113.01
3	D	473	LEU	N-CA-C	-8.22	103.25	113.20
1	A	201	THR	N-CA-C	8.14	122.26	109.81
1	J	201	THR	N-CA-C	8.12	122.22	109.81
3	M	717	GLN	CA-C-N	-8.03	109.80	119.84
3	M	717	GLN	C-N-CA	-8.03	109.80	119.84
3	D	717	GLN	CA-C-N	-8.03	109.80	119.84
3	D	717	GLN	C-N-CA	-8.03	109.80	119.84
2	C	564	MET	N-CA-C	-8.02	102.62	111.36
2	L	564	MET	N-CA-C	-8.01	102.63	111.36
2	C	576	ALA	CA-C-N	7.99	129.83	119.84
2	C	576	ALA	C-N-CA	7.99	129.83	119.84
2	L	576	ALA	CA-C-N	7.99	129.82	119.84
2	L	576	ALA	C-N-CA	7.99	129.82	119.84
2	C	240	THR	CA-C-N	-7.97	109.71	122.23
2	C	240	THR	C-N-CA	-7.97	109.71	122.23
2	C	1061	GLU	N-CA-C	-7.96	101.56	111.11
2	L	1061	GLU	N-CA-C	-7.96	101.56	111.11
5	H	173	GLU	N-CA-C	7.95	127.74	110.80
3	M	1425	THR	N-CA-C	-7.95	102.30	110.97
5	Q	173	GLU	N-CA-C	7.94	127.72	110.80
2	L	240	THR	CA-C-N	-7.93	109.78	122.23
2	L	240	THR	C-N-CA	-7.93	109.78	122.23
3	D	1425	THR	N-CA-C	-7.92	102.34	110.97
2	C	1032	PHE	N-CA-C	-7.80	103.28	114.12
2	L	350	ARG	N-CA-C	-7.79	102.62	113.37
3	D	44	LEU	CA-C-N	-7.79	106.66	121.54
3	D	44	LEU	C-N-CA	-7.79	106.66	121.54
2	L	1032	PHE	N-CA-C	-7.78	103.30	114.12
3	M	44	LEU	CA-C-N	-7.78	106.68	121.54
3	M	44	LEU	C-N-CA	-7.78	106.68	121.54
2	C	350	ARG	N-CA-C	-7.77	102.64	113.37
3	M	89	ARG	CA-C-N	-7.77	108.61	122.74
3	M	89	ARG	C-N-CA	-7.77	108.61	122.74
3	M	1238	MET	N-CA-C	-7.76	101.79	111.11
3	D	1238	MET	N-CA-C	-7.76	101.80	111.11
3	D	89	ARG	CA-C-N	-7.75	108.63	122.74
3	D	89	ARG	C-N-CA	-7.75	108.63	122.74
1	B	102	ARG	N-CA-C	-7.72	98.89	110.24
1	K	102	ARG	N-CA-C	-7.72	98.89	110.24
1	K	177	VAL	N-CA-C	7.71	118.90	108.11
1	B	177	VAL	N-CA-C	7.71	118.90	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	476	GLU	N-CA-C	-7.66	101.67	111.02
3	M	476	GLU	N-CA-C	-7.65	101.69	111.02
3	M	1128	VAL	N-CA-C	-7.61	93.50	109.34
3	D	1128	VAL	N-CA-C	-7.61	93.52	109.34
3	D	1010	ASN	N-CA-C	-7.58	102.16	111.33
3	M	1010	ASN	N-CA-C	-7.57	102.17	111.33
3	M	1216	SER	N-CA-C	-7.57	101.10	110.41
3	D	1216	SER	N-CA-C	-7.56	101.11	110.41
3	M	1087	ARG	CA-C-N	7.44	132.60	120.63
3	M	1087	ARG	C-N-CA	7.44	132.60	120.63
2	C	585	GLU	N-CA-C	-7.43	103.17	111.71
1	K	103	ALA	N-CA-C	7.43	120.36	109.07
1	B	103	ALA	N-CA-C	7.41	120.34	109.07
3	D	1087	ARG	CA-C-N	7.41	132.56	120.63
3	D	1087	ARG	C-N-CA	7.41	132.56	120.63
3	M	122	GLU	N-CA-C	-7.41	103.71	112.89
3	M	512	MET	N-CA-C	-7.40	100.28	110.35
2	L	585	GLU	N-CA-C	-7.40	103.20	111.71
3	D	122	GLU	N-CA-C	-7.39	103.72	112.89
3	D	512	MET	N-CA-C	-7.38	100.31	110.35
5	H	194	GLU	N-CA-C	-7.35	103.27	112.90
5	Q	194	GLU	N-CA-C	-7.35	103.27	112.90
3	D	132	TYR	N-CA-C	-7.33	100.23	110.35
3	M	132	TYR	N-CA-C	-7.33	100.23	110.35
2	C	1094	ALA	N-CA-C	-7.30	102.12	111.02
2	L	1094	ALA	N-CA-C	-7.27	102.15	111.02
3	M	1322	GLY	N-CA-C	-7.21	106.03	115.47
2	C	557	ARG	N-CA-C	-7.21	101.94	111.24
2	L	557	ARG	N-CA-C	-7.21	101.94	111.24
5	Q	153	THR	N-CA-C	-7.20	104.52	112.72
5	H	153	THR	N-CA-C	-7.18	104.53	112.72
3	D	1322	GLY	N-CA-C	-7.16	106.09	115.47
1	B	131	THR	N-CA-C	-7.14	99.35	110.42
3	D	771	SER	N-CA-C	-7.13	99.33	109.24
2	C	321	GLU	N-CA-C	-7.13	105.42	112.97
3	M	532	GLY	CA-C-N	7.13	131.38	121.26
3	M	532	GLY	C-N-CA	7.13	131.38	121.26
3	M	771	SER	N-CA-C	-7.13	99.33	109.24
2	L	321	GLU	N-CA-C	-7.12	105.42	112.97
3	D	532	GLY	CA-C-N	7.12	131.37	121.26
3	D	532	GLY	C-N-CA	7.12	131.37	121.26
3	M	155	ASP	N-CA-C	-7.12	103.58	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	155	ASP	N-CA-C	-7.11	103.58	112.90
1	K	131	THR	N-CA-C	-7.11	99.40	110.42
3	D	1345	GLU	N-CA-C	-7.10	103.72	112.88
3	M	1345	GLU	N-CA-C	-7.10	103.72	112.88
3	M	833	GLU	N-CA-C	-7.06	104.24	112.92
3	D	833	GLU	N-CA-C	-7.05	104.25	112.92
3	M	153	LEU	N-CA-C	-7.03	103.66	113.37
3	D	1493	LYS	N-CA-C	-7.03	104.02	112.59
3	M	1493	LYS	N-CA-C	-7.02	104.03	112.59
3	D	877	PRO	N-CA-C	-7.01	105.10	113.86
3	D	153	LEU	N-CA-C	-7.01	103.70	113.37
3	M	877	PRO	N-CA-C	-7.01	105.10	113.86
1	B	93	LYS	N-CA-C	-6.97	103.84	114.16
1	K	93	LYS	N-CA-C	-6.96	103.86	114.16
3	M	1108	ARG	N-CA-C	-6.92	99.63	110.36
3	D	1108	ARG	N-CA-C	-6.91	99.66	110.36
3	M	997	THR	N-CA-C	-6.89	102.93	111.75
2	L	344	PHE	N-CA-C	-6.87	103.87	111.36
3	M	1258	ARG	N-CA-C	-6.86	104.94	113.38
3	D	1258	ARG	N-CA-C	-6.86	104.95	113.38
2	C	344	PHE	N-CA-C	-6.85	103.90	111.36
3	D	997	THR	N-CA-C	-6.84	103.00	111.75
3	D	1403	LEU	N-CA-C	-6.83	102.13	110.88
3	M	1403	LEU	N-CA-C	-6.82	102.15	110.88
2	C	807	ARG	N-CA-C	6.76	118.80	108.52
2	L	807	ARG	N-CA-C	6.75	118.78	108.52
1	J	67	THR	N-CA-C	6.75	119.24	110.53
1	A	67	THR	N-CA-C	6.71	119.18	110.53
1	A	205	VAL	N-CA-C	6.68	118.07	107.98
1	J	205	VAL	N-CA-C	6.67	118.06	107.98
3	D	637	LEU	N-CA-C	-6.66	103.77	114.09
3	M	637	LEU	N-CA-C	-6.65	103.78	114.09
3	D	996	TRP	N-CA-C	-6.64	105.30	113.41
3	M	996	TRP	N-CA-C	-6.63	105.32	113.41
3	D	472	LYS	N-CA-C	-6.59	103.92	112.23
1	B	124	ASN	N-CA-C	6.59	124.38	109.81
1	K	124	ASN	N-CA-C	6.59	124.38	109.81
4	N	88	GLU	N-CA-C	-6.59	105.06	113.23
4	E	88	GLU	N-CA-C	-6.58	105.07	113.23
3	M	472	LYS	N-CA-C	-6.58	103.94	112.23
1	K	140	MET	N-CA-C	6.57	120.32	108.69
1	B	140	MET	N-CA-C	6.55	120.28	108.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	693	GLU	N-CA-C	-6.55	103.55	113.89
3	M	693	GLU	N-CA-C	-6.53	103.57	113.89
1	A	48	ILE	CA-C-N	6.49	127.95	119.84
1	A	48	ILE	C-N-CA	6.49	127.95	119.84
1	A	61	VAL	N-CA-C	6.48	117.21	107.75
1	J	48	ILE	CA-C-N	6.48	127.94	119.84
1	J	48	ILE	C-N-CA	6.48	127.94	119.84
1	J	61	VAL	N-CA-C	6.47	117.19	107.75
2	L	901	TYR	N-CA-C	6.47	119.01	109.24
2	C	901	TYR	N-CA-C	6.46	118.99	109.24
3	D	1318	TYR	N-CA-C	6.45	118.85	111.11
3	M	1318	TYR	N-CA-C	6.43	118.83	111.11
2	L	695	LEU	N-CA-C	-6.42	105.34	113.43
2	C	695	LEU	N-CA-C	-6.41	105.36	113.43
3	D	1280	VAL	N-CA-C	6.40	118.02	108.23
2	C	412	ALA	N-CA-C	-6.39	105.44	112.72
2	L	273	GLY	N-CA-C	-6.39	104.77	113.27
2	C	273	GLY	N-CA-C	-6.38	104.79	113.27
3	M	1280	VAL	N-CA-C	6.38	117.98	108.23
3	M	104	PHE	N-CA-C	6.37	119.73	109.02
2	L	412	ALA	N-CA-C	-6.37	105.46	112.72
1	K	24	VAL	N-CA-C	6.37	116.99	108.27
3	D	1174	LEU	N-CA-C	-6.35	104.48	112.93
3	D	104	PHE	N-CA-C	6.35	119.69	109.02
3	M	1174	LEU	N-CA-C	-6.35	104.48	112.93
1	B	24	VAL	N-CA-C	6.35	116.97	108.27
2	L	533	ASP	N-CA-C	-6.32	105.67	113.19
1	A	68	ILE	CA-C-N	6.30	126.25	119.76
1	A	68	ILE	C-N-CA	6.30	126.25	119.76
2	C	533	ASP	N-CA-C	-6.30	105.69	113.19
2	L	717	LEU	N-CA-C	-6.29	101.93	111.56
2	C	717	LEU	N-CA-C	-6.29	101.94	111.56
2	C	995	MET	N-CA-C	6.28	121.03	112.68
1	J	68	ILE	CA-C-N	6.28	126.23	119.76
1	J	68	ILE	C-N-CA	6.28	126.23	119.76
3	D	817	GLU	N-CA-C	-6.27	106.59	114.56
3	M	817	GLU	N-CA-C	-6.27	106.60	114.56
3	D	625	TYR	N-CA-C	-6.27	104.26	112.41
1	B	172	SER	CA-C-N	-6.26	112.01	119.84
1	B	172	SER	C-N-CA	-6.26	112.01	119.84
4	E	87	LYS	N-CA-C	-6.26	104.90	112.54
2	C	1112	PHE	N-CA-C	6.26	119.30	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	625	TYR	N-CA-C	-6.26	104.28	112.41
2	L	995	MET	N-CA-C	6.25	121.00	112.68
2	L	1112	PHE	N-CA-C	6.25	119.29	110.23
4	N	87	LYS	N-CA-C	-6.24	104.93	112.54
2	C	895	TYR	N-CA-C	-6.24	104.54	111.71
2	L	895	TYR	N-CA-C	-6.23	104.54	111.71
1	K	172	SER	CA-C-N	-6.23	112.05	119.84
1	K	172	SER	C-N-CA	-6.23	112.05	119.84
2	L	430	VAL	N-CA-C	6.22	122.27	109.34
2	C	430	VAL	N-CA-C	6.21	122.26	109.34
2	L	1017	THR	N-CA-C	-6.19	104.79	112.90
4	E	92	LEU	N-CA-C	-6.18	103.89	112.30
2	C	1017	THR	N-CA-C	-6.17	104.81	112.90
2	C	878	SER	N-CA-C	-6.17	103.71	111.11
3	D	1491	THR	N-CA-C	-6.17	103.88	112.45
3	M	1491	THR	N-CA-C	-6.16	103.89	112.45
2	C	631	SER	N-CA-C	-6.16	100.83	109.69
3	D	456	MET	N-CA-C	-6.15	104.65	111.36
3	M	959	GLU	N-CA-C	-6.15	104.14	112.26
2	L	631	SER	N-CA-C	-6.15	100.84	109.69
2	L	878	SER	N-CA-C	-6.14	103.74	111.11
2	C	523	ILE	N-CA-C	6.14	117.63	108.23
3	D	959	GLU	N-CA-C	-6.14	104.15	112.26
3	M	456	MET	N-CA-C	-6.14	104.67	111.36
2	L	523	ILE	N-CA-C	6.14	117.62	108.23
3	D	918	ALA	N-CA-C	-6.14	104.59	111.28
4	N	92	LEU	N-CA-C	-6.14	103.87	113.02
3	M	918	ALA	N-CA-C	-6.12	104.61	111.28
1	A	163	ASN	N-CA-C	-6.09	105.49	113.17
1	A	165	ILE	N-CA-C	6.09	114.92	108.95
2	C	886	LEU	N-CA-C	-6.09	105.56	112.87
1	J	174	VAL	N-CA-C	6.09	118.55	109.17
2	L	886	LEU	N-CA-C	-6.08	105.57	112.87
1	A	174	VAL	N-CA-C	6.08	118.53	109.17
3	M	1035	ILE	N-CA-C	-6.08	105.80	111.45
1	J	163	ASN	N-CA-C	-6.07	105.53	113.17
1	J	165	ILE	N-CA-C	6.07	114.89	108.95
3	D	1035	ILE	N-CA-C	-6.06	105.82	111.45
3	D	644	LEU	CA-C-N	6.06	127.41	119.84
3	D	644	LEU	C-N-CA	6.06	127.41	119.84
3	M	644	LEU	CA-C-N	6.05	127.40	119.84
3	M	644	LEU	C-N-CA	6.05	127.40	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	757	ALA	N-CA-C	-6.02	104.04	111.33
3	D	757	ALA	N-CA-C	-6.00	104.07	111.33
2	C	593	ALA	N-CA-C	-5.98	101.78	111.04
2	L	593	ALA	N-CA-C	-5.98	101.78	111.04
3	D	113	GLY	CA-C-N	5.96	132.93	121.54
3	D	113	GLY	C-N-CA	5.96	132.93	121.54
3	M	1492	LEU	N-CA-C	-5.96	105.97	113.18
1	K	81	ASN	N-CA-C	-5.96	106.55	113.88
5	Q	418	LYS	N-CA-C	-5.96	104.86	111.71
3	D	1086	LEU	CA-C-N	-5.94	112.81	120.65
3	D	1086	LEU	C-N-CA	-5.94	112.81	120.65
3	D	1492	LEU	N-CA-C	-5.94	105.99	113.18
1	B	81	ASN	N-CA-C	-5.94	106.58	113.88
2	L	1090	LYS	N-CA-C	-5.94	103.99	111.11
5	H	418	LYS	N-CA-C	-5.93	104.89	111.71
3	M	113	GLY	CA-C-N	5.93	132.87	121.54
3	M	113	GLY	C-N-CA	5.93	132.87	121.54
3	M	1344	VAL	N-CA-C	-5.93	107.51	113.20
2	C	1090	LYS	N-CA-C	-5.93	104.00	111.11
3	M	955	VAL	N-CA-C	5.92	116.97	107.73
3	D	955	VAL	N-CA-C	5.91	116.96	107.73
3	D	1344	VAL	N-CA-C	-5.91	107.52	113.20
3	M	1086	LEU	CA-C-N	-5.91	112.85	120.65
3	M	1086	LEU	C-N-CA	-5.91	112.85	120.65
2	C	268	ASP	N-CA-C	5.91	115.28	108.49
3	D	35	ARG	N-CA-C	-5.89	105.19	112.38
2	L	268	ASP	N-CA-C	5.89	115.26	108.49
3	D	1272	ALA	N-CA-C	-5.89	104.02	110.91
3	M	35	ARG	N-CA-C	-5.88	105.21	112.38
3	M	1272	ALA	N-CA-C	-5.87	104.04	110.91
2	L	85	GLU	N-CA-C	-5.86	105.62	112.89
1	A	16	GLN	N-CA-C	-5.86	104.59	110.97
5	H	171	VAL	N-CA-C	5.85	121.52	109.34
1	J	16	GLN	N-CA-C	-5.85	104.59	110.97
5	Q	171	VAL	N-CA-C	5.85	121.51	109.34
2	L	416	GLY	N-CA-C	-5.84	104.61	112.14
2	C	85	GLU	N-CA-C	-5.84	105.65	112.89
2	C	416	GLY	N-CA-C	-5.84	104.61	112.14
2	L	333	ILE	N-CA-C	-5.83	100.19	108.58
2	C	333	ILE	N-CA-C	-5.82	100.20	108.58
3	M	1495	ILE	N-CA-C	-5.81	105.11	113.07
1	A	172	SER	CA-C-N	5.79	125.48	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	SER	C-N-CA	5.79	125.48	119.05
3	D	1495	ILE	N-CA-C	-5.79	105.13	113.07
1	J	198	ARG	N-CA-C	5.78	118.28	110.88
5	Q	261	ALA	N-CA-C	-5.76	106.09	113.23
1	A	198	ARG	N-CA-C	5.75	118.25	110.88
1	J	172	SER	CA-C-N	5.75	125.43	119.05
1	J	172	SER	C-N-CA	5.75	125.43	119.05
3	M	1034	GLN	N-CA-C	-5.75	106.14	114.12
5	H	261	ALA	N-CA-C	-5.74	106.11	113.23
3	D	865	THR	N-CA-C	-5.72	101.45	109.69
3	D	1034	GLN	N-CA-C	-5.72	106.17	114.12
3	M	865	THR	N-CA-C	-5.72	101.46	109.69
1	J	24	VAL	N-CA-C	5.71	116.70	108.48
1	A	24	VAL	N-CA-C	5.70	116.69	108.48
3	D	912	LYS	N-CA-C	-5.68	102.00	111.37
1	B	162	ILE	N-CA-C	5.67	116.37	108.89
1	K	162	ILE	N-CA-C	5.66	116.36	108.89
3	M	912	LYS	N-CA-C	-5.66	102.03	111.37
3	M	1031	ASN	CA-C-N	5.66	126.91	119.84
3	M	1031	ASN	C-N-CA	5.66	126.91	119.84
3	M	1323	GLN	N-CA-C	5.65	122.30	109.81
3	D	726	ILE	N-CA-C	5.65	116.44	108.36
3	M	464	LEU	N-CA-C	-5.64	98.79	110.80
3	D	1031	ASN	CA-C-N	5.63	126.88	119.84
3	D	1031	ASN	C-N-CA	5.63	126.88	119.84
3	D	1323	GLN	N-CA-C	5.63	122.26	109.81
3	D	464	LEU	N-CA-C	-5.63	98.80	110.80
3	M	726	ILE	N-CA-C	5.63	116.41	108.36
5	H	174	VAL	N-CA-C	5.63	121.05	109.34
5	Q	174	VAL	N-CA-C	5.62	121.03	109.34
1	K	90	LEU	N-CA-C	5.61	117.83	107.73
3	M	1172	HIS	N-CA-C	-5.61	104.86	110.97
1	B	90	LEU	N-CA-C	5.59	117.80	107.73
3	D	521	PRO	N-CA-C	5.59	117.52	110.70
3	M	521	PRO	N-CA-C	5.59	117.52	110.70
3	D	1172	HIS	N-CA-C	-5.59	104.88	110.97
2	L	510	THR	N-CA-C	5.59	118.56	109.06
2	C	510	THR	N-CA-C	5.58	118.55	109.06
2	L	351	LEU	N-CA-C	-5.58	107.48	114.56
3	M	523	ASP	CA-C-N	5.58	132.19	121.54
3	M	523	ASP	C-N-CA	5.58	132.19	121.54
1	B	25	LEU	N-CA-C	-5.57	98.27	108.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	351	LEU	N-CA-C	-5.57	107.49	114.56
3	D	523	ASP	CA-C-N	5.57	132.17	121.54
3	D	523	ASP	C-N-CA	5.57	132.17	121.54
1	B	43	ILE	N-CA-C	-5.56	106.91	113.42
1	K	43	ILE	N-CA-C	-5.56	106.91	113.42
2	L	120	LEU	N-CA-C	5.56	116.69	108.86
1	K	25	LEU	N-CA-C	-5.56	98.30	108.02
2	C	120	LEU	N-CA-C	5.54	116.66	108.86
3	D	455	ARG	N-CA-C	5.52	117.49	108.55
2	C	732	ALA	N-CA-C	-5.51	105.37	111.71
3	M	455	ARG	N-CA-C	5.51	117.48	108.55
1	J	47	SER	N-CA-C	5.51	118.44	108.69
3	D	462	GLN	N-CA-C	-5.50	106.07	112.89
2	L	143	SER	CA-C-N	5.50	126.71	119.84
2	L	143	SER	C-N-CA	5.50	126.71	119.84
2	C	135	VAL	N-CA-C	5.50	116.58	108.45
1	A	47	SER	N-CA-C	5.49	118.41	108.69
2	C	597	ALA	N-CA-C	5.49	115.49	108.24
3	M	462	GLN	N-CA-C	-5.49	106.08	112.89
2	C	143	SER	CA-C-N	5.49	126.70	119.84
2	C	143	SER	C-N-CA	5.49	126.70	119.84
2	L	732	ALA	N-CA-C	-5.48	105.41	111.71
2	L	135	VAL	N-CA-C	5.48	116.56	108.45
2	C	722	ILE	N-CA-C	5.47	120.71	109.34
2	L	722	ILE	N-CA-C	5.46	120.70	109.34
3	D	1094	LEU	CA-C-N	5.46	127.54	120.44
3	D	1094	LEU	C-N-CA	5.46	127.54	120.44
2	L	597	ALA	N-CA-C	5.45	115.43	108.24
3	M	1094	LEU	CA-C-N	5.45	127.52	120.44
3	M	1094	LEU	C-N-CA	5.45	127.52	120.44
2	C	661	SER	N-CA-C	5.44	117.11	108.79
2	C	934	PHE	N-CA-C	5.43	118.13	109.65
2	L	661	SER	N-CA-C	5.43	117.10	108.79
2	L	934	PHE	N-CA-C	5.43	118.12	109.65
1	K	172	SER	N-CA-C	-5.42	97.82	109.81
1	A	26	GLU	N-CA-C	5.41	121.77	109.81
3	M	1046	GLN	N-CA-C	5.41	118.56	109.95
3	M	115	LEU	CA-C-N	5.41	132.44	122.92
3	M	115	LEU	C-N-CA	5.41	132.44	122.92
3	M	470	LEU	N-CA-C	-5.41	105.55	111.82
1	J	26	GLU	N-CA-C	5.40	121.74	109.81
3	D	1046	GLN	N-CA-C	5.40	118.53	109.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	172	SER	N-CA-C	-5.40	97.89	109.81
3	D	115	LEU	CA-C-N	5.40	132.42	122.92
3	D	115	LEU	C-N-CA	5.40	132.42	122.92
3	D	720	LEU	N-CA-C	5.39	117.16	108.32
2	L	76	PRO	CA-C-N	5.38	125.05	119.56
2	L	76	PRO	C-N-CA	5.38	125.05	119.56
2	L	1084	SER	N-CA-C	-5.38	104.86	111.75
2	C	76	PRO	CA-C-N	5.38	125.05	119.56
2	C	76	PRO	C-N-CA	5.38	125.05	119.56
3	M	720	LEU	N-CA-C	5.38	117.14	108.32
2	L	762	LYS	N-CA-C	5.38	122.25	110.80
2	C	762	LYS	N-CA-C	5.37	122.23	110.80
3	D	1447	LEU	N-CA-C	-5.36	105.60	111.82
2	C	1084	SER	N-CA-C	-5.36	104.89	111.75
3	D	470	LEU	N-CA-C	-5.35	105.53	111.36
1	J	118	ALA	N-CA-C	-5.35	99.41	110.80
3	M	1370	ILE	N-CA-C	-5.34	106.21	111.77
3	D	1370	ILE	N-CA-C	-5.34	106.22	111.77
1	A	118	ALA	N-CA-C	-5.34	99.43	110.80
3	D	1496	GLU	N-CA-C	-5.34	106.74	113.20
1	J	26	GLU	CA-C-N	-5.34	113.17	119.84
1	J	26	GLU	C-N-CA	-5.34	113.17	119.84
3	M	1496	GLU	N-CA-C	-5.33	106.75	113.20
3	M	1447	LEU	N-CA-C	-5.33	105.64	111.82
1	A	26	GLU	CA-C-N	-5.32	113.19	119.84
1	A	26	GLU	C-N-CA	-5.32	113.19	119.84
1	J	140	MET	N-CA-C	5.32	117.77	109.52
1	A	140	MET	N-CA-C	5.32	117.76	109.52
2	C	583	LEU	N-CA-C	-5.30	105.91	112.38
3	M	1124	GLN	N-CA-C	5.30	118.13	109.59
3	D	1228	SER	N-CA-C	-5.30	105.17	111.69
1	K	105	GLY	N-CA-C	-5.29	101.54	112.34
3	D	1124	GLN	N-CA-C	5.29	118.11	109.59
3	D	831	GLY	N-CA-C	5.29	115.02	110.21
1	B	105	GLY	N-CA-C	-5.28	101.56	112.34
2	L	583	LEU	N-CA-C	-5.28	105.94	112.38
3	M	1228	SER	N-CA-C	-5.28	105.19	111.69
2	L	210	GLU	N-CA-C	-5.28	106.52	113.12
3	D	533	GLY	CA-C-N	5.28	131.62	121.54
3	D	533	GLY	C-N-CA	5.28	131.62	121.54
3	M	533	GLY	CA-C-N	5.28	131.62	121.54
3	M	533	GLY	C-N-CA	5.28	131.62	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	210	GLU	N-CA-C	-5.28	106.53	113.12
2	L	551	GLU	N-CA-C	-5.27	104.58	112.54
2	C	869	VAL	N-CA-C	5.27	116.25	108.45
2	L	869	VAL	N-CA-C	5.26	116.23	108.45
3	M	1053	PHE	N-CA-C	5.26	117.92	110.50
2	C	547	ILE	CA-C-N	5.25	126.41	119.84
2	C	547	ILE	C-N-CA	5.25	126.41	119.84
3	D	1053	PHE	N-CA-C	5.25	117.90	110.50
2	C	551	GLU	N-CA-C	-5.25	104.61	112.54
3	M	831	GLY	N-CA-C	5.25	114.98	110.21
5	Q	148	ALA	N-CA-C	-5.25	105.47	111.14
2	C	308	ARG	N-CA-C	-5.24	104.99	111.33
3	M	1171	VAL	N-CA-C	-5.24	104.65	110.62
2	L	547	ILE	CA-C-N	5.24	126.39	119.84
2	L	547	ILE	C-N-CA	5.24	126.39	119.84
2	L	802	GLY	N-CA-C	5.24	117.08	110.38
2	C	802	GLY	N-CA-C	5.23	117.08	110.38
5	H	148	ALA	N-CA-C	-5.22	105.50	111.14
3	D	1171	VAL	N-CA-C	-5.22	104.67	110.62
2	L	308	ARG	N-CA-C	-5.21	105.02	111.33
2	L	813	VAL	N-CA-C	5.21	114.77	107.37
3	M	954	ALA	N-CA-C	-5.21	100.30	108.63
1	B	165	ILE	N-CA-C	5.20	113.10	108.63
1	K	165	ILE	N-CA-C	5.20	113.10	108.63
2	C	525	ALA	CA-C-N	5.20	126.34	119.84
2	C	525	ALA	C-N-CA	5.20	126.34	119.84
3	D	1350	ASP	N-CA-C	-5.19	107.33	113.97
2	C	591	SER	N-CA-C	-5.19	106.97	113.72
3	D	954	ALA	N-CA-C	-5.19	100.33	108.63
2	L	591	SER	N-CA-C	-5.19	106.97	113.72
2	C	813	VAL	N-CA-C	5.18	114.73	107.37
2	L	169	GLY	CA-C-N	5.18	127.04	120.51
2	L	169	GLY	C-N-CA	5.18	127.04	120.51
3	M	1350	ASP	N-CA-C	-5.17	107.35	113.97
2	L	525	ALA	CA-C-N	5.17	126.31	119.84
2	L	525	ALA	C-N-CA	5.17	126.31	119.84
2	C	169	GLY	CA-C-N	5.17	127.02	120.51
2	C	169	GLY	C-N-CA	5.17	127.02	120.51
5	H	276	PRO	N-CA-C	-5.16	103.67	111.41
2	C	69	LEU	N-CA-C	5.16	116.80	108.34
5	Q	276	PRO	N-CA-C	-5.16	103.67	111.41
2	L	69	LEU	N-CA-C	5.15	116.79	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	766	GLU	CA-C-N	5.14	126.27	119.84
2	C	766	GLU	C-N-CA	5.14	126.27	119.84
1	K	139	TYR	N-CA-C	-5.14	100.92	109.46
1	B	139	TYR	N-CA-C	-5.14	100.93	109.46
2	C	142	ARG	N-CA-C	-5.13	102.69	110.24
3	D	1112	CYS	N-CA-C	-5.13	107.53	112.97
2	L	142	ARG	N-CA-C	-5.11	102.73	110.24
2	C	563	ASN	N-CA-C	-5.11	108.31	114.75
2	L	766	GLU	CA-C-N	5.11	126.22	119.84
2	L	766	GLU	C-N-CA	5.11	126.22	119.84
2	L	801	VAL	N-CA-C	-5.11	106.59	112.98
3	M	1112	CYS	N-CA-C	-5.10	107.56	112.97
2	L	563	ASN	N-CA-C	-5.10	108.33	114.75
2	L	1024	LYS	N-CA-C	-5.08	107.37	113.21
2	C	801	VAL	N-CA-C	-5.08	106.64	112.98
3	D	537	THR	N-CA-C	5.06	115.73	108.74
2	C	1024	LYS	N-CA-C	-5.06	107.39	113.21
1	B	88	ARG	N-CA-C	5.05	117.20	109.07
3	M	537	THR	N-CA-C	5.05	115.71	108.74
1	K	88	ARG	N-CA-C	5.05	117.20	109.07
2	C	853	LEU	N-CA-C	5.04	117.26	110.31
1	K	213	GLN	N-CA-C	-5.04	107.31	113.50
1	B	213	GLN	N-CA-C	-5.03	107.31	113.50
3	D	827	ILE	N-CA-C	-5.03	108.94	113.71
3	M	513	ILE	N-CA-C	5.02	116.58	108.85
2	L	853	LEU	N-CA-C	5.02	117.24	110.31
2	L	357	GLU	N-CA-C	-5.01	107.44	113.21
2	C	256	TYR	N-CA-C	-5.01	105.48	112.45
2	C	357	GLU	N-CA-C	-5.01	107.45	113.21
2	L	256	TYR	N-CA-C	-5.00	105.50	112.45
1	J	104	GLU	N-CA-C	5.00	117.59	109.24

There are no chirality outliers.

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	242	LEU	Peptide
2	C	244	PRO	Peptide
2	C	416	GLY	Peptide
2	C	417	GLY	Peptide
2	C	418	LEU	Peptide
2	C	419	THR	Peptide

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Mol	Chain	Res	Type	Group
2	C	422	ARG	Peptide
2	C	423	ALA	Peptide
3	D	115	LEU	Peptide
3	D	521	PRO	Peptide
3	D	526	PRO	Peptide
3	D	529	GLN	Peptide
3	D	531	ASP	Peptide
3	D	534	ARG	Peptide
3	D	91	GLY	Peptide
2	L	242	LEU	Peptide
2	L	244	PRO	Peptide
2	L	416	GLY	Peptide
2	L	417	GLY	Peptide
2	L	418	LEU	Peptide
2	L	419	THR	Peptide
2	L	422	ARG	Peptide
2	L	423	ALA	Peptide
3	M	115	LEU	Peptide
3	M	521	PRO	Peptide
3	M	526	PRO	Peptide
3	M	529	GLN	Peptide
3	M	531	ASP	Peptide
3	M	534	ARG	Peptide
3	M	91	GLY	Peptide

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	672	0	241	17	0
1	B	660	0	238	16	0
1	J	672	0	241	18	0
1	K	660	0	238	16	0
2	C	3252	0	1190	140	0
2	L	3252	0	1190	141	0
3	D	3549	0	1281	177	0
3	M	3549	0	1281	182	0
4	E	276	0	96	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	N	276	0	96	19	0
5	H	966	0	342	17	0
5	Q	966	0	342	19	0
6	D	1	0	0	0	0
6	M	1	0	0	0	0
7	D	2	0	0	0	0
7	M	2	0	0	0	0
All	All	18756	0	6776	768	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 30.

All (768) 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)
3:M:44:LEU:C	3:M:45:PHE:N	1.70	1.46
3:D:44:LEU:C	3:D:45:PHE:N	1.70	1.45
3:M:933:ALA:C	3:M:935:LYS:H	1.80	0.88
2:L:542:LEU:C	2:L:544:THR:H	1.83	0.86
3:M:44:LEU:C	3:M:46:ASP:H	1.85	0.85
3:D:933:ALA:C	3:D:935:LYS:H	1.81	0.85
2:C:542:LEU:C	2:C:544:THR:H	1.83	0.85
3:M:152:LEU:C	3:M:154:THR:H	1.85	0.84
3:D:152:LEU:C	3:D:154:THR:H	1.85	0.84
3:D:44:LEU:C	3:D:46:ASP:H	1.85	0.84
2:L:533:ASP:C	2:L:535:SER:H	1.86	0.83
3:D:578:VAL:C	3:D:580:ALA:H	1.87	0.82
3:M:578:VAL:C	3:M:580:ALA:H	1.87	0.82
2:C:681:GLY:C	2:C:683:ASN:H	1.88	0.82
2:L:1033:GLY:HA2	3:M:620:GLY:HA2	1.60	0.82
2:C:1033:GLY:HA2	3:D:620:GLY:HA2	1.60	0.82
2:L:681:GLY:C	2:L:683:ASN:H	1.88	0.81
2:C:1033:GLY:CA	3:D:620:GLY:HA2	2.10	0.81
2:L:559:LEU:C	2:L:561:GLY:H	1.89	0.81
2:C:349:ALA:C	2:C:351:LEU:H	1.89	0.81
3:D:1069:GLU:C	3:D:1071:PHE:H	1.89	0.81
2:C:533:ASP:C	2:C:535:SER:H	1.86	0.81
2:L:1033:GLY:CA	3:M:620:GLY:HA2	2.10	0.81
2:C:559:LEU:C	2:C:561:GLY:H	1.89	0.81
3:M:44:LEU:C	3:M:45:PHE:CA	2.53	0.80
3:M:1069:GLU:C	3:M:1071:PHE:H	1.89	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:44:LEU:C	3:D:45:PHE:CA	2.54	0.80
2:L:349:ALA:C	2:L:351:LEU:H	1.89	0.77
5:H:151:LEU:C	5:H:153:THR:H	1.93	0.77
2:L:383:ARG:C	2:L:385:PHE:H	1.93	0.76
3:M:604:THR:C	3:M:606:ILE:H	1.94	0.76
3:D:604:THR:C	3:D:606:ILE:H	1.94	0.75
2:C:383:ARG:C	2:C:385:PHE:H	1.93	0.75
5:Q:151:LEU:C	5:Q:153:THR:H	1.93	0.75
3:D:1022:VAL:C	3:D:1024:ALA:H	1.96	0.74
3:M:1022:VAL:C	3:M:1024:ALA:H	1.96	0.73
2:L:1100:GLN:C	2:L:1102:LEU:H	1.97	0.73
3:M:975:GLU:C	3:M:977:ALA:H	1.96	0.73
2:L:544:THR:C	2:L:546:LEU:H	1.97	0.73
2:C:1100:GLN:C	2:C:1102:LEU:H	1.97	0.72
3:D:975:GLU:C	3:D:977:ALA:H	1.96	0.72
2:C:544:THR:C	2:C:546:LEU:H	1.97	0.71
5:H:276:PRO:C	5:H:278:HIS:H	1.98	0.71
2:C:1092:LEU:C	2:C:1094:ALA:H	1.97	0.71
4:E:25:LYS:C	4:E:27:ALA:H	1.98	0.71
4:N:25:LYS:C	4:N:27:ALA:H	1.98	0.70
2:C:347:GLY:C	2:C:349:ALA:H	1.99	0.70
3:D:1060:SER:C	3:D:1062:ARG:H	1.98	0.70
2:L:1092:LEU:C	2:L:1094:ALA:N	2.48	0.70
3:M:1060:SER:C	3:M:1062:ARG:H	1.98	0.70
2:L:347:GLY:C	2:L:349:ALA:H	1.99	0.69
2:L:406:HIS:C	2:L:408:ARG:H	2.01	0.69
3:M:1448:THR:C	3:M:1450:ALA:H	2.01	0.69
5:Q:276:PRO:C	5:Q:278:HIS:H	1.98	0.69
2:L:1092:LEU:C	2:L:1094:ALA:H	1.97	0.69
3:D:734:GLU:C	3:D:736:PHE:H	2.01	0.69
3:D:1448:THR:C	3:D:1450:ALA:H	2.01	0.69
2:L:437:ARG:C	2:L:439:CYS:H	2.02	0.68
3:M:734:GLU:C	3:M:736:PHE:H	2.01	0.68
2:C:406:HIS:C	2:C:408:ARG:H	2.01	0.68
2:L:542:LEU:C	2:L:544:THR:N	2.51	0.68
2:C:430:VAL:C	2:C:432:ARG:H	2.02	0.68
2:C:437:ARG:C	2:C:439:CYS:H	2.02	0.67
3:M:1191:PRO:C	3:M:1193:THR:H	2.01	0.67
2:L:430:VAL:C	2:L:432:ARG:H	2.02	0.67
3:D:1191:PRO:C	3:D:1193:THR:H	2.01	0.67
3:M:957:PRO:C	3:M:959:GLU:H	2.03	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:70:THR:C	4:E:72:ARG:H	2.02	0.67
5:H:270:ALA:C	5:H:272:THR:H	2.02	0.67
3:D:957:PRO:C	3:D:959:GLU:H	2.03	0.67
2:L:549:PHE:C	2:L:551:GLU:H	2.03	0.66
4:N:70:THR:C	4:N:72:ARG:H	2.02	0.66
2:C:561:GLY:C	2:C:563:ASN:H	2.04	0.66
5:Q:270:ALA:C	5:Q:272:THR:H	2.02	0.66
3:M:855:HIS:C	3:M:857:LEU:H	2.04	0.66
2:L:561:GLY:C	2:L:563:ASN:H	2.04	0.65
2:C:1100:GLN:C	2:C:1102:LEU:N	2.53	0.65
4:E:11:GLY:C	4:E:13:VAL:H	2.05	0.65
3:D:152:LEU:C	3:D:154:THR:N	2.54	0.65
4:N:11:GLY:C	4:N:13:VAL:H	2.05	0.65
2:C:549:PHE:C	2:C:551:GLU:H	2.03	0.65
2:L:450:GLY:C	2:L:452:ILE:H	2.04	0.64
2:C:450:GLY:C	2:C:452:ILE:H	2.04	0.64
3:M:845:ASN:C	3:M:847:ASP:H	2.06	0.64
2:C:178:ALA:C	2:C:180:GLY:H	2.05	0.64
3:M:639:LEU:C	3:M:641:GLN:H	2.05	0.64
3:M:688:TRP:C	3:M:690:ALA:H	2.05	0.64
3:D:688:TRP:C	3:D:690:ALA:H	2.05	0.64
2:L:178:ALA:C	2:L:180:GLY:H	2.05	0.64
3:M:119:SER:C	3:M:121:THR:H	2.05	0.64
3:D:757:ALA:C	3:D:759:ALA:H	2.04	0.64
2:L:523:ILE:C	2:L:525:ALA:N	2.51	0.64
3:M:503:LEU:C	3:M:505:SER:H	2.06	0.64
2:C:559:LEU:C	2:C:561:GLY:N	2.55	0.64
2:C:1092:LEU:C	2:C:1094:ALA:N	2.48	0.64
3:D:639:LEU:C	3:D:641:GLN:H	2.05	0.64
3:M:1141:GLU:C	3:M:1143:GLY:H	2.06	0.64
2:L:581:THR:C	2:L:583:LEU:H	2.06	0.64
3:D:44:LEU:C	3:D:46:ASP:N	2.56	0.63
2:L:559:LEU:C	2:L:561:GLY:N	2.55	0.63
2:C:581:THR:C	2:C:583:LEU:H	2.06	0.63
3:D:855:HIS:C	3:D:857:LEU:H	2.04	0.63
3:M:757:ALA:C	3:M:759:ALA:H	2.04	0.63
2:C:483:VAL:C	2:C:485:TYR:H	2.07	0.63
3:D:119:SER:C	3:D:121:THR:H	2.05	0.63
3:D:503:LEU:C	3:D:505:SER:H	2.06	0.63
3:D:1340:GLY:C	3:D:1342:GLU:H	2.07	0.63
2:L:325:ILE:C	2:L:327:HIS:H	2.06	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:111:ASP:C	2:C:113:VAL:H	2.07	0.63
3:M:1340:GLY:C	3:M:1342:GLU:H	2.06	0.63
2:C:325:ILE:C	2:C:327:HIS:H	2.06	0.63
2:C:424:GLY:C	2:C:426:ASP:H	2.06	0.63
1:A:217:ILE:C	1:A:219:LYS:H	2.06	0.63
2:L:406:HIS:C	2:L:408:ARG:N	2.55	0.63
2:L:424:GLY:C	2:L:426:ASP:H	2.06	0.63
3:D:1032:PRO:C	3:D:1034:GLN:H	2.08	0.62
3:D:933:ALA:C	3:D:935:LYS:N	2.50	0.62
2:L:808:ARG:C	2:L:810:ASP:H	2.07	0.62
3:D:467:GLU:C	3:D:469:ASP:H	2.08	0.62
3:M:44:LEU:C	3:M:46:ASP:N	2.55	0.62
2:C:523:ILE:C	2:C:525:ALA:N	2.51	0.62
2:C:808:ARG:C	2:C:810:ASP:H	2.07	0.62
2:L:111:ASP:C	2:L:113:VAL:H	2.07	0.62
3:M:1226:ALA:C	3:M:1228:SER:H	2.06	0.62
3:D:44:LEU:CA	3:D:45:PHE:N	2.62	0.62
3:D:877:PRO:C	3:D:879:ARG:H	2.08	0.62
1:J:217:ILE:C	1:J:219:LYS:H	2.06	0.62
2:L:1015:LEU:C	2:L:1017:THR:H	2.08	0.62
2:L:1100:GLN:C	2:L:1102:LEU:N	2.53	0.62
3:M:509:PRO:C	3:M:511:TRP:H	2.08	0.62
2:C:943:VAL:C	2:C:945:ALA:N	2.58	0.61
2:C:1015:LEU:C	2:C:1017:THR:H	2.08	0.61
3:M:643:GLY:HA3	3:M:727:GLN:H	1.65	0.61
3:D:845:ASN:C	3:D:847:ASP:H	2.05	0.61
3:D:1226:ALA:C	3:D:1228:SER:H	2.06	0.61
3:M:467:GLU:C	3:M:469:ASP:H	2.08	0.61
3:D:643:GLY:HA3	3:D:727:GLN:H	1.65	0.61
3:M:117:ASP:C	3:M:119:SER:H	2.07	0.61
3:D:1069:GLU:C	3:D:1071:PHE:N	2.58	0.61
3:D:1141:GLU:C	3:D:1143:GLY:H	2.06	0.61
3:M:44:LEU:CA	3:M:45:PHE:N	2.62	0.61
3:M:924:MET:C	3:M:926:LYS:H	2.09	0.61
3:D:924:MET:C	3:D:926:LYS:H	2.09	0.61
3:M:1069:GLU:C	3:M:1071:PHE:N	2.58	0.61
2:C:383:ARG:C	2:C:385:PHE:N	2.59	0.61
3:D:117:ASP:C	3:D:119:SER:H	2.07	0.61
2:L:383:ARG:C	2:L:385:PHE:N	2.59	0.61
5:Q:151:LEU:C	5:Q:153:THR:N	2.59	0.61
2:C:1023:GLY:C	2:C:1025:ALA:H	2.09	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:943:VAL:C	2:L:945:ALA:N	2.58	0.60
3:M:1032:PRO:C	3:M:1034:GLN:H	2.07	0.60
3:D:578:VAL:C	3:D:580:ALA:N	2.56	0.60
3:M:877:PRO:C	3:M:879:ARG:H	2.08	0.60
2:C:406:HIS:C	2:C:408:ARG:N	2.55	0.60
2:L:424:GLY:C	2:L:426:ASP:N	2.58	0.60
2:L:483:VAL:C	2:L:485:TYR:H	2.07	0.60
3:M:487:ALA:C	3:M:489:ARG:H	2.10	0.60
3:D:108:VAL:C	3:D:110:SER:N	2.58	0.60
3:M:108:VAL:C	3:M:110:SER:N	2.57	0.60
2:C:885:ILE:C	2:C:887:GLU:N	2.56	0.60
2:C:542:LEU:C	2:C:544:THR:N	2.51	0.59
2:L:349:ALA:C	2:L:351:LEU:N	2.56	0.59
2:L:1023:GLY:C	2:L:1025:ALA:H	2.09	0.59
2:C:889:HIS:C	2:C:891:GLY:N	2.58	0.59
2:L:447:ALA:C	2:L:449:ILE:H	2.10	0.59
2:C:570:PRO:C	2:C:572:ILE:H	2.09	0.59
2:C:885:ILE:C	2:C:887:GLU:H	2.09	0.59
2:L:885:ILE:C	2:L:887:GLU:H	2.09	0.59
3:D:509:PRO:C	3:D:511:TRP:H	2.08	0.59
3:M:1289:ARG:C	3:M:1291:SER:H	2.10	0.59
2:C:424:GLY:C	2:C:426:ASP:N	2.58	0.59
3:D:119:SER:C	3:D:121:THR:N	2.58	0.59
3:D:993:ILE:C	3:D:995:LEU:H	2.11	0.59
3:D:1332:PRO:C	3:D:1334:GLN:H	2.10	0.59
2:L:380:ALA:C	2:L:382:LEU:H	2.10	0.59
1:A:217:ILE:C	1:A:219:LYS:N	2.61	0.59
2:C:447:ALA:C	2:C:449:ILE:H	2.10	0.59
3:D:1289:ARG:C	3:D:1291:SER:H	2.10	0.59
3:M:578:VAL:C	3:M:580:ALA:N	2.56	0.59
2:C:349:ALA:C	2:C:351:LEU:N	2.56	0.58
2:C:380:ALA:C	2:C:382:LEU:H	2.10	0.58
2:L:885:ILE:C	2:L:887:GLU:N	2.56	0.58
2:L:570:PRO:C	2:L:572:ILE:H	2.09	0.58
1:J:217:ILE:C	1:J:219:LYS:N	2.61	0.58
3:M:933:ALA:C	3:M:935:LYS:N	2.50	0.58
1:B:34:VAL:C	1:B:36:LEU:N	2.61	0.58
2:C:532:MET:C	2:C:534:VAL:H	2.12	0.58
2:L:336:VAL:C	2:L:338:GLU:H	2.11	0.58
2:C:533:ASP:C	2:C:535:SER:N	2.57	0.58
2:C:571:LEU:C	2:C:573:ARG:H	2.11	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:487:ALA:C	3:D:489:ARG:H	2.10	0.58
2:L:532:MET:C	2:L:534:VAL:H	2.12	0.58
2:C:892:LEU:C	2:C:894:GLY:H	2.12	0.58
2:L:356:ARG:C	2:L:358:ARG:H	2.11	0.58
2:L:889:HIS:C	2:L:891:GLY:N	2.58	0.58
3:M:845:ASN:C	3:M:847:ASP:N	2.58	0.58
2:L:571:LEU:C	2:L:573:ARG:H	2.11	0.57
3:M:119:SER:C	3:M:121:THR:N	2.58	0.57
3:M:1340:GLY:C	3:M:1342:GLU:N	2.62	0.57
3:M:470:LEU:C	3:M:472:LYS:H	2.13	0.57
3:M:993:ILE:C	3:M:995:LEU:H	2.11	0.57
2:C:336:VAL:C	2:C:338:GLU:H	2.11	0.57
3:M:152:LEU:C	3:M:154:THR:N	2.54	0.57
3:D:465:LEU:C	3:D:467:GLU:H	2.12	0.57
3:D:685:ASP:C	3:D:687:VAL:H	2.13	0.57
2:L:892:LEU:C	2:L:894:GLY:H	2.12	0.57
2:L:1033:GLY:HA3	3:M:620:GLY:HA2	1.86	0.56
3:M:1332:PRO:C	3:M:1334:GLN:H	2.11	0.56
2:C:356:ARG:C	2:C:358:ARG:H	2.11	0.56
3:D:1196:THR:C	3:D:1198:TYR:H	2.12	0.56
1:J:79:ILE:C	1:J:81:ASN:H	2.13	0.56
3:M:685:ASP:C	3:M:687:VAL:H	2.13	0.56
3:D:1020:LEU:C	3:D:1022:VAL:H	2.14	0.56
3:M:465:LEU:C	3:M:467:GLU:H	2.12	0.56
5:H:322:THR:C	5:H:324:LYS:H	2.14	0.56
5:Q:322:THR:C	5:Q:324:LYS:H	2.14	0.56
1:K:34:VAL:C	1:K:36:LEU:N	2.61	0.56
2:C:396:ASP:C	2:C:398:THR:H	2.15	0.56
2:C:1033:GLY:HA3	3:D:620:GLY:HA2	1.86	0.56
3:D:604:THR:C	3:D:606:ILE:N	2.62	0.56
3:D:541:ASN:C	3:D:543:LEU:N	2.61	0.55
1:A:79:ILE:C	1:A:81:ASN:H	2.13	0.55
3:D:108:VAL:C	3:D:110:SER:H	2.14	0.55
3:D:470:LEU:C	3:D:472:LYS:H	2.13	0.55
3:D:960:LYS:C	3:D:962:ARG:H	2.15	0.55
3:M:957:PRO:C	3:M:959:GLU:N	2.65	0.55
3:M:1020:LEU:C	3:M:1022:VAL:H	2.14	0.55
3:M:960:LYS:C	3:M:962:ARG:H	2.15	0.55
3:M:1196:THR:C	3:M:1198:TYR:H	2.12	0.55
2:C:723:THR:C	2:C:725:ASP:H	2.14	0.55
3:M:950:GLY:C	3:M:952:ASP:N	2.63	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:VAL:H	2:C:608:GLY:CA	2.20	0.55
3:D:1332:PRO:C	3:D:1334:GLN:N	2.64	0.55
2:L:198:ARG:C	2:L:200:LEU:H	2.15	0.55
3:D:924:MET:C	3:D:926:LYS:N	2.64	0.55
3:D:957:PRO:C	3:D:959:GLU:N	2.65	0.55
3:D:1340:GLY:C	3:D:1342:GLU:N	2.62	0.55
1:J:71:VAL:H	2:L:608:GLY:CA	2.20	0.55
2:L:533:ASP:C	2:L:535:SER:N	2.57	0.55
2:L:919:ALA:C	2:L:921:ALA:N	2.64	0.55
3:M:1332:PRO:C	3:M:1334:GLN:N	2.64	0.55
3:M:108:VAL:C	3:M:110:SER:H	2.14	0.55
2:L:723:THR:C	2:L:725:ASP:H	2.15	0.54
2:C:198:ARG:C	2:C:200:LEU:H	2.15	0.54
3:D:960:LYS:C	3:D:962:ARG:N	2.65	0.54
2:L:302:VAL:C	2:L:304:LEU:H	2.15	0.54
2:L:523:ILE:C	2:L:525:ALA:H	2.15	0.54
3:M:541:ASN:C	3:M:543:LEU:N	2.61	0.54
2:L:396:ASP:C	2:L:398:THR:H	2.15	0.54
2:C:302:VAL:C	2:C:304:LEU:H	2.15	0.54
2:C:523:ILE:C	2:C:525:ALA:H	2.15	0.54
3:M:924:MET:C	3:M:926:LYS:N	2.64	0.54
1:B:31:GLY:C	1:B:33:GLY:H	2.15	0.54
2:L:111:ASP:C	2:L:113:VAL:N	2.65	0.54
5:H:151:LEU:C	5:H:153:THR:N	2.59	0.54
2:C:1041:GLU:C	2:C:1043:TYR:N	2.64	0.54
2:C:681:GLY:C	2:C:683:ASN:N	2.55	0.54
2:C:919:ALA:C	2:C:921:ALA:N	2.64	0.54
2:L:892:LEU:C	2:L:894:GLY:N	2.66	0.53
3:M:1228:SER:C	3:M:1230:GLY:H	2.16	0.53
2:C:89:THR:C	2:C:91:GLN:H	2.17	0.53
3:D:950:GLY:C	3:D:952:ASP:N	2.63	0.53
3:M:1191:PRO:C	3:M:1193:THR:N	2.67	0.53
4:N:25:LYS:C	4:N:27:ALA:N	2.66	0.53
2:C:774:LEU:C	2:C:776:SER:N	2.66	0.53
3:D:593:ASN:CA	3:D:594:PRO:C	2.81	0.53
1:K:31:GLY:C	1:K:33:GLY:H	2.15	0.53
3:M:593:ASN:CA	3:M:594:PRO:C	2.81	0.53
2:C:892:LEU:C	2:C:894:GLY:N	2.66	0.53
3:D:845:ASN:C	3:D:847:ASP:N	2.58	0.53
3:D:1228:SER:C	3:D:1230:GLY:H	2.16	0.53
2:L:581:THR:C	2:L:583:LEU:N	2.65	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:532:MET:C	2:C:534:VAL:N	2.67	0.53
3:M:1060:SER:C	3:M:1062:ARG:N	2.67	0.53
1:B:172:SER:C	1:B:174:VAL:H	2.17	0.53
2:C:27:LYS:C	2:C:29:ALA:N	2.67	0.53
1:J:223:ASN:C	1:J:225:PHE:N	2.65	0.53
2:L:89:THR:C	2:L:91:GLN:H	2.16	0.53
3:D:1060:SER:C	3:D:1062:ARG:N	2.67	0.53
3:D:1448:THR:C	3:D:1450:ALA:N	2.67	0.53
1:K:223:ASN:C	1:K:225:PHE:H	2.17	0.53
2:L:774:LEU:C	2:L:776:SER:N	2.66	0.53
3:M:1223:VAL:C	3:M:1225:ALA:N	2.65	0.53
3:M:960:LYS:C	3:M:962:ARG:N	2.65	0.52
3:D:100:ALA:C	3:D:102:ILE:H	2.18	0.52
1:K:105:GLY:HA2	1:K:136:GLY:HA3	1.91	0.52
2:L:1041:GLU:C	2:L:1043:TYR:N	2.64	0.52
3:M:100:ALA:C	3:M:102:ILE:H	2.18	0.52
3:M:1226:ALA:C	3:M:1228:SER:N	2.68	0.52
2:L:532:MET:C	2:L:534:VAL:N	2.67	0.52
1:A:122:ILE:C	1:A:124:ASN:H	2.18	0.52
3:D:1331:ASP:C	3:D:1333:HIS:N	2.65	0.52
2:L:544:THR:C	2:L:546:LEU:N	2.63	0.52
1:A:223:ASN:C	1:A:225:PHE:N	2.65	0.52
4:E:43:GLU:C	4:E:45:ARG:N	2.67	0.52
3:M:1448:THR:C	3:M:1450:ALA:N	2.67	0.52
1:B:223:ASN:C	1:B:225:PHE:H	2.17	0.52
2:C:581:THR:C	2:C:583:LEU:N	2.65	0.52
3:M:102:ILE:C	3:M:104:PHE:N	2.64	0.52
4:E:43:GLU:C	4:E:45:ARG:H	2.18	0.52
3:D:1022:VAL:C	3:D:1024:ALA:N	2.61	0.52
1:K:172:SER:C	1:K:174:VAL:H	2.17	0.52
2:L:583:LEU:C	2:L:585:GLU:N	2.68	0.52
3:M:877:PRO:C	3:M:879:ARG:N	2.68	0.52
2:C:111:ASP:C	2:C:113:VAL:N	2.65	0.52
3:D:102:ILE:C	3:D:104:PHE:N	2.64	0.52
3:M:1022:VAL:C	3:M:1024:ALA:N	2.61	0.52
3:D:1321:ALA:C	3:D:1323:GLN:H	2.16	0.51
1:J:122:ILE:C	1:J:124:ASN:H	2.18	0.51
2:C:1083:GLU:C	2:C:1085:PHE:N	2.66	0.51
3:M:1331:ASP:C	3:M:1333:HIS:N	2.65	0.51
1:B:105:GLY:HA2	1:B:136:GLY:HA3	1.91	0.51
2:C:272:ALA:C	2:C:274:ARG:N	2.67	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:148:GLU:C	3:M:150:ARG:H	2.18	0.51
3:D:1226:ALA:C	3:D:1228:SER:N	2.68	0.51
1:K:223:ASN:C	1:K:225:PHE:N	2.68	0.51
2:L:1083:GLU:C	2:L:1085:PHE:N	2.66	0.51
2:C:342:ASP:C	2:C:344:PHE:H	2.18	0.51
2:C:437:ARG:C	2:C:439:CYS:N	2.69	0.51
3:D:1223:VAL:C	3:D:1225:ALA:N	2.65	0.51
5:H:378:GLU:C	5:H:380:GLU:H	2.19	0.51
3:D:150:ARG:C	3:D:152:LEU:H	2.19	0.51
5:Q:378:GLU:C	5:Q:380:GLU:H	2.19	0.51
2:L:342:ASP:C	2:L:344:PHE:H	2.18	0.51
3:M:508:ARG:C	3:M:510:GLU:H	2.19	0.51
3:M:841:PHE:C	3:M:843:PHE:H	2.19	0.51
3:M:688:TRP:C	3:M:690:ALA:N	2.69	0.51
5:Q:179:LYS:C	5:Q:181:LEU:H	2.19	0.51
3:D:148:GLU:C	3:D:150:ARG:H	2.18	0.51
3:D:877:PRO:C	3:D:879:ARG:N	2.68	0.51
3:M:1321:ALA:C	3:M:1323:GLN:H	2.16	0.51
5:H:216:LYS:C	5:H:218:THR:H	2.19	0.50
3:M:117:ASP:C	3:M:119:SER:N	2.69	0.50
5:Q:421:ARG:C	5:Q:423:LEU:H	2.19	0.50
3:D:117:ASP:C	3:D:119:SER:N	2.70	0.50
3:M:150:ARG:C	3:M:152:LEU:H	2.19	0.50
4:N:43:GLU:C	4:N:45:ARG:N	2.68	0.50
1:J:118:ALA:C	1:J:120:VAL:H	2.20	0.50
3:D:1090:ASP:C	3:D:1092:GLY:N	2.69	0.50
5:Q:216:LYS:C	5:Q:218:THR:H	2.19	0.50
2:C:583:LEU:C	2:C:585:GLU:N	2.68	0.50
3:D:508:ARG:C	3:D:510:GLU:H	2.19	0.50
3:D:989:TYR:C	3:D:991:GLN:N	2.66	0.50
2:L:1085:PHE:C	2:L:1087:VAL:N	2.66	0.50
3:M:1090:ASP:C	3:M:1092:GLY:N	2.69	0.50
4:N:43:GLU:C	4:N:45:ARG:H	2.18	0.50
3:D:841:PHE:C	3:D:843:PHE:H	2.19	0.50
2:L:437:ARG:C	2:L:439:CYS:N	2.69	0.50
2:L:976:ASP:C	2:L:978:ARG:H	2.19	0.50
3:M:580:ALA:C	3:M:582:ILE:N	2.69	0.50
3:D:487:ALA:C	3:D:489:ARG:N	2.70	0.50
3:D:740:PHE:C	3:D:742:GLY:H	2.20	0.50
5:H:421:ARG:C	5:H:423:LEU:H	2.19	0.50
1:J:156:HIS:C	1:J:158:ILE:H	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:34:TYR:C	3:M:36:THR:N	2.66	0.50
3:M:487:ALA:C	3:M:489:ARG:N	2.70	0.50
3:D:1196:THR:C	3:D:1198:TYR:N	2.70	0.50
2:L:774:LEU:C	2:L:776:SER:H	2.20	0.50
2:L:1001:VAL:C	2:L:1003:ASP:N	2.68	0.50
1:A:111:ALA:C	1:A:113:ASP:H	2.20	0.49
3:D:34:TYR:C	3:D:36:THR:N	2.66	0.49
3:D:1191:PRO:C	3:D:1193:THR:N	2.67	0.49
4:E:84:ARG:C	4:E:86:GLN:N	2.70	0.49
5:H:179:LYS:C	5:H:181:LEU:H	2.19	0.49
1:J:70:GLY:HA3	1:J:135:GLY:HA3	1.93	0.49
2:L:342:ASP:C	2:L:344:PHE:N	2.70	0.49
3:M:930:LEU:C	3:M:932:ASP:N	2.69	0.49
3:M:1141:GLU:C	3:M:1143:GLY:N	2.68	0.49
2:C:342:ASP:C	2:C:344:PHE:N	2.70	0.49
4:E:86:GLN:C	4:E:89:MET:H	2.20	0.49
1:K:34:VAL:C	1:K:36:LEU:H	2.21	0.49
2:L:27:LYS:C	2:L:29:ALA:N	2.67	0.49
3:M:619:LEU:C	3:M:621:LYS:H	2.20	0.49
3:M:1260:ILE:C	3:M:1262:LEU:N	2.68	0.49
4:N:86:GLN:C	4:N:89:MET:H	2.20	0.49
5:Q:270:ALA:C	5:Q:272:THR:N	2.69	0.49
2:C:178:ALA:C	2:C:180:GLY:N	2.70	0.49
2:C:976:ASP:C	2:C:978:ARG:H	2.19	0.49
2:C:1085:PHE:C	2:C:1087:VAL:N	2.66	0.49
3:D:688:TRP:C	3:D:690:ALA:N	2.69	0.49
1:A:70:GLY:HA3	1:A:135:GLY:HA3	1.93	0.49
2:C:1001:VAL:C	2:C:1003:ASP:N	2.68	0.49
3:M:470:LEU:C	3:M:472:LYS:N	2.71	0.49
3:M:740:PHE:C	3:M:742:GLY:H	2.20	0.49
3:M:1196:THR:C	3:M:1198:TYR:N	2.70	0.49
1:A:156:HIS:C	1:A:158:ILE:H	2.20	0.49
2:C:583:LEU:C	2:C:585:GLU:H	2.21	0.49
2:C:774:LEU:C	2:C:776:SER:H	2.20	0.49
1:J:111:ALA:C	1:J:113:ASP:H	2.20	0.49
3:M:937:TYR:C	3:M:939:PHE:N	2.70	0.49
1:B:223:ASN:C	1:B:225:PHE:N	2.68	0.49
3:D:580:ALA:C	3:D:582:ILE:N	2.69	0.49
3:D:1260:ILE:C	3:D:1262:LEU:N	2.68	0.49
2:L:178:ALA:C	2:L:180:GLY:N	2.70	0.49
2:L:272:ALA:C	2:L:274:ARG:N	2.67	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:VAL:C	1:B:36:LEU:H	2.21	0.49
3:D:639:LEU:C	3:D:641:GLN:N	2.71	0.49
3:D:757:ALA:C	3:D:759:ALA:N	2.70	0.49
2:C:325:ILE:C	2:C:327:HIS:N	2.71	0.49
3:D:619:LEU:C	3:D:621:LYS:H	2.20	0.49
3:D:892:ASP:C	3:D:894:LYS:N	2.70	0.49
5:H:211:VAL:C	5:H:213:ILE:H	2.20	0.49
1:K:79:ILE:C	1:K:81:ASN:N	2.70	0.49
3:D:710:ARG:C	3:D:712:GLY:N	2.65	0.48
3:D:1172:HIS:C	3:D:1174:LEU:N	2.70	0.48
3:D:1220:ALA:C	3:D:1222:GLY:N	2.68	0.48
2:L:20:GLU:C	2:L:22:GLN:N	2.71	0.48
3:D:815:ALA:C	3:D:817:GLU:H	2.21	0.48
5:H:276:PRO:C	5:H:278:HIS:N	2.65	0.48
3:M:710:ARG:C	3:M:712:GLY:N	2.65	0.48
3:M:815:ALA:C	3:M:817:GLU:H	2.21	0.48
2:L:325:ILE:C	2:L:327:HIS:N	2.71	0.48
2:L:919:ALA:C	2:L:921:ALA:H	2.21	0.48
2:L:1033:GLY:HA2	3:M:620:GLY:CA	2.37	0.48
3:M:1220:ALA:C	3:M:1222:GLY:N	2.68	0.48
3:M:1321:ALA:C	3:M:1323:GLN:N	2.71	0.48
2:C:965:GLU:C	2:C:967:PHE:N	2.71	0.48
3:D:930:LEU:C	3:D:932:ASP:N	2.69	0.48
3:D:993:ILE:C	3:D:995:LEU:N	2.71	0.48
1:A:118:ALA:C	1:A:120:VAL:H	2.20	0.48
2:L:583:LEU:C	2:L:585:GLU:H	2.21	0.48
2:L:946:ARG:C	2:L:948:GLU:N	2.71	0.48
2:L:1041:GLU:C	2:L:1043:TYR:H	2.21	0.48
3:M:996:TRP:C	3:M:998:GLU:N	2.69	0.48
4:N:84:ARG:C	4:N:86:GLN:N	2.70	0.48
2:L:582:GLY:C	2:L:584:GLU:N	2.68	0.48
3:M:892:ASP:C	3:M:894:LYS:N	2.70	0.48
2:C:20:GLU:C	2:C:22:GLN:N	2.71	0.48
2:C:430:VAL:C	2:C:432:ARG:N	2.72	0.48
3:D:1141:GLU:C	3:D:1143:GLY:N	2.68	0.48
3:M:975:GLU:C	3:M:977:ALA:N	2.65	0.48
3:M:1386:ASP:C	3:M:1388:ARG:H	2.22	0.48
3:M:1462:LEU:C	3:M:1464:GLU:N	2.69	0.48
5:Q:211:VAL:C	5:Q:213:ILE:H	2.20	0.48
2:C:561:GLY:C	2:C:563:ASN:N	2.71	0.48
3:D:22:SER:C	3:D:24:GLY:H	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:602:SER:C	3:M:604:THR:H	2.22	0.48
3:M:1172:HIS:C	3:M:1174:LEU:N	2.70	0.48
3:D:1386:ASP:C	3:D:1388:ARG:H	2.22	0.47
2:C:919:ALA:C	2:C:921:ALA:H	2.21	0.47
2:C:1041:GLU:C	2:C:1043:TYR:H	2.21	0.47
3:D:602:SER:C	3:D:604:THR:H	2.22	0.47
4:E:70:THR:C	4:E:72:ARG:N	2.69	0.47
4:E:83:ASP:C	4:E:85:LEU:H	2.22	0.47
1:A:189:ARG:C	1:A:191:ASP:H	2.22	0.47
2:C:570:PRO:C	2:C:572:ILE:N	2.72	0.47
2:C:692:GLU:C	2:C:694:LEU:N	2.70	0.47
2:C:946:ARG:C	2:C:948:GLU:N	2.71	0.47
1:J:71:VAL:C	2:L:608:GLY:HA2	2.40	0.47
3:D:937:TYR:C	3:D:939:PHE:N	2.70	0.47
3:D:731:LEU:C	3:D:733:CYS:N	2.70	0.47
3:M:22:SER:C	3:M:24:GLY:H	2.22	0.47
3:M:731:LEU:C	3:M:733:CYS:N	2.70	0.47
3:M:764:LEU:C	3:M:766:ALA:N	2.73	0.47
3:M:937:TYR:C	3:M:939:PHE:H	2.23	0.47
1:B:79:ILE:C	1:B:81:ASN:N	2.70	0.47
2:C:544:THR:C	2:C:546:LEU:N	2.63	0.47
2:L:570:PRO:C	2:L:572:ILE:N	2.72	0.47
3:M:467:GLU:C	3:M:469:ASP:N	2.73	0.47
3:M:757:ALA:C	3:M:759:ALA:N	2.70	0.47
3:M:989:TYR:C	3:M:991:GLN:N	2.66	0.47
3:M:1098:LEU:C	3:M:1100:ASP:N	2.72	0.47
2:C:302:VAL:C	2:C:304:LEU:N	2.73	0.47
3:D:937:TYR:C	3:D:939:PHE:H	2.23	0.47
3:M:1009:LYS:C	3:M:1011:PHE:N	2.70	0.47
1:A:71:VAL:C	2:C:608:GLY:HA2	2.40	0.47
2:C:808:ARG:C	2:C:810:ASP:N	2.73	0.47
3:D:470:LEU:C	3:D:472:LYS:N	2.71	0.47
3:D:1462:LEU:C	3:D:1464:GLU:N	2.69	0.47
1:J:79:ILE:C	1:J:81:ASN:N	2.72	0.47
2:L:1015:LEU:C	2:L:1017:THR:N	2.73	0.47
3:D:1321:ALA:C	3:D:1323:GLN:N	2.71	0.47
4:E:17:TYR:C	4:E:19:LEU:N	2.72	0.47
2:L:549:PHE:C	2:L:551:GLU:N	2.72	0.47
5:Q:179:LYS:C	5:Q:181:LEU:N	2.71	0.47
2:C:320:HIS:C	2:C:322:VAL:H	2.23	0.46
3:D:996:TRP:C	3:D:998:GLU:N	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1098:LEU:C	3:D:1100:ASP:N	2.72	0.46
4:E:67:GLU:C	4:E:69:LEU:H	2.24	0.46
4:N:17:TYR:C	4:N:19:LEU:N	2.72	0.46
4:N:67:GLU:C	4:N:69:LEU:H	2.24	0.46
1:J:189:ARG:C	1:J:191:ASP:H	2.22	0.46
4:N:84:ARG:C	4:N:87:LYS:H	2.24	0.46
2:C:582:GLY:C	2:C:584:GLU:N	2.68	0.46
2:C:1001:VAL:C	2:C:1003:ASP:H	2.23	0.46
3:D:764:LEU:C	3:D:766:ALA:H	2.24	0.46
3:D:885:ILE:C	3:D:887:GLY:N	2.73	0.46
2:L:463:ALA:C	2:L:465:GLY:N	2.72	0.46
2:L:681:GLY:C	2:L:683:ASN:N	2.55	0.46
2:L:808:ARG:C	2:L:810:ASP:N	2.73	0.46
3:M:993:ILE:C	3:M:995:LEU:N	2.71	0.46
4:N:83:ASP:C	4:N:85:LEU:H	2.22	0.46
5:Q:276:PRO:C	5:Q:278:HIS:N	2.65	0.46
2:C:663:GLU:C	2:C:665:PHE:H	2.24	0.46
3:D:82:ARG:C	3:D:84:ILE:H	2.23	0.46
4:E:11:GLY:C	4:E:13:VAL:N	2.71	0.46
2:L:1001:VAL:C	2:L:1003:ASP:H	2.23	0.46
2:C:549:PHE:C	2:C:551:GLU:N	2.72	0.46
3:D:941:LEU:C	3:D:943:THR:N	2.71	0.46
3:D:1032:PRO:C	3:D:1034:GLN:N	2.74	0.46
3:M:855:HIS:C	3:M:857:LEU:N	2.70	0.46
3:D:465:LEU:C	3:D:467:GLU:N	2.72	0.46
5:H:179:LYS:C	5:H:181:LEU:N	2.71	0.46
2:L:302:VAL:C	2:L:304:LEU:N	2.73	0.46
3:M:56:TYR:C	3:M:58:CYS:H	2.24	0.46
3:D:1129:THR:C	3:D:1131:THR:H	2.24	0.46
3:D:1270:ALA:C	3:D:1272:ALA:H	2.23	0.46
3:M:1331:ASP:C	3:M:1333:HIS:H	2.24	0.46
3:D:1020:LEU:C	3:D:1022:VAL:N	2.74	0.46
3:D:1331:ASP:C	3:D:1333:HIS:H	2.24	0.46
4:E:25:LYS:C	4:E:27:ALA:N	2.66	0.46
3:M:541:ASN:C	3:M:543:LEU:H	2.24	0.46
3:M:1270:ALA:C	3:M:1272:ALA:H	2.23	0.46
2:C:943:VAL:C	2:C:945:ALA:H	2.24	0.46
2:L:692:GLU:C	2:L:694:LEU:N	2.70	0.46
3:M:604:THR:C	3:M:606:ILE:N	2.62	0.46
3:M:1129:THR:C	3:M:1131:THR:H	2.24	0.46
2:C:463:ALA:C	2:C:465:GLY:N	2.72	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:917:LEU:C	2:C:919:ALA:N	2.73	0.45
3:D:541:ASN:C	3:D:543:LEU:H	2.24	0.45
3:D:1090:ASP:C	3:D:1092:GLY:H	2.23	0.45
2:L:943:VAL:C	2:L:945:ALA:H	2.24	0.45
3:M:82:ARG:C	3:M:84:ILE:H	2.23	0.45
3:M:1353:GLN:C	3:M:1355:VAL:N	2.74	0.45
4:N:70:THR:C	4:N:72:ARG:N	2.69	0.45
3:M:734:GLU:C	3:M:736:PHE:N	2.68	0.45
2:C:347:GLY:C	2:C:349:ALA:N	2.70	0.45
2:C:884:GLN:C	2:C:886:LEU:N	2.75	0.45
2:L:965:GLU:C	2:L:967:PHE:N	2.71	0.45
3:M:1032:PRO:C	3:M:1034:GLN:N	2.74	0.45
5:Q:94:ASP:C	5:Q:96:VAL:H	2.25	0.45
2:C:520:GLU:C	2:C:522:VAL:N	2.75	0.45
3:M:1090:ASP:C	3:M:1092:GLY:H	2.23	0.45
4:N:57:ASP:C	4:N:59:ASN:H	2.25	0.45
1:B:172:SER:C	1:B:174:VAL:N	2.75	0.45
4:E:84:ARG:C	4:E:87:LYS:H	2.24	0.45
2:L:380:ALA:C	2:L:382:LEU:N	2.75	0.45
2:L:561:GLY:C	2:L:563:ASN:N	2.71	0.45
2:C:1033:GLY:HA2	3:D:620:GLY:CA	2.37	0.45
3:D:1353:GLN:C	3:D:1355:VAL:N	2.74	0.45
2:L:320:HIS:C	2:L:322:VAL:H	2.23	0.45
2:L:732:ALA:C	2:L:734:LEU:N	2.75	0.45
2:L:450:GLY:C	2:L:452:ILE:N	2.70	0.45
2:L:663:GLU:C	2:L:665:PHE:H	2.24	0.45
3:M:509:PRO:C	3:M:511:TRP:N	2.75	0.45
3:M:571:LYS:C	3:M:573:MET:N	2.74	0.45
2:C:915:LYS:C	2:C:917:LEU:N	2.73	0.45
3:D:31:THR:C	3:D:33:ASN:H	2.25	0.45
3:D:571:LYS:C	3:D:573:MET:N	2.74	0.45
2:C:63:GLY:HA3	2:C:102:HIS:CA	2.47	0.45
5:H:94:ASP:C	5:H:96:VAL:H	2.25	0.45
3:D:56:TYR:C	3:D:58:CYS:H	2.24	0.45
3:D:491:LYS:C	3:D:493:ARG:N	2.73	0.45
2:L:884:GLN:C	2:L:886:LEU:N	2.75	0.45
3:M:690:ALA:C	3:M:692:GLU:N	2.75	0.45
2:C:447:ALA:C	2:C:449:ILE:N	2.75	0.44
2:C:679:PHE:C	2:C:681:GLY:N	2.75	0.44
2:L:63:GLY:HA3	2:L:102:HIS:CA	2.47	0.44
3:M:138:LYS:C	3:M:140:ALA:H	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:941:LEU:C	3:M:943:THR:N	2.71	0.44
3:D:21:TRP:C	3:D:23:TYR:N	2.73	0.44
3:D:503:LEU:C	3:D:505:SER:N	2.75	0.44
2:C:1055:ILE:C	2:C:1057:SER:H	2.25	0.44
3:D:509:PRO:C	3:D:511:TRP:N	2.75	0.44
3:D:1289:ARG:C	3:D:1291:SER:N	2.76	0.44
5:H:94:ASP:C	5:H:96:VAL:N	2.76	0.44
2:L:693:GLU:C	2:L:695:LEU:H	2.25	0.44
2:L:915:LYS:C	2:L:917:LEU:N	2.73	0.44
3:M:639:LEU:C	3:M:641:GLN:N	2.71	0.44
2:C:335:THR:C	2:C:337:GLY:N	2.76	0.44
3:D:472:LYS:C	3:D:474:GLU:H	2.26	0.44
3:D:1467:ILE:C	3:D:1469:GLY:H	2.26	0.44
2:L:335:THR:C	2:L:337:GLY:N	2.76	0.44
2:L:679:PHE:C	2:L:681:GLY:N	2.75	0.44
2:L:925:TYR:C	2:L:927:GLY:N	2.75	0.44
3:M:885:ILE:C	3:M:887:GLY:N	2.73	0.44
1:A:134:GLU:C	1:A:136:GLY:H	2.25	0.44
3:D:934:LEU:C	3:D:938:GLY:HA3	2.43	0.44
3:D:1352:ILE:C	3:D:1354:LYS:N	2.74	0.44
2:L:1055:ILE:C	2:L:1057:SER:H	2.25	0.44
3:M:21:TRP:C	3:M:23:TYR:N	2.73	0.44
3:M:1020:LEU:C	3:M:1022:VAL:N	2.74	0.44
3:M:1100:ASP:C	3:M:1102:ALA:N	2.75	0.44
5:Q:94:ASP:C	5:Q:96:VAL:N	2.76	0.44
2:C:336:VAL:C	2:C:338:GLU:N	2.76	0.44
2:L:723:THR:C	2:L:725:ASP:N	2.76	0.44
3:M:764:LEU:C	3:M:766:ALA:H	2.24	0.44
5:Q:421:ARG:C	5:Q:423:LEU:N	2.76	0.44
3:D:550:ARG:C	3:D:552:ASN:N	2.76	0.44
5:H:421:ARG:C	5:H:423:LEU:N	2.76	0.44
1:K:172:SER:C	1:K:174:VAL:N	2.75	0.44
3:M:31:THR:C	3:M:33:ASN:H	2.25	0.44
3:M:472:LYS:C	3:M:474:GLU:H	2.25	0.44
2:C:925:TYR:C	2:C:927:GLY:N	2.75	0.43
3:D:84:ILE:C	3:D:86:ARG:H	2.26	0.43
3:D:138:LYS:C	3:D:140:ALA:H	2.25	0.43
1:K:70:GLY:HA3	1:K:135:GLY:HA3	2.00	0.43
2:L:520:GLU:C	2:L:522:VAL:N	2.75	0.43
1:A:79:ILE:C	1:A:81:ASN:N	2.72	0.43
1:A:156:HIS:C	1:A:158:ILE:N	2.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:550:ARG:C	3:M:552:ASN:N	2.76	0.43
3:M:1067:VAL:C	3:M:1069:GLU:N	2.75	0.43
2:C:277:ALA:C	2:C:279:GLU:H	2.26	0.43
3:D:1009:LYS:C	3:D:1011:PHE:N	2.70	0.43
3:M:934:LEU:C	3:M:938:GLY:HA3	2.43	0.43
4:E:83:ASP:C	4:E:85:LEU:N	2.76	0.43
2:C:776:SER:C	2:C:778:PHE:N	2.75	0.43
3:D:764:LEU:C	3:D:766:ALA:N	2.72	0.43
4:E:57:ASP:C	4:E:59:ASN:H	2.24	0.43
4:E:81:PRO:C	4:E:83:ASP:N	2.74	0.43
1:J:223:ASN:C	1:J:225:PHE:H	2.26	0.43
1:K:217:ILE:C	1:K:219:LYS:N	2.75	0.43
2:L:122:THR:C	2:L:124:ASP:N	2.75	0.43
3:M:691:LEU:C	3:M:693:GLU:H	2.27	0.43
1:B:59:GLU:C	1:B:61:VAL:H	2.26	0.43
2:C:380:ALA:C	2:C:382:LEU:N	2.75	0.43
3:D:34:TYR:C	3:D:36:THR:H	2.26	0.43
1:K:59:GLU:C	1:K:61:VAL:H	2.26	0.43
5:Q:211:VAL:C	5:Q:213:ILE:N	2.76	0.43
2:C:23:VAL:C	2:C:25:SER:N	2.76	0.43
2:C:723:THR:C	2:C:725:ASP:N	2.76	0.43
3:D:975:GLU:C	3:D:977:ALA:N	2.65	0.43
3:M:503:LEU:C	3:M:505:SER:N	2.75	0.43
3:M:1352:ILE:C	3:M:1354:LYS:N	2.74	0.43
4:N:11:GLY:C	4:N:13:VAL:N	2.71	0.43
4:N:23:VAL:C	4:N:25:LYS:H	2.27	0.43
4:E:23:VAL:C	4:E:25:LYS:H	2.27	0.43
1:J:134:GLU:C	1:J:136:GLY:H	2.25	0.43
2:L:23:VAL:C	2:L:25:SER:N	2.76	0.43
3:M:84:ILE:C	3:M:86:ARG:H	2.26	0.43
3:M:102:ILE:C	3:M:104:PHE:H	2.27	0.43
3:M:1228:SER:C	3:M:1230:GLY:N	2.76	0.43
2:C:450:GLY:C	2:C:452:ILE:N	2.70	0.43
4:N:83:ASP:C	4:N:85:LEU:N	2.76	0.43
1:A:223:ASN:C	1:A:225:PHE:H	2.26	0.43
1:B:70:GLY:HA3	1:B:135:GLY:HA3	2.00	0.43
2:C:693:GLU:C	2:C:695:LEU:H	2.26	0.43
2:C:1015:LEU:C	2:C:1017:THR:N	2.73	0.43
3:D:1228:SER:C	3:D:1230:GLY:N	2.76	0.43
2:L:277:ALA:C	2:L:279:GLU:H	2.26	0.43
2:L:447:ALA:C	2:L:449:ILE:N	2.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:1467:ILE:C	3:M:1469:GLY:H	2.26	0.43
2:C:1035:MET:C	2:C:1037:VAL:N	2.74	0.42
3:D:22:SER:C	3:D:24:GLY:N	2.77	0.42
2:L:917:LEU:C	2:L:919:ALA:N	2.73	0.42
3:M:643:GLY:HA3	3:M:727:GLN:N	2.33	0.42
3:M:853:VAL:C	3:M:855:HIS:N	2.77	0.42
2:C:732:ALA:C	2:C:734:LEU:N	2.75	0.42
3:D:101:HIS:C	3:D:103:TRP:H	2.27	0.42
3:D:892:ASP:C	3:D:894:LYS:H	2.26	0.42
3:M:1289:ARG:C	3:M:1291:SER:N	2.76	0.42
5:Q:146:VAL:C	5:Q:148:ALA:N	2.75	0.42
3:D:691:LEU:C	3:D:693:GLU:H	2.27	0.42
5:H:150:ILE:C	5:H:152:GLY:H	2.27	0.42
1:J:156:HIS:C	1:J:158:ILE:N	2.77	0.42
2:L:324:ASP:C	2:L:326:ASP:N	2.76	0.42
2:L:1090:LYS:C	2:L:1092:LEU:N	2.75	0.42
2:C:772:ARG:C	2:C:774:LEU:H	2.27	0.42
2:C:1090:LYS:C	2:C:1092:LEU:N	2.75	0.42
5:Q:150:ILE:C	5:Q:152:GLY:H	2.27	0.42
3:D:902:MET:C	3:D:904:VAL:H	2.27	0.42
3:D:1425:THR:C	3:D:1427:SER:N	2.77	0.42
5:H:211:VAL:C	5:H:213:ILE:N	2.76	0.42
2:L:198:ARG:C	2:L:200:LEU:N	2.77	0.42
2:L:861:LEU:C	2:L:863:ASP:N	2.77	0.42
3:M:480:GLU:C	3:M:482:LYS:N	2.76	0.42
3:M:902:MET:C	3:M:904:VAL:H	2.27	0.42
3:D:480:GLU:C	3:D:482:LYS:N	2.76	0.42
3:D:1407:LEU:C	3:D:1409:ALA:H	2.28	0.42
2:L:1023:GLY:C	2:L:1025:ALA:N	2.77	0.42
3:M:34:TYR:C	3:M:36:THR:H	2.26	0.42
3:M:101:HIS:C	3:M:103:TRP:H	2.27	0.42
3:M:465:LEU:C	3:M:467:GLU:N	2.72	0.42
3:M:1407:LEU:C	3:M:1409:ALA:H	2.28	0.42
3:D:479:GLU:C	3:D:481:MET:N	2.78	0.42
3:D:987:GLU:C	3:D:989:TYR:N	2.77	0.42
2:L:221:LEU:C	2:L:223:ASP:H	2.28	0.42
3:M:892:ASP:C	3:M:894:LYS:H	2.26	0.42
3:M:930:LEU:C	3:M:932:ASP:H	2.27	0.42
3:D:855:HIS:C	3:D:857:LEU:N	2.70	0.42
2:L:948:GLU:C	2:L:950:LEU:N	2.77	0.42
3:M:491:LYS:C	3:M:493:ARG:N	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:81:PRO:C	4:N:83:ASP:N	2.74	0.42
1:B:134:GLU:C	1:B:136:GLY:N	2.78	0.42
2:C:198:ARG:C	2:C:200:LEU:N	2.77	0.42
2:C:221:LEU:C	2:C:223:ASP:H	2.28	0.42
2:L:772:ARG:C	2:L:774:LEU:H	2.28	0.42
3:M:460:ALA:C	3:M:463:GLU:H	2.28	0.42
3:M:685:ASP:C	3:M:687:VAL:N	2.78	0.42
3:M:943:THR:C	3:M:945:SER:H	2.28	0.42
3:M:987:GLU:C	3:M:989:TYR:N	2.77	0.42
3:M:1019:PRO:C	3:M:1021:TYR:N	2.76	0.42
2:C:274:ARG:C	2:C:276:LYS:H	2.28	0.41
3:D:690:ALA:C	3:D:692:GLU:N	2.75	0.41
1:K:79:ILE:C	1:K:81:ASN:H	2.28	0.41
2:L:89:THR:C	2:L:91:GLN:N	2.78	0.41
2:L:356:ARG:C	2:L:358:ARG:N	2.77	0.41
3:M:568:ARG:C	3:M:570:GLU:N	2.78	0.41
2:C:948:GLU:C	2:C:950:LEU:N	2.77	0.41
3:D:711:LEU:C	3:D:713:ILE:H	2.28	0.41
3:D:1067:VAL:C	3:D:1069:GLU:N	2.75	0.41
2:L:1050:GLN:C	2:L:1052:MET:N	2.77	0.41
3:M:471:GLU:C	3:M:474:GLU:H	2.28	0.41
1:B:79:ILE:C	1:B:81:ASN:H	2.28	0.41
2:C:1050:GLN:C	2:C:1052:MET:N	2.77	0.41
3:D:989:TYR:C	3:D:991:GLN:H	2.28	0.41
4:E:84:ARG:C	4:E:86:GLN:H	2.27	0.41
2:L:171:TRP:H	2:L:187:ASN:CA	2.33	0.41
3:M:22:SER:C	3:M:24:GLY:N	2.77	0.41
4:N:84:ARG:C	4:N:86:GLN:H	2.27	0.41
1:K:134:GLU:C	1:K:136:GLY:N	2.78	0.41
2:C:89:THR:C	2:C:91:GLN:N	2.78	0.41
2:C:772:ARG:C	2:C:774:LEU:N	2.77	0.41
3:D:1100:ASP:C	3:D:1102:ALA:N	2.75	0.41
3:M:479:GLU:C	3:M:481:MET:N	2.78	0.41
3:M:989:TYR:C	3:M:991:GLN:H	2.28	0.41
2:C:861:LEU:C	2:C:863:ASP:N	2.77	0.41
2:C:1033:GLY:HA2	3:D:619:LEU:C	2.46	0.41
3:D:148:GLU:C	3:D:150:ARG:N	2.79	0.41
3:D:460:ALA:C	3:D:463:GLU:H	2.28	0.41
2:L:891:GLY:C	2:L:893:ALA:N	2.77	0.41
2:L:274:ARG:C	2:L:276:LYS:H	2.28	0.41
2:L:772:ARG:C	2:L:774:LEU:N	2.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ARG:C	1:A:191:ASP:N	2.79	0.41
1:B:115:THR:C	1:B:117:SER:H	2.29	0.41
2:C:122:THR:C	2:C:124:ASP:N	2.75	0.41
2:C:504:GLU:C	2:C:506:ASP:H	2.28	0.41
3:D:943:THR:C	3:D:945:SER:H	2.28	0.41
4:E:19:LEU:C	4:E:21:VAL:N	2.79	0.41
1:K:31:GLY:C	1:K:33:GLY:N	2.79	0.41
1:K:115:THR:C	1:K:117:SER:H	2.29	0.41
2:L:1033:GLY:HA2	3:M:619:LEU:C	2.46	0.41
2:L:1035:MET:C	2:L:1037:VAL:N	2.74	0.41
3:M:711:LEU:C	3:M:713:ILE:H	2.28	0.41
3:M:1071:PHE:C	3:M:1073:SER:N	2.78	0.41
3:M:1372:VAL:C	3:M:1374:GLN:N	2.78	0.41
2:C:32:ALA:C	2:C:34:VAL:H	2.29	0.41
2:C:571:LEU:C	2:C:573:ARG:N	2.76	0.41
3:D:471:GLU:C	3:D:474:GLU:H	2.28	0.41
3:D:643:GLY:HA3	3:D:727:GLN:N	2.33	0.41
3:D:1019:PRO:C	3:D:1021:TYR:N	2.76	0.41
2:C:680:ASP:C	2:C:682:TYR:N	2.79	0.40
3:D:930:LEU:C	3:D:932:ASP:H	2.27	0.40
1:J:59:GLU:C	1:J:61:VAL:H	2.29	0.40
1:J:189:ARG:C	1:J:191:ASP:N	2.79	0.40
2:L:571:LEU:C	2:L:573:ARG:N	2.76	0.40
2:L:680:ASP:C	2:L:682:TYR:N	2.79	0.40
3:M:545:ARG:C	3:M:547:LEU:N	2.79	0.40
3:D:102:ILE:C	3:D:104:PHE:H	2.27	0.40
3:D:1372:VAL:C	3:D:1374:GLN:N	2.78	0.40
2:L:976:ASP:C	2:L:978:ARG:N	2.79	0.40
3:M:985:ASP:C	3:M:987:GLU:N	2.78	0.40
3:D:1353:GLN:C	3:D:1355:VAL:H	2.29	0.40
2:L:696:LYS:C	2:L:698:ASP:H	2.29	0.40
3:M:148:GLU:C	3:M:150:ARG:N	2.79	0.40
1:B:217:ILE:C	1:B:219:LYS:N	2.75	0.40
3:D:150:ARG:C	3:D:152:LEU:N	2.79	0.40
3:D:472:LYS:C	3:D:474:GLU:N	2.78	0.40
3:M:138:LYS:C	3:M:140:ALA:N	2.79	0.40
3:M:647:ARG:C	3:M:649:ALA:N	2.79	0.40
3:M:1425:THR:C	3:M:1427:SER:N	2.77	0.40
1:B:112:GLY:C	1:B:114:PHE:N	2.79	0.40
2:C:277:ALA:C	2:C:279:GLU:N	2.80	0.40
2:C:391:LEU:C	2:C:393:GLN:N	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:734:GLU:C	3:D:736:PHE:N	2.68	0.40
3:D:1438:ALA:C	3:D:1440:PHE:N	2.80	0.40
2:L:776:SER:C	2:L:778:PHE:N	2.75	0.40
2:L:1064:ASN:C	2:L:1066:ALA:N	2.79	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 X-ray entries followed by that with respect to entries of similar resolution.

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	222/314 (71%)	95 (43%)	65 (29%)	62 (28%)	0	0
1	B	218/314 (69%)	110 (50%)	53 (24%)	55 (25%)	0	1
1	J	222/314 (71%)	95 (43%)	65 (29%)	62 (28%)	0	0
1	K	218/314 (69%)	110 (50%)	53 (24%)	55 (25%)	0	1
2	C	1072/1118 (96%)	439 (41%)	296 (28%)	337 (31%)	0	0
2	L	1072/1118 (96%)	439 (41%)	294 (27%)	339 (32%)	0	0
3	D	1175/1524 (77%)	456 (39%)	307 (26%)	412 (35%)	0	0
3	M	1175/1524 (77%)	456 (39%)	309 (26%)	410 (35%)	0	0
4	E	90/99 (91%)	40 (44%)	24 (27%)	26 (29%)	0	0
4	N	90/99 (91%)	40 (44%)	24 (27%)	26 (29%)	0	0
5	H	318/332 (96%)	209 (66%)	57 (18%)	52 (16%)	0	3
5	Q	318/332 (96%)	209 (66%)	57 (18%)	52 (16%)	0	3
All	All	6190/7402 (84%)	2698 (44%)	1604 (26%)	1888 (30%)	0	0

All (1888) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	GLU
1	A	64	GLU
1	A	76	VAL
1	A	125	PRO
1	A	137	LYS
1	A	148	VAL
1	A	153	ALA
1	A	158	ILE
1	A	162	ILE
1	A	172	SER
1	A	176	ARG
1	A	182	GLU
1	A	188	GLN
1	A	199	ILE
1	A	208	LEU
1	A	216	ALA
1	A	226	ALA
1	B	7	LYS
1	B	15	THR
1	B	29	GLU
1	B	54	THR
1	B	75	VAL
1	B	91	ASP
1	B	104	GLU
1	B	106	PRO
1	B	114	PHE
1	B	128	HIS
1	B	135	GLY
1	B	158	ILE
1	B	171	PHE
1	B	181	VAL
1	B	185	ARG
1	B	186	LEU
1	B	191	ASP
1	B	195	LEU
1	B	200	TRP
1	B	224	TYR
2	C	17	PRO
2	C	22	GLN
2	C	27	LYS
2	C	31	GLN
2	C	33	ASP
2	C	40	GLU

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Mol	Chain	Res	Type
2	C	42	VAL
2	C	46	ALA
2	C	47	ALA
2	C	54	ILE
2	C	70	GLU
2	C	80	GLN
2	C	88	LEU
2	C	102	HIS
2	C	109	LYS
2	C	111	ASP
2	C	114	PHE
2	C	115	LEU
2	C	136	ILE
2	C	137	VAL
2	C	153	ALA
2	C	155	PRO
2	C	168	ARG
2	C	182	VAL
2	C	187	ASN
2	C	199	VAL
2	C	221	LEU
2	C	244	PRO
2	C	263	ASP
2	C	264	PRO
2	C	269	LEU
2	C	275	TYR
2	C	278	GLU
2	C	288	ARG
2	C	322	VAL
2	C	336	VAL
2	C	370	ALA
2	C	392	SER
2	C	395	LYS
2	C	397	GLU
2	C	398	THR
2	C	402	SER
2	C	409	ARG
2	C	418	LEU
2	C	420	ARG
2	C	425	PHE
2	C	430	VAL
2	C	431	HIS

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Mol	Chain	Res	Type
2	C	432	ARG
2	C	434	HIS
2	C	444	PRO
2	C	449	ILE
2	C	451	LEU
2	C	457	ALA
2	C	483	VAL
2	C	496	ILE
2	C	498	GLN
2	C	503	LEU
2	C	518	ARG
2	C	522	VAL
2	C	526	PRO
2	C	530	GLU
2	C	532	MET
2	C	537	LYS
2	C	541	SER
2	C	543	ASN
2	C	545	ASN
2	C	548	PRO
2	C	574	ALA
2	C	580	MET
2	C	587	VAL
2	C	588	VAL
2	C	599	GLU
2	C	603	VAL
2	C	604	VAL
2	C	612	ALA
2	C	616	GLU
2	C	629	ALA
2	C	633	GLN
2	C	641	PRO
2	C	643	VAL
2	C	644	ARG
2	C	656	ALA
2	C	657	ASP
2	C	663	GLU
2	C	677	MET
2	C	713	ARG
2	C	714	ASP
2	C	715	THR
2	C	728	HIS

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Mol	Chain	Res	Type
2	C	735	ARG
2	C	738	ASP
2	C	760	SER
2	C	762	LYS
2	C	767	PRO
2	C	788	THR
2	C	804	LEU
2	C	831	ARG
2	C	832	LYS
2	C	840	ALA
2	C	848	VAL
2	C	849	VAL
2	C	871	LEU
2	C	880	MET
2	C	884	GLN
2	C	885	ILE
2	C	919	ALA
2	C	920	GLU
2	C	944	LEU
2	C	957	LYS
2	C	964	LYS
2	C	965	GLU
2	C	967	PHE
2	C	973	VAL
2	C	974	LEU
2	C	984	GLU
2	C	999	HIS
2	C	1000	MET
2	C	1011	GLY
2	C	1012	PRO
2	C	1021	LEU
2	C	1027	PHE
2	C	1035	MET
2	C	1038	TRP
2	C	1053	LEU
2	C	1075	ASP
2	C	1078	GLU
2	C	1104	GLU
3	D	5	VAL
3	D	10	ILE
3	D	12	LEU
3	D	13	ALA

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Mol	Chain	Res	Type
3	D	26	VAL
3	D	28	LYS
3	D	33	ASN
3	D	41	ARG
3	D	52	PRO
3	D	64	LYS
3	D	97	THR
3	D	98	PRO
3	D	100	ALA
3	D	109	PRO
3	D	110	SER
3	D	117	ASP
3	D	119	SER
3	D	126	VAL
3	D	131	LYS
3	D	140	ALA
3	D	141	VAL
3	D	143	ASP
3	D	146	PRO
3	D	147	VAL
3	D	454	ALA
3	D	477	LEU
3	D	478	LEU
3	D	479	GLU
3	D	484	PRO
3	D	486	ARG
3	D	487	ALA
3	D	488	ARG
3	D	491	LYS
3	D	526	PRO
3	D	530	VAL
3	D	531	ASP
3	D	535	PHE
3	D	547	LEU
3	D	548	ILE
3	D	564	GLU
3	D	565	ILE
3	D	571	LYS
3	D	582	ILE
3	D	607	LEU
3	D	626	SER
3	D	630	VAL

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Mol	Chain	Res	Type
3	D	633	VAL
3	D	638	LYS
3	D	646	LYS
3	D	647	ARG
3	D	648	MET
3	D	649	ALA
3	D	650	LEU
3	D	655	PRO
3	D	662	GLU
3	D	665	ALA
3	D	668	PRO
3	D	672	ALA
3	D	678	GLU
3	D	679	ARG
3	D	682	ASP
3	D	684	LYS
3	D	696	HIS
3	D	702	LEU
3	D	718	PRO
3	D	725	SER
3	D	730	PRO
3	D	731	LEU
3	D	739	ASP
3	D	762	GLN
3	D	770	LEU
3	D	782	SER
3	D	793	THR
3	D	795	VAL
3	D	797	LYS
3	D	799	LYS
3	D	807	ALA
3	D	808	THR
3	D	811	GLU
3	D	815	ALA
3	D	821	VAL
3	D	825	ALA
3	D	826	PRO
3	D	828	VAL
3	D	829	VAL
3	D	835	SER
3	D	838	ARG
3	D	840	LYS

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Mol	Chain	Res	Type
3	D	842	VAL
3	D	848	GLU
3	D	849	ALA
3	D	862	ASP
3	D	875	THR
3	D	898	GLU
3	D	899	LEU
3	D	900	ILE
3	D	905	PRO
3	D	908	LYS
3	D	919	PHE
3	D	924	MET
3	D	925	GLU
3	D	947	ILE
3	D	948	THR
3	D	953	ASP
3	D	961	GLN
3	D	966	GLU
3	D	1000	THR
3	D	1006	ALA
3	D	1016	PRO
3	D	1023	MET
3	D	1028	ALA
3	D	1029	ARG
3	D	1040	GLY
3	D	1045	MET
3	D	1054	GLU
3	D	1059	SER
3	D	1061	PHE
3	D	1067	VAL
3	D	1109	GLU
3	D	1111	ASP
3	D	1113	GLY
3	D	1116	ASN
3	D	1141	GLU
3	D	1149	LEU
3	D	1152	GLU
3	D	1178	ALA
3	D	1190	SER
3	D	1194	CYS
3	D	1195	GLN
3	D	1201	CYS

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Mol	Chain	Res	Type
3	D	1203	LYS
3	D	1208	ASP
3	D	1209	LEU
3	D	1210	SER
3	D	1219	GLU
3	D	1223	VAL
3	D	1224	VAL
3	D	1225	ALA
3	D	1231	GLU
3	D	1232	PRO
3	D	1234	THR
3	D	1236	LEU
3	D	1239	ARG
3	D	1268	PRO
3	D	1276	GLU
3	D	1281	VAL
3	D	1296	SER
3	D	1300	SER
3	D	1306	PRO
3	D	1313	VAL
3	D	1320	GLU
3	D	1321	ALA
3	D	1323	GLN
3	D	1330	ILE
3	D	1347	TYR
3	D	1364	HIS
3	D	1366	LYS
3	D	1367	HIS
3	D	1373	ARG
3	D	1374	GLN
3	D	1375	MET
3	D	1384	PRO
3	D	1388	ARG
3	D	1394	VAL
3	D	1396	GLU
3	D	1408	ILE
3	D	1424	VAL
3	D	1436	SER
3	D	1439	SER
3	D	1442	ASN
3	D	1445	HIS
3	D	1448	THR

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Mol	Chain	Res	Type
3	D	1451	ALA
3	D	1452	ILE
3	D	1455	LYS
3	D	1457	ASP
3	D	1458	GLU
3	D	1462	LEU
3	D	1464	GLU
3	D	1483	PHE
3	D	1487	VAL
4	E	16	LYS
4	E	21	VAL
4	E	30	LEU
4	E	34	ARG
4	E	42	PRO
4	E	50	THR
4	E	51	LEU
4	E	60	ALA
4	E	61	VAL
4	E	77	GLU
4	E	90	GLU
5	H	171	VAL
5	H	203	ILE
5	H	211	VAL
5	H	220	ARG
5	H	249	LYS
5	H	251	SER
5	H	328	GLU
5	H	329	PRO
5	H	333	GLU
5	H	335	PRO
5	H	352	ASN
5	H	407	VAL
5	H	409	ARG
5	H	420	LEU
5	H	432	LYS
1	J	59	GLU
1	J	64	GLU
1	J	76	VAL
1	J	125	PRO
1	J	137	LYS
1	J	148	VAL
1	J	153	ALA

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Mol	Chain	Res	Type
1	J	158	ILE
1	J	162	ILE
1	J	172	SER
1	J	176	ARG
1	J	182	GLU
1	J	188	GLN
1	J	199	ILE
1	J	208	LEU
1	J	216	ALA
1	J	226	ALA
1	K	7	LYS
1	K	15	THR
1	K	29	GLU
1	K	54	THR
1	K	75	VAL
1	K	91	ASP
1	K	104	GLU
1	K	106	PRO
1	K	114	PHE
1	K	128	HIS
1	K	135	GLY
1	K	158	ILE
1	K	171	PHE
1	K	181	VAL
1	K	185	ARG
1	K	186	LEU
1	K	191	ASP
1	K	195	LEU
1	K	200	TRP
1	K	224	TYR
2	L	17	PRO
2	L	22	GLN
2	L	27	LYS
2	L	31	GLN
2	L	33	ASP
2	L	40	GLU
2	L	42	VAL
2	L	46	ALA
2	L	47	ALA
2	L	54	ILE
2	L	70	GLU
2	L	80	GLN

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Mol	Chain	Res	Type
2	L	88	LEU
2	L	102	HIS
2	L	109	LYS
2	L	111	ASP
2	L	114	PHE
2	L	115	LEU
2	L	136	ILE
2	L	137	VAL
2	L	153	ALA
2	L	155	PRO
2	L	168	ARG
2	L	182	VAL
2	L	187	ASN
2	L	199	VAL
2	L	221	LEU
2	L	244	PRO
2	L	263	ASP
2	L	264	PRO
2	L	269	LEU
2	L	275	TYR
2	L	278	GLU
2	L	288	ARG
2	L	322	VAL
2	L	336	VAL
2	L	370	ALA
2	L	392	SER
2	L	395	LYS
2	L	397	GLU
2	L	398	THR
2	L	402	SER
2	L	409	ARG
2	L	418	LEU
2	L	420	ARG
2	L	425	PHE
2	L	430	VAL
2	L	431	HIS
2	L	432	ARG
2	L	434	HIS
2	L	444	PRO
2	L	449	ILE
2	L	451	LEU
2	L	457	ALA

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Mol	Chain	Res	Type
2	L	483	VAL
2	L	496	ILE
2	L	498	GLN
2	L	503	LEU
2	L	518	ARG
2	L	522	VAL
2	L	526	PRO
2	L	530	GLU
2	L	532	MET
2	L	537	LYS
2	L	541	SER
2	L	543	ASN
2	L	545	ASN
2	L	548	PRO
2	L	574	ALA
2	L	580	MET
2	L	587	VAL
2	L	588	VAL
2	L	599	GLU
2	L	603	VAL
2	L	604	VAL
2	L	612	ALA
2	L	616	GLU
2	L	629	ALA
2	L	633	GLN
2	L	641	PRO
2	L	643	VAL
2	L	644	ARG
2	L	656	ALA
2	L	657	ASP
2	L	663	GLU
2	L	677	MET
2	L	713	ARG
2	L	714	ASP
2	L	715	THR
2	L	728	HIS
2	L	735	ARG
2	L	738	ASP
2	L	760	SER
2	L	762	LYS
2	L	767	PRO
2	L	788	THR

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Mol	Chain	Res	Type
2	L	804	LEU
2	L	831	ARG
2	L	832	LYS
2	L	840	ALA
2	L	848	VAL
2	L	849	VAL
2	L	871	LEU
2	L	880	MET
2	L	884	GLN
2	L	885	ILE
2	L	919	ALA
2	L	920	GLU
2	L	944	LEU
2	L	957	LYS
2	L	964	LYS
2	L	965	GLU
2	L	967	PHE
2	L	973	VAL
2	L	974	LEU
2	L	984	GLU
2	L	999	HIS
2	L	1000	MET
2	L	1011	GLY
2	L	1012	PRO
2	L	1021	LEU
2	L	1027	PHE
2	L	1035	MET
2	L	1038	TRP
2	L	1053	LEU
2	L	1075	ASP
2	L	1078	GLU
2	L	1104	GLU
3	M	5	VAL
3	M	10	ILE
3	M	12	LEU
3	M	13	ALA
3	M	26	VAL
3	M	28	LYS
3	M	33	ASN
3	M	41	ARG
3	M	52	PRO
3	M	64	LYS

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Mol	Chain	Res	Type
3	M	97	THR
3	M	98	PRO
3	M	100	ALA
3	M	109	PRO
3	M	110	SER
3	M	117	ASP
3	M	119	SER
3	M	126	VAL
3	M	131	LYS
3	M	140	ALA
3	M	141	VAL
3	M	143	ASP
3	M	146	PRO
3	M	147	VAL
3	M	454	ALA
3	M	477	LEU
3	M	478	LEU
3	M	479	GLU
3	M	484	PRO
3	M	486	ARG
3	M	487	ALA
3	M	488	ARG
3	M	491	LYS
3	M	526	PRO
3	M	530	VAL
3	M	531	ASP
3	M	535	PHE
3	M	547	LEU
3	M	548	ILE
3	M	564	GLU
3	M	565	ILE
3	M	571	LYS
3	M	582	ILE
3	M	607	LEU
3	M	626	SER
3	M	630	VAL
3	M	633	VAL
3	M	638	LYS
3	M	646	LYS
3	M	647	ARG
3	M	648	MET
3	M	649	ALA

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Mol	Chain	Res	Type
3	M	650	LEU
3	M	655	PRO
3	M	662	GLU
3	M	665	ALA
3	M	668	PRO
3	M	672	ALA
3	M	678	GLU
3	M	679	ARG
3	M	682	ASP
3	M	684	LYS
3	M	696	HIS
3	M	702	LEU
3	M	718	PRO
3	M	725	SER
3	M	730	PRO
3	M	731	LEU
3	M	739	ASP
3	M	762	GLN
3	M	770	LEU
3	M	782	SER
3	M	793	THR
3	M	795	VAL
3	M	797	LYS
3	M	799	LYS
3	M	807	ALA
3	M	808	THR
3	M	811	GLU
3	M	815	ALA
3	M	821	VAL
3	M	825	ALA
3	M	826	PRO
3	M	828	VAL
3	M	829	VAL
3	M	835	SER
3	M	838	ARG
3	M	840	LYS
3	M	842	VAL
3	M	848	GLU
3	M	849	ALA
3	M	862	ASP
3	M	875	THR
3	M	898	GLU

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Mol	Chain	Res	Type
3	M	899	LEU
3	M	900	ILE
3	M	905	PRO
3	M	908	LYS
3	M	919	PHE
3	M	924	MET
3	M	925	GLU
3	M	947	ILE
3	M	948	THR
3	M	953	ASP
3	M	961	GLN
3	M	966	GLU
3	M	1000	THR
3	M	1006	ALA
3	M	1016	PRO
3	M	1023	MET
3	M	1028	ALA
3	M	1029	ARG
3	M	1040	GLY
3	M	1045	MET
3	M	1054	GLU
3	M	1059	SER
3	M	1061	PHE
3	M	1067	VAL
3	M	1109	GLU
3	M	1111	ASP
3	M	1113	GLY
3	M	1116	ASN
3	M	1141	GLU
3	M	1149	LEU
3	M	1152	GLU
3	M	1178	ALA
3	M	1190	SER
3	M	1194	CYS
3	M	1195	GLN
3	M	1201	CYS
3	M	1203	LYS
3	M	1208	ASP
3	M	1209	LEU
3	M	1210	SER
3	M	1219	GLU
3	M	1223	VAL

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Mol	Chain	Res	Type
3	M	1224	VAL
3	M	1225	ALA
3	M	1231	GLU
3	M	1232	PRO
3	M	1234	THR
3	M	1236	LEU
3	M	1239	ARG
3	M	1268	PRO
3	M	1276	GLU
3	M	1281	VAL
3	M	1296	SER
3	M	1300	SER
3	M	1306	PRO
3	M	1313	VAL
3	M	1320	GLU
3	M	1321	ALA
3	M	1323	GLN
3	M	1330	ILE
3	M	1347	TYR
3	M	1364	HIS
3	M	1366	LYS
3	M	1367	HIS
3	M	1373	ARG
3	M	1374	GLN
3	M	1375	MET
3	M	1384	PRO
3	M	1388	ARG
3	M	1394	VAL
3	M	1396	GLU
3	M	1408	ILE
3	M	1424	VAL
3	M	1436	SER
3	M	1439	SER
3	M	1442	ASN
3	M	1445	HIS
3	M	1448	THR
3	M	1451	ALA
3	M	1452	ILE
3	M	1455	LYS
3	M	1457	ASP
3	M	1458	GLU
3	M	1462	LEU

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Mol	Chain	Res	Type
3	M	1464	GLU
3	M	1483	PHE
3	M	1487	VAL
4	N	16	LYS
4	N	21	VAL
4	N	30	LEU
4	N	34	ARG
4	N	42	PRO
4	N	50	THR
4	N	51	LEU
4	N	60	ALA
4	N	61	VAL
4	N	77	GLU
4	N	90	GLU
5	Q	171	VAL
5	Q	203	ILE
5	Q	211	VAL
5	Q	220	ARG
5	Q	249	LYS
5	Q	251	SER
5	Q	328	GLU
5	Q	329	PRO
5	Q	333	GLU
5	Q	335	PRO
5	Q	352	ASN
5	Q	407	VAL
5	Q	409	ARG
5	Q	420	LEU
5	Q	432	LYS
1	A	13	ALA
1	A	36	LEU
1	A	44	LEU
1	A	46	SER
1	A	54	THR
1	A	65	PHE
1	A	107	LYS
1	A	112	GLY
1	A	123	MET
1	A	126	ASP
1	A	132	LEU
1	A	138	LEU
1	A	164	ALA

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Mol	Chain	Res	Type
1	A	189	ARG
1	A	209	GLU
1	A	211	LEU
1	A	215	VAL
1	A	224	TYR
1	A	228	PRO
1	B	35	THR
1	B	53	VAL
1	B	70	GLY
1	B	78	ILE
1	B	112	GLY
1	B	117	SER
1	B	137	LYS
1	B	138	LEU
1	B	152	PRO
1	B	196	THR
1	B	201	THR
1	B	202	ASP
1	B	204	SER
1	B	208	LEU
2	C	24	GLU
2	C	28	LYS
2	C	43	GLY
2	C	81	ASP
2	C	108	ILE
2	C	112	GLU
2	C	133	ASP
2	C	144	PRO
2	C	157	ARG
2	C	177	GLU
2	C	179	SER
2	C	237	ARG
2	C	316	GLY
2	C	326	ASP
2	C	338	GLU
2	C	381	ALA
2	C	391	LEU
2	C	393	GLN
2	C	423	ALA
2	C	427	VAL
2	C	438	ILE
2	C	445	GLU

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Mol	Chain	Res	Type
2	C	450	GLY
2	C	458	TYR
2	C	460	ARG
2	C	489	SER
2	C	494	TYR
2	C	502	PRO
2	C	508	ILE
2	C	514	VAL
2	C	529	VAL
2	C	534	VAL
2	C	536	PRO
2	C	550	LEU
2	C	560	MET
2	C	582	GLY
2	C	589	ARG
2	C	600	ASP
2	C	605	LYS
2	C	608	GLY
2	C	620	LEU
2	C	635	THR
2	C	655	LEU
2	C	666	LEU
2	C	685	GLU
2	C	698	ASP
2	C	761	PHE
2	C	769	PRO
2	C	775	ARG
2	C	787	ASP
2	C	791	ARG
2	C	793	PRO
2	C	808	ARG
2	C	809	GLY
2	C	855	VAL
2	C	857	ASP
2	C	876	VAL
2	C	877	PRO
2	C	894	GLY
2	C	928	LYS
2	C	933	GLY
2	C	945	ALA
2	C	960	GLU
2	C	968	ASP

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Mol	Chain	Res	Type
2	C	972	VAL
2	C	981	GLU
2	C	987	ILE
2	C	1001	VAL
2	C	1037	VAL
2	C	1046	ALA
2	C	1056	LYS
2	C	1060	ILE
2	C	1066	ALA
2	C	1079	PRO
2	C	1082	PRO
2	C	1083	GLU
2	C	1093	GLN
2	C	1096	ALA
2	C	1106	ASP
2	C	1113	GLU
2	C	1114	GLY
3	D	7	LYS
3	D	14	SER
3	D	18	ILE
3	D	32	ILE
3	D	37	LEU
3	D	43	GLY
3	D	45	PHE
3	D	47	GLU
3	D	67	ARG
3	D	72	VAL
3	D	85	VAL
3	D	99	ALA
3	D	102	ILE
3	D	127	LEU
3	D	129	PHE
3	D	139	GLY
3	D	464	LEU
3	D	480	GLU
3	D	485	SER
3	D	498	VAL
3	D	502	PHE
3	D	506	GLY
3	D	540	LEU
3	D	545	ARG
3	D	558	LEU

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Mol	Chain	Res	Type
3	D	567	ILE
3	D	586	ARG
3	D	595	GLY
3	D	601	ARG
3	D	605	ASP
3	D	609	GLY
3	D	621	LYS
3	D	640	HIS
3	D	643	GLY
3	D	681	ARG
3	D	686	GLU
3	D	689	ASP
3	D	695	ILE
3	D	712	GLY
3	D	715	ALA
3	D	723	GLY
3	D	724	GLN
3	D	735	ALA
3	D	776	GLU
3	D	783	ARG
3	D	784	ASP
3	D	794	GLN
3	D	796	ARG
3	D	803	GLY
3	D	819	GLY
3	D	822	ALA
3	D	864	VAL
3	D	872	ARG
3	D	892	ASP
3	D	893	GLU
3	D	897	GLN
3	D	913	ASP
3	D	920	LEU
3	D	928	ALA
3	D	936	TYR
3	D	958	GLU
3	D	964	LEU
3	D	994	GLN
3	D	1001	GLU
3	D	1020	LEU
3	D	1042	ARG
3	D	1056	PRO

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Mol	Chain	Res	Type
3	D	1070	TYR
3	D	1099	VAL
3	D	1142	SER
3	D	1146	GLY
3	D	1173	PHE
3	D	1175	ILE
3	D	1179	GLU
3	D	1180	ALA
3	D	1188	VAL
3	D	1200	VAL
3	D	1212	ALA
3	D	1215	VAL
3	D	1233	GLY
3	D	1237	THR
3	D	1263	PHE
3	D	1273	VAL
3	D	1287	GLU
3	D	1328	GLY
3	D	1339	LYS
3	D	1353	GLN
3	D	1360	GLY
3	D	1361	VAL
3	D	1365	ASP
3	D	1381	VAL
3	D	1386	ASP
3	D	1397	LYS
3	D	1430	SER
3	D	1449	GLU
3	D	1454	GLY
3	D	1466	VAL
3	D	1473	PRO
3	D	1475	GLY
4	E	6	ILE
4	E	10	PHE
4	E	12	MET
4	E	15	SER
4	E	22	VAL
4	E	23	VAL
4	E	24	ALA
4	E	41	GLU
5	H	108	LEU
5	H	111	LEU

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Mol	Chain	Res	Type
5	H	152	GLY
5	H	172	GLU
5	H	173	GLU
5	H	176	GLY
5	H	186	LYS
5	H	277	VAL
5	H	315	ASP
5	H	331	SER
5	H	349	PRO
5	H	351	GLU
5	H	387	ARG
5	H	406	GLY
5	H	410	GLU
5	H	419	ALA
5	H	431	ARG
1	J	13	ALA
1	J	36	LEU
1	J	44	LEU
1	J	46	SER
1	J	54	THR
1	J	65	PHE
1	J	107	LYS
1	J	112	GLY
1	J	123	MET
1	J	126	ASP
1	J	132	LEU
1	J	138	LEU
1	J	164	ALA
1	J	189	ARG
1	J	209	GLU
1	J	211	LEU
1	J	215	VAL
1	J	224	TYR
1	J	228	PRO
1	K	35	THR
1	K	53	VAL
1	K	70	GLY
1	K	78	ILE
1	K	112	GLY
1	K	117	SER
1	K	137	LYS
1	K	138	LEU

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Mol	Chain	Res	Type
1	K	152	PRO
1	K	196	THR
1	K	201	THR
1	K	202	ASP
1	K	204	SER
1	K	208	LEU
2	L	24	GLU
2	L	28	LYS
2	L	43	GLY
2	L	81	ASP
2	L	108	ILE
2	L	112	GLU
2	L	133	ASP
2	L	144	PRO
2	L	157	ARG
2	L	177	GLU
2	L	179	SER
2	L	237	ARG
2	L	316	GLY
2	L	326	ASP
2	L	338	GLU
2	L	381	ALA
2	L	391	LEU
2	L	393	GLN
2	L	423	ALA
2	L	427	VAL
2	L	438	ILE
2	L	445	GLU
2	L	450	GLY
2	L	458	TYR
2	L	460	ARG
2	L	489	SER
2	L	494	TYR
2	L	502	PRO
2	L	508	ILE
2	L	514	VAL
2	L	529	VAL
2	L	534	VAL
2	L	536	PRO
2	L	550	LEU
2	L	560	MET
2	L	582	GLY

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Mol	Chain	Res	Type
2	L	589	ARG
2	L	600	ASP
2	L	605	LYS
2	L	608	GLY
2	L	620	LEU
2	L	635	THR
2	L	655	LEU
2	L	666	LEU
2	L	685	GLU
2	L	698	ASP
2	L	761	PHE
2	L	769	PRO
2	L	775	ARG
2	L	787	ASP
2	L	791	ARG
2	L	793	PRO
2	L	808	ARG
2	L	809	GLY
2	L	855	VAL
2	L	857	ASP
2	L	876	VAL
2	L	877	PRO
2	L	894	GLY
2	L	928	LYS
2	L	933	GLY
2	L	945	ALA
2	L	960	GLU
2	L	968	ASP
2	L	972	VAL
2	L	981	GLU
2	L	987	ILE
2	L	1001	VAL
2	L	1037	VAL
2	L	1046	ALA
2	L	1056	LYS
2	L	1060	ILE
2	L	1066	ALA
2	L	1079	PRO
2	L	1082	PRO
2	L	1083	GLU
2	L	1093	GLN
2	L	1096	ALA

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Mol	Chain	Res	Type
2	L	1106	ASP
2	L	1113	GLU
2	L	1114	GLY
3	M	7	LYS
3	M	14	SER
3	M	18	ILE
3	M	32	ILE
3	M	37	LEU
3	M	43	GLY
3	M	45	PHE
3	M	47	GLU
3	M	67	ARG
3	M	72	VAL
3	M	85	VAL
3	M	99	ALA
3	M	102	ILE
3	M	127	LEU
3	M	129	PHE
3	M	139	GLY
3	M	464	LEU
3	M	480	GLU
3	M	485	SER
3	M	498	VAL
3	M	502	PHE
3	M	506	GLY
3	M	540	LEU
3	M	545	ARG
3	M	558	LEU
3	M	567	ILE
3	M	586	ARG
3	M	595	GLY
3	M	601	ARG
3	M	605	ASP
3	M	609	GLY
3	M	621	LYS
3	M	640	HIS
3	M	643	GLY
3	M	681	ARG
3	M	686	GLU
3	M	689	ASP
3	M	695	ILE
3	M	712	GLY

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Mol	Chain	Res	Type
3	M	715	ALA
3	M	723	GLY
3	M	724	GLN
3	M	735	ALA
3	M	776	GLU
3	M	783	ARG
3	M	784	ASP
3	M	794	GLN
3	M	796	ARG
3	M	803	GLY
3	M	819	GLY
3	M	822	ALA
3	M	864	VAL
3	M	872	ARG
3	M	892	ASP
3	M	893	GLU
3	M	897	GLN
3	M	913	ASP
3	M	920	LEU
3	M	928	ALA
3	M	936	TYR
3	M	958	GLU
3	M	964	LEU
3	M	994	GLN
3	M	1001	GLU
3	M	1020	LEU
3	M	1042	ARG
3	M	1056	PRO
3	M	1070	TYR
3	M	1099	VAL
3	M	1142	SER
3	M	1146	GLY
3	M	1173	PHE
3	M	1175	ILE
3	M	1179	GLU
3	M	1180	ALA
3	M	1188	VAL
3	M	1200	VAL
3	M	1212	ALA
3	M	1215	VAL
3	M	1233	GLY
3	M	1237	THR

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Mol	Chain	Res	Type
3	M	1263	PHE
3	M	1273	VAL
3	M	1287	GLU
3	M	1328	GLY
3	M	1339	LYS
3	M	1353	GLN
3	M	1360	GLY
3	M	1361	VAL
3	M	1365	ASP
3	M	1381	VAL
3	M	1386	ASP
3	M	1397	LYS
3	M	1430	SER
3	M	1449	GLU
3	M	1454	GLY
3	M	1466	VAL
3	M	1473	PRO
3	M	1475	GLY
4	N	6	ILE
4	N	10	PHE
4	N	12	MET
4	N	15	SER
4	N	22	VAL
4	N	23	VAL
4	N	24	ALA
4	N	41	GLU
5	Q	108	LEU
5	Q	111	LEU
5	Q	152	GLY
5	Q	172	GLU
5	Q	173	GLU
5	Q	176	GLY
5	Q	186	LYS
5	Q	277	VAL
5	Q	315	ASP
5	Q	331	SER
5	Q	349	PRO
5	Q	351	GLU
5	Q	387	ARG
5	Q	406	GLY
5	Q	410	GLU
5	Q	419	ALA

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Mol	Chain	Res	Type
5	Q	431	ARG
1	A	7	LYS
1	A	31	GLY
1	A	49	PRO
1	A	74	ASP
1	A	96	SER
1	A	101	LEU
1	A	105	GLY
1	A	109	VAL
1	A	111	ALA
1	A	131	THR
1	A	161	ARG
1	B	32	PHE
1	B	95	ALA
1	B	116	PRO
1	B	132	LEU
1	B	134	GLU
1	B	161	ARG
2	C	14	PRO
2	C	18	LEU
2	C	19	THR
2	C	53	PRO
2	C	166	PRO
2	C	362	GLY
2	C	401	LEU
2	C	410	ILE
2	C	433	THR
2	C	453	THR
2	C	462	ASP
2	C	467	ILE
2	C	486	MET
2	C	507	ARG
2	C	512	ARG
2	C	561	GLY
2	C	575	GLN
2	C	594	ALA
2	C	613	VAL
2	C	625	LEU
2	C	645	VAL
2	C	686	ASP
2	C	696	LYS
2	C	821	GLU

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Mol	Chain	Res	Type
2	C	856	GLU
2	C	873	PRO
2	C	909	ALA
2	C	924	LEU
2	C	936	VAL
2	C	997	LEU
2	C	1020	PRO
2	C	1030	GLN
2	C	1058	ASP
2	C	1069	ALA
2	C	1100	GLN
2	C	1109	VAL
3	D	25	GLU
3	D	44	LEU
3	D	53	ILE
3	D	68	PHE
3	D	133	ILE
3	D	149	LYS
3	D	463	GLU
3	D	561	GLY
3	D	566	ILE
3	D	569	ASN
3	D	579	ASP
3	D	698	LYS
3	D	714	GLN
3	D	818	ARG
3	D	847	ASP
3	D	858	LEU
3	D	904	VAL
3	D	938	GLY
3	D	945	SER
3	D	965	GLU
3	D	967	ALA
3	D	1009	LYS
3	D	1047	LYS
3	D	1048	PRO
3	D	1049	SER
3	D	1098	LEU
3	D	1103	HIS
3	D	1105	ILE
3	D	1128	VAL
3	D	1135	ARG

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Mol	Chain	Res	Type
3	D	1192	LEU
3	D	1315	ASP
3	D	1359	GLN
3	D	1368	ILE
3	D	1387	SER
3	D	1389	LEU
3	D	1416	ALA
3	D	1435	LEU
3	D	1459	LEU
3	D	1465	ASN
3	D	1468	LEU
3	D	1485	GLN
4	E	18	ARG
4	E	71	GLY
4	E	84	ARG
5	H	181	LEU
5	H	297	LEU
5	H	327	GLN
5	H	353	LEU
1	J	7	LYS
1	J	31	GLY
1	J	49	PRO
1	J	74	ASP
1	J	96	SER
1	J	101	LEU
1	J	105	GLY
1	J	109	VAL
1	J	111	ALA
1	J	131	THR
1	J	161	ARG
1	K	32	PHE
1	K	95	ALA
1	K	116	PRO
1	K	132	LEU
1	K	134	GLU
1	K	161	ARG
2	L	14	PRO
2	L	18	LEU
2	L	19	THR
2	L	53	PRO
2	L	166	PRO
2	L	362	GLY

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Mol	Chain	Res	Type
2	L	401	LEU
2	L	410	ILE
2	L	433	THR
2	L	453	THR
2	L	462	ASP
2	L	467	ILE
2	L	486	MET
2	L	507	ARG
2	L	512	ARG
2	L	561	GLY
2	L	575	GLN
2	L	594	ALA
2	L	613	VAL
2	L	625	LEU
2	L	645	VAL
2	L	686	ASP
2	L	696	LYS
2	L	821	GLU
2	L	856	GLU
2	L	873	PRO
2	L	909	ALA
2	L	924	LEU
2	L	936	VAL
2	L	997	LEU
2	L	1020	PRO
2	L	1030	GLN
2	L	1058	ASP
2	L	1069	ALA
2	L	1100	GLN
2	L	1109	VAL
3	M	25	GLU
3	M	44	LEU
3	M	53	ILE
3	M	68	PHE
3	M	133	ILE
3	M	149	LYS
3	M	463	GLU
3	M	561	GLY
3	M	566	ILE
3	M	569	ASN
3	M	579	ASP
3	M	698	LYS

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Mol	Chain	Res	Type
3	M	714	GLN
3	M	818	ARG
3	M	847	ASP
3	M	858	LEU
3	M	883	ALA
3	M	904	VAL
3	M	938	GLY
3	M	945	SER
3	M	965	GLU
3	M	967	ALA
3	M	1009	LYS
3	M	1047	LYS
3	M	1048	PRO
3	M	1049	SER
3	M	1098	LEU
3	M	1103	HIS
3	M	1105	ILE
3	M	1128	VAL
3	M	1135	ARG
3	M	1192	LEU
3	M	1315	ASP
3	M	1359	GLN
3	M	1368	ILE
3	M	1387	SER
3	M	1389	LEU
3	M	1416	ALA
3	M	1435	LEU
3	M	1459	LEU
3	M	1465	ASN
3	M	1468	LEU
3	M	1485	GLN
4	N	18	ARG
4	N	71	GLY
4	N	84	ARG
5	Q	181	LEU
5	Q	297	LEU
5	Q	327	GLN
5	Q	353	LEU
1	A	78	ILE
1	A	91	ASP
1	A	128	HIS
1	A	152	PRO

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Mol	Chain	Res	Type
1	A	218	LEU
1	B	13	ALA
1	B	20	TYR
1	B	21	GLY
1	B	22	GLU
1	B	46	SER
1	B	48	ILE
1	B	76	VAL
1	B	113	ASP
2	C	35	PRO
2	C	87	ASP
2	C	106	GLY
2	C	148	PHE
2	C	167	LYS
2	C	175	GLU
2	C	205	GLU
2	C	303	PHE
2	C	317	VAL
2	C	318	PRO
2	C	376	ARG
2	C	394	PHE
2	C	521	PRO
2	C	562	SER
2	C	572	ILE
2	C	607	ASP
2	C	636	ALA
2	C	659	PRO
2	C	675	ALA
2	C	682	TYR
2	C	716	LYS
2	C	739	GLU
2	C	756	VAL
2	C	777	ILE
2	C	786	LYS
2	C	796	GLU
2	C	822	VAL
2	C	830	LYS
2	C	833	LEU
2	C	834	GLN
2	C	942	GLU
2	C	943	VAL
2	C	1039	ALA

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Mol	Chain	Res	Type
2	C	1072	LYS
2	C	1089	VAL
3	D	6	ARG
3	D	101	HIS
3	D	135	LEU
3	D	136	ASP
3	D	457	GLY
3	D	468	LEU
3	D	490	ALA
3	D	496	LEU
3	D	520	LEU
3	D	546	ARG
3	D	554	LEU
3	D	570	GLU
3	D	592	THR
3	D	594	PRO
3	D	608	SER
3	D	644	LEU
3	D	666	PHE
3	D	673	ALA
3	D	721	VAL
3	D	765	SER
3	D	785	ILE
3	D	843	PHE
3	D	883	ALA
3	D	934	LEU
3	D	944	THR
3	D	976	GLN
3	D	1069	GLU
3	D	1101	VAL
3	D	1115	THR
3	D	1177	ALA
3	D	1193	THR
3	D	1274	ILE
3	D	1277	ILE
3	D	1342	GLU
3	D	1352	ILE
3	D	1354	LYS
3	D	1377	LYS
3	D	1432	LYS
3	D	1460	ILE
4	E	26	ARG

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Mol	Chain	Res	Type
4	E	73	LEU
4	E	79	LEU
5	H	110	THR
5	H	217	TYR
5	H	222	LEU
5	H	271	ARG
5	H	310	MET
5	H	323	LEU
5	H	354	PRO
5	H	393	GLY
5	H	403	ALA
1	J	78	ILE
1	J	91	ASP
1	J	128	HIS
1	J	152	PRO
1	J	218	LEU
1	K	13	ALA
1	K	20	TYR
1	K	21	GLY
1	K	22	GLU
1	K	46	SER
1	K	48	ILE
1	K	76	VAL
1	K	113	ASP
2	L	35	PRO
2	L	87	ASP
2	L	106	GLY
2	L	148	PHE
2	L	167	LYS
2	L	175	GLU
2	L	205	GLU
2	L	303	PHE
2	L	317	VAL
2	L	318	PRO
2	L	376	ARG
2	L	394	PHE
2	L	521	PRO
2	L	562	SER
2	L	572	ILE
2	L	607	ASP
2	L	636	ALA
2	L	659	PRO

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Mol	Chain	Res	Type
2	L	675	ALA
2	L	682	TYR
2	L	716	LYS
2	L	739	GLU
2	L	756	VAL
2	L	777	ILE
2	L	786	LYS
2	L	796	GLU
2	L	822	VAL
2	L	830	LYS
2	L	833	LEU
2	L	834	GLN
2	L	942	GLU
2	L	943	VAL
2	L	1039	ALA
2	L	1072	LYS
2	L	1089	VAL
3	M	6	ARG
3	M	101	HIS
3	M	135	LEU
3	M	136	ASP
3	M	457	GLY
3	M	468	LEU
3	M	490	ALA
3	M	496	LEU
3	M	520	LEU
3	M	546	ARG
3	M	554	LEU
3	M	570	GLU
3	M	592	THR
3	M	594	PRO
3	M	608	SER
3	M	644	LEU
3	M	666	PHE
3	M	673	ALA
3	M	721	VAL
3	M	765	SER
3	M	785	ILE
3	M	843	PHE
3	M	934	LEU
3	M	944	THR
3	M	976	GLN

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Mol	Chain	Res	Type
3	M	1069	GLU
3	M	1101	VAL
3	M	1115	THR
3	M	1177	ALA
3	M	1193	THR
3	M	1274	ILE
3	M	1277	ILE
3	M	1342	GLU
3	M	1352	ILE
3	M	1354	LYS
3	M	1377	LYS
3	M	1432	LYS
3	M	1460	ILE
4	N	26	ARG
4	N	73	LEU
4	N	79	LEU
5	Q	110	THR
5	Q	217	TYR
5	Q	222	LEU
5	Q	271	ARG
5	Q	310	MET
5	Q	323	LEU
5	Q	354	PRO
5	Q	393	GLY
5	Q	403	ALA
1	A	41	ARG
1	A	45	LEU
1	A	53	VAL
1	A	127	LEU
1	A	139	TYR
1	A	203	GLY
1	B	119	ASP
1	B	154	GLU
1	B	175	ARG
1	B	187	GLY
2	C	15	LEU
2	C	21	ILE
2	C	73	ILE
2	C	124	ASP
2	C	149	THR
2	C	231	PRO
2	C	235	MET

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Mol	Chain	Res	Type
2	C	243	ARG
2	C	377	PRO
2	C	407	LYS
2	C	576	ALA
2	C	624	PRO
2	C	681	GLY
2	C	889	HIS
2	C	925	TYR
2	C	958	SER
2	C	966	LEU
2	C	977	GLY
2	C	1047	HIS
2	C	1063	ARG
2	C	1101	THR
3	D	150	ARG
3	D	743	ASP
3	D	774	SER
3	D	816	TYR
3	D	906	GLN
3	D	929	ARG
3	D	972	ARG
3	D	1012	GLU
3	D	1107	VAL
3	D	1133	ARG
3	D	1136	LYS
3	D	1207	TYR
3	D	1229	ILE
3	D	1299	PHE
3	D	1317	ASP
3	D	1324	PRO
4	E	55	TYR
5	H	138	ASP
5	H	154	ALA
5	H	355	SER
1	J	41	ARG
1	J	45	LEU
1	J	53	VAL
1	J	127	LEU
1	J	139	TYR
1	J	203	GLY
1	K	119	ASP
1	K	154	GLU

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Mol	Chain	Res	Type
1	K	175	ARG
1	K	187	GLY
2	L	15	LEU
2	L	21	ILE
2	L	73	ILE
2	L	124	ASP
2	L	149	THR
2	L	231	PRO
2	L	235	MET
2	L	243	ARG
2	L	377	PRO
2	L	407	LYS
2	L	576	ALA
2	L	624	PRO
2	L	681	GLY
2	L	889	HIS
2	L	925	TYR
2	L	958	SER
2	L	966	LEU
2	L	977	GLY
2	L	1047	HIS
2	L	1063	ARG
2	L	1101	THR
3	M	150	ARG
3	M	743	ASP
3	M	774	SER
3	M	816	TYR
3	M	906	GLN
3	M	929	ARG
3	M	972	ARG
3	M	1012	GLU
3	M	1107	VAL
3	M	1133	ARG
3	M	1136	LYS
3	M	1207	TYR
3	M	1229	ILE
3	M	1299	PHE
3	M	1317	ASP
3	M	1324	PRO
4	N	55	TYR
5	Q	138	ASP
5	Q	154	ALA

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Mol	Chain	Res	Type
5	Q	355	SER
1	A	58	ILE
1	A	75	VAL
2	C	9	ILE
2	C	23	VAL
2	C	197	LEU
2	C	390	GLN
2	C	403	SER
2	C	602	GLU
2	C	794	PRO
2	C	835	VAL
2	C	858	MET
2	C	859	PRO
3	D	504	ASP
3	D	623	VAL
3	D	882	PHE
3	D	884	ARG
3	D	981	GLY
3	D	987	GLU
3	D	989	TYR
3	D	1007	VAL
3	D	1213	ARG
3	D	1290	LEU
3	D	1319	VAL
3	D	1443	THR
3	D	1478	SER
5	H	244	TYR
5	H	302	SER
1	J	58	ILE
1	J	75	VAL
2	L	9	ILE
2	L	23	VAL
2	L	197	LEU
2	L	390	GLN
2	L	403	SER
2	L	500	ASN
2	L	602	GLU
2	L	794	PRO
2	L	835	VAL
2	L	858	MET
2	L	859	PRO
2	L	947	ALA

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Mol	Chain	Res	Type
3	M	504	ASP
3	M	623	VAL
3	M	882	PHE
3	M	884	ARG
3	M	981	GLY
3	M	987	GLU
3	M	1007	VAL
3	M	1213	ARG
3	M	1290	LEU
3	M	1319	VAL
3	M	1443	THR
3	M	1478	SER
5	Q	244	TYR
5	Q	302	SER
2	C	181	VAL
2	C	287	GLY
2	C	304	LEU
2	C	443	THR
2	C	520	GLU
2	C	912	PRO
2	C	1033	GLY
3	D	108	VAL
3	D	144	GLY
3	D	1032	PRO
3	D	1221	VAL
3	D	1392	GLY
2	L	181	VAL
2	L	287	GLY
2	L	304	LEU
2	L	443	THR
2	L	520	GLU
2	L	912	PRO
2	L	1033	GLY
3	M	108	VAL
3	M	144	GLY
3	M	1032	PRO
3	M	1221	VAL
3	M	1392	GLY
1	A	21	GLY
1	A	92	PRO
1	B	129	ILE
1	B	199	ILE

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Mol	Chain	Res	Type
2	C	119	PRO
2	C	192	PRO
2	C	446	GLY
2	C	678	PRO
2	C	727	PRO
3	D	719	VAL
3	D	792	ILE
3	D	992	VAL
3	D	1372	VAL
3	D	1415	VAL
3	D	1461	GLY
5	H	210	VAL
5	H	356	PRO
1	J	21	GLY
1	J	92	PRO
1	K	129	ILE
1	K	199	ILE
2	L	119	PRO
2	L	192	PRO
2	L	446	GLY
2	L	678	PRO
2	L	727	PRO
3	M	719	VAL
3	M	761	ILE
3	M	792	ILE
3	M	992	VAL
3	M	1372	VAL
3	M	1415	VAL
3	M	1461	GLY
5	Q	210	VAL
5	Q	356	PRO
1	B	124	ASN
2	C	151	ASP
2	C	319	GLY
2	C	415	PRO
2	C	621	VAL
2	C	674	VAL
2	C	799	ILE
2	C	982	PRO
2	C	1077	PRO
2	C	1099	VAL
3	D	683	ILE

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Mol	Chain	Res	Type
3	D	761	ILE
3	D	809	PRO
3	D	856	GLY
1	K	124	ASN
2	L	151	ASP
2	L	319	GLY
2	L	415	PRO
2	L	621	VAL
2	L	674	VAL
2	L	799	ILE
2	L	982	PRO
2	L	1077	PRO
2	L	1099	VAL
3	M	683	ILE
3	M	809	PRO
3	M	856	GLY
2	C	852	ILE
2	C	1055	ILE
3	D	38	LYS
2	L	852	ILE
2	L	1055	ILE
3	M	38	LYS
2	C	757	GLY
2	C	1016	ILE
2	C	1076	VAL
3	D	137	PRO
3	D	599	PRO
3	D	632	VAL
3	D	974	ILE
3	D	1423	GLY
3	D	1467	ILE
2	L	757	GLY
2	L	1016	ILE
2	L	1076	VAL
3	M	137	PRO
3	M	632	VAL
3	M	974	ILE
3	M	1423	GLY
3	M	1467	ILE

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	D	11
3	M	11

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Mol	Chain	Number of breaks
2	C	8
2	L	8
5	H	1
5	Q	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	44:LEU	C	45:PHE	N	1.70
1	M	44:LEU	C	45:PHE	N	1.70
1	D	532:GLY	C	533:GLY	N	1.61
1	M	532:GLY	C	533:GLY	N	1.61
1	C	416:GLY	C	417:GLY	N	1.19
1	L	416:GLY	C	417:GLY	N	1.19
1	D	93:ILE	C	94:GLU	N	1.17
1	M	93:ILE	C	94:GLU	N	1.17
1	D	115:LEU	C	116:LEU	N	1.16
1	M	115:LEU	C	116:LEU	N	1.16
1	C	423:ALA	C	424:GLY	N	1.13
1	L	423:ALA	C	424:GLY	N	1.13
1	D	113:GLY	C	114:THR	N	1.12
1	M	113:GLY	C	114:THR	N	1.12
1	D	1087:ARG	C	1088:THR	N	1.11
1	M	1087:ARG	C	1088:THR	N	1.11
1	D	521:PRO	C	522:PRO	N	1.09
1	D	526:PRO	C	527:MET	N	1.09
1	M	521:PRO	C	522:PRO	N	1.09
1	M	526:PRO	C	527:MET	N	1.09
1	D	529:GLN	C	530:VAL	N	1.06
1	M	529:GLN	C	530:VAL	N	1.06
1	H	239:VAL	C	240:GLU	N	1.05
1	Q	239:VAL	C	240:GLU	N	1.05
1	C	418:LEU	C	419:THR	N	1.01
1	C	419:THR	C	420:ARG	N	1.01
1	C	422:ARG	C	423:ALA	N	1.01
1	L	418:LEU	C	419:THR	N	1.01
1	L	419:THR	C	420:ARG	N	1.01
1	L	422:ARG	C	423:ALA	N	1.01
1	D	531:ASP	C	532:GLY	N	1.00
1	M	531:ASP	C	532:GLY	N	1.00
1	C	240:THR	C	241:LEU	N	0.99
1	L	240:THR	C	241:LEU	N	0.98
1	C	417:GLY	C	418:LEU	N	0.95

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	417:GLY	C	418:LEU	N	0.95
1	C	244:PRO	C	245:GLY	N	0.92
1	D	91:GLY	C	92:HIS	N	0.92
1	L	244:PRO	C	245:GLY	N	0.92
1	M	91:GLY	C	92:HIS	N	0.92

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.