



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 16, 2023 – 10:28 AM EDT

PDB ID : 2A69
Title : Crystal structure of the T. Thermophilus RNA polymerase holoenzyme in complex with antibiotic rifapentin
Authors : Artsimovitch, I.; Vassilyeva, M.N.; Svetlov, D.; Svetlov, V.; Perederina, A.; Igarashi, N.; Matsugaki, N.; Wakatsuki, S.; Tahirov, T.H.; Vassilyev, D.G.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2005-07-02
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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](#) ①) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.35
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

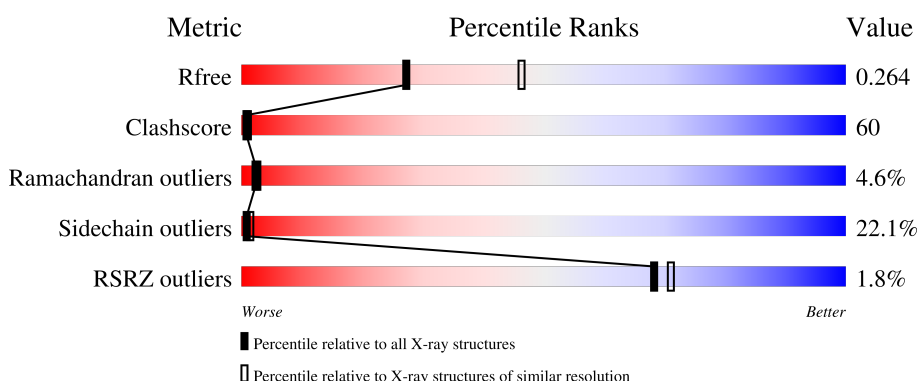
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	315	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 17%; height: 10px; background-color: green;"></div> <div style="width: 44%; height: 10px; background-color: yellow;"></div> <div style="width: 10%; height: 10px; background-color: orange;"></div> <div style="width: 27%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">17% 44% 10% • 27%</p>
1	B	315	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red;"></div> <div style="width: 18%; height: 10px; background-color: green;"></div> <div style="width: 43%; height: 10px; background-color: yellow;"></div> <div style="width: 11%; height: 10px; background-color: orange;"></div> <div style="width: 27%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">4% 18% 43% 11% 27%</p>
1	K	315	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 23%; height: 10px; background-color: green;"></div> <div style="width: 40%; height: 10px; background-color: yellow;"></div> <div style="width: 9%; height: 10px; background-color: orange;"></div> <div style="width: 27%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">% 23% 40% 9% • 27%</p>
1	L	315	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red;"></div> <div style="width: 19%; height: 10px; background-color: green;"></div> <div style="width: 43%; height: 10px; background-color: yellow;"></div> <div style="width: 10%; height: 10px; background-color: orange;"></div> <div style="width: 27%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">2% 19% 43% 10% 27%</p>
2	C	1119	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 22%; height: 10px; background-color: green;"></div> <div style="width: 59%; height: 10px; background-color: yellow;"></div> <div style="width: 18%; height: 10px; background-color: orange;"></div> <div style="width: 1%; height: 10px; background-color: red;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">% 22% 59% 18% • 2%</p>

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Mol	Chain	Length	Quality of chain
2	M	1119	<p>24% 59% 16%</p>
3	D	1524	<p>23% 52% 16% 2% 9%</p>
3	N	1524	<p>25% 51% 14% 2% 9%</p>
4	E	99	<p>28% 49% 18% 5%</p>
4	O	99	<p>27% 49% 18%</p>
5	F	423	<p>20% 46% 14% 2% 18%</p>
5	P	423	<p>20% 49% 11% 2% 18%</p>

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 60572 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 DNA-directed RNA polymerase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
1	B	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
1	K	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
1	L	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			

- Molecule 2 is a protein called DNA-directed RNA polymerase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	1119	Total	C	N	O	S	0	0	0
			8829	5581	1577	1647	24			
2	M	1119	Total	C	N	O	S	0	0	0
			8829	5581	1577	1647	24			

- Molecule 3 is a protein called DNA-directed RNA polymerase beta' chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	1392	Total	C	N	O	S	0	0	0
			10797	6819	1925	2020	33			
3	N	1392	Total	C	N	O	S	0	0	0
			10797	6819	1925	2020	33			

- Molecule 4 is a protein called RNA polymerase omega chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	E	95	Total	C	N	O	S	0	0	0
			769	488	133	144	4			
4	O	95	Total	C	N	O	S	0	0	0
			769	488	133	144	4			

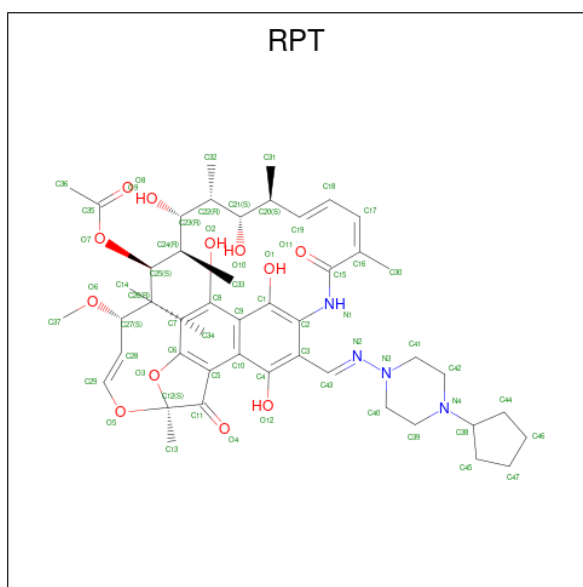
- Molecule 5 is a protein called RNA polymerase sigma factor rpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	F	345	Total 2771	C 1744	N 504	O 519	S 4	0	0	0
5	P	345	Total 2771	C 1744	N 504	O 519	S 4	0	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	33	Total 33	Mg 33	0	0
6	B	21	Total 21	Mg 21	0	0
6	C	73	Total 73	Mg 73	0	0
6	D	106	Total 106	Mg 106	0	0
6	E	5	Total 5	Mg 5	0	0
6	F	28	Total 28	Mg 28	0	0
6	K	19	Total 19	Mg 19	0	0
6	L	17	Total 17	Mg 17	0	0
6	M	65	Total 65	Mg 65	0	0
6	N	92	Total 92	Mg 92	0	0
6	O	8	Total 8	Mg 8	0	0
6	P	20	Total 20	Mg 20	0	0

- Molecule 7 is RIFAPENTINE (three-letter code: RPT) (formula: C₄₇H₆₄N₄O₁₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
7	C	1	Total	C	N	O	0	0
			63	47	4	12		
7	M	1	Total	C	N	O	0	0
			63	47	4	12		

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	2	Total	Zn	0	0
			2	2		
8	N	2	Total	Zn	0	0
			2	2		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	239	Total	O	0	0
			239	239		
9	B	258	Total	O	0	0
			258	258		
9	C	979	Total	O	0	0
			979	979		
9	D	1252	Total	O	0	0
			1252	1252		
9	E	117	Total	O	0	0
			117	117		

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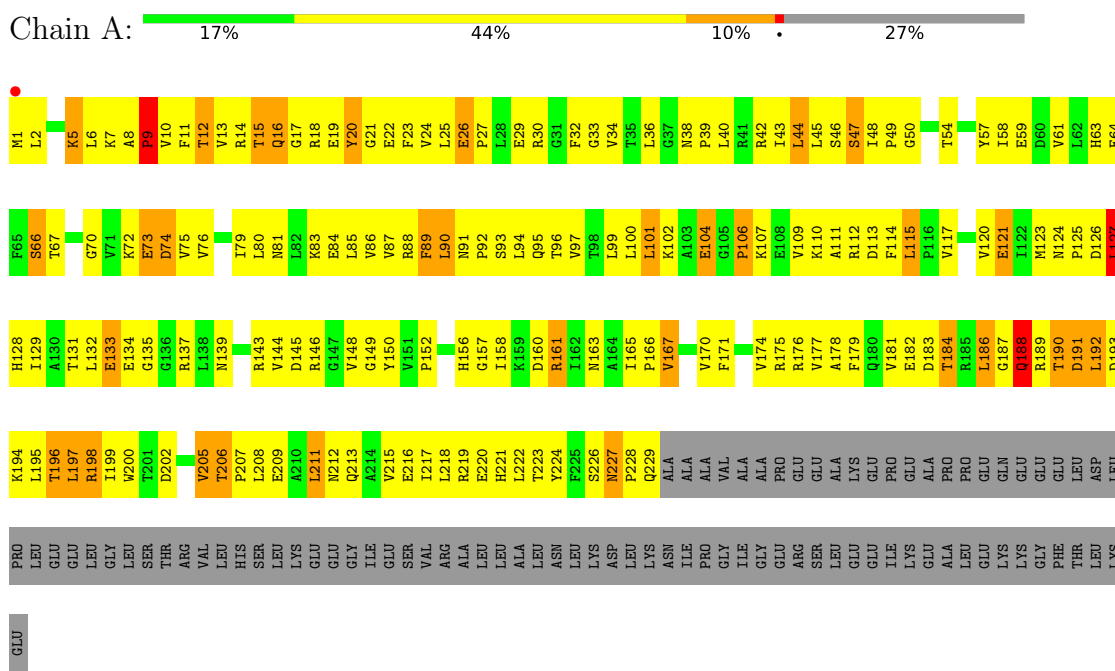
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	F	420	Total 420	O 420	0	0
9	K	183	Total 183	O 183	0	0
9	L	219	Total 219	O 219	0	0
9	M	998	Total 998	O 998	0	0
9	N	1265	Total 1265	O 1265	0	0
9	O	108	Total 108	O 108	0	0
9	P	361	Total 361	O 361	0	0

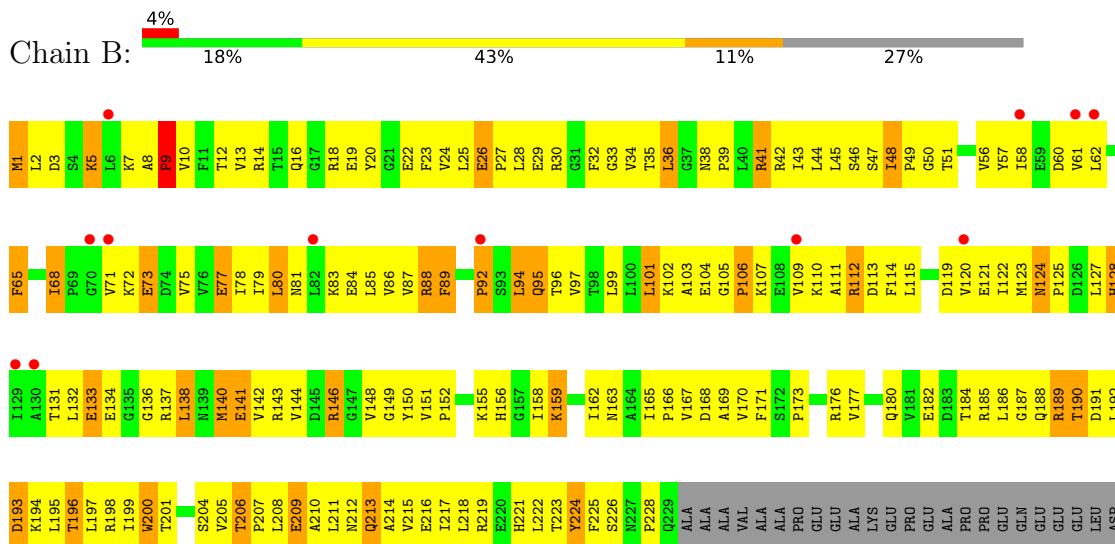
3 Residue-property plots

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

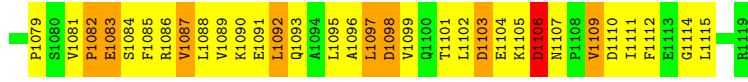
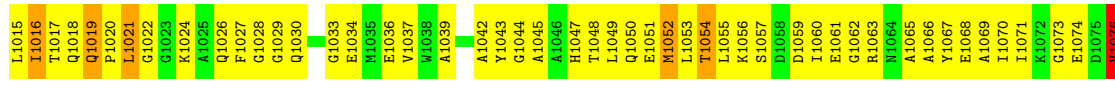
- Molecule 1: DNA-directed RNA polymerase alpha chain



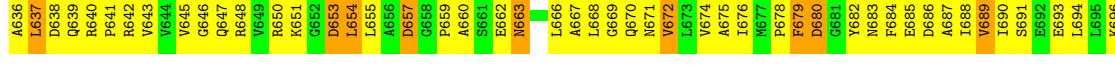
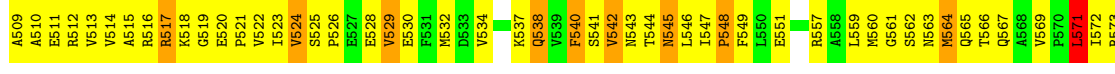
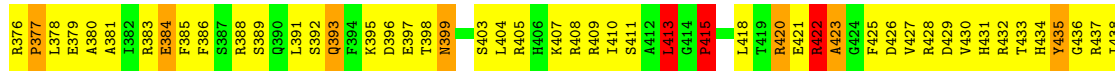
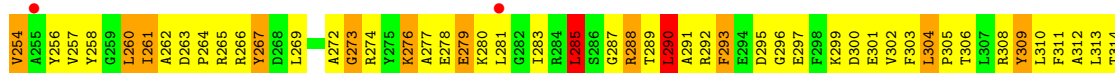
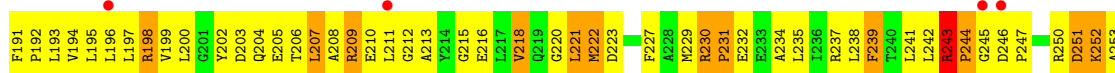
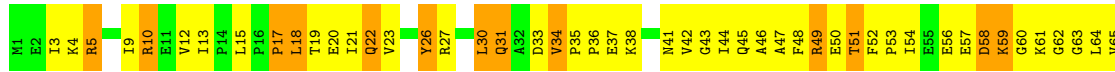
- Molecule 1: DNA-directed RNA polymerase alpha chain



V65	V66	V67	V68	V69	V70	V71	V72	V73	V74	V75	V76	V77	V78	V79	V80	V81	V82	V83	V84	V85	V86	V87	V88	V89	V90	V91	V92	V93	V94	V95	V96	V97	V98	V99	V100	V101	V102	V103	V104	V105	V106	V107	V108	V109	V110	V111	V112	V113	V114	V115	V116	V117	V118	V119	V120	V121	V122	V123	V124	V125						
L66	D67	L68	L69	L70	L71	L72	L73	L74	L75	L76	L77	L78	L79	L80	L81	L82	L83	L84	L85	L86	L87	L88	L89	L90	L91	L92	L93	L94	L95	L96	L97	L98	L99	L100	L101	L102	L103	L104	L105	L106	L107	L108	L109	L110	L111	L112	L113	L114	L115	L116	L117	L118	L119	L120	L121	L122	L123	L124	L125							
S126	F127	R188	R189	K190	A132	D133	V134	V135	L136	V137	S138	L139	L140	H141	R142	S143	P144	V145	V146	Y147	D150	P150	L151	P152	A153	H154	P155	G156	R157	Y158	L159	D160	D223	F227	I162	I163	A228	P164	L165	P166	K167	R168	G169	P170	W171	I172	D173	L174	E175	L236	L241	L242	R243	M179	G180	D244	R250	D251	K185	A253						
M187	K188	R189	K190	L193	V194	L195	L196	L197	L198	V199	L200	G201	Y202	Y203	Q204	E205	P144	T206	L207	A208	R209	E210	L211	G212	A213	Y214	G215	V218	L221	M222	D223	F227	I162	I163	A228	P164	L165	P166	K167	R168	G169	P170	W171	I172	D173	L174	E175	L236	L241	L242	R243	M179	G180	D244	R250	D251	K185	A253								
V254	A255	Y256	Y257	G258	L260	L261	A262	D263	P264	R265	L266	D267	D268	D269	Q270	E271	A272	G273	R274	Y275	E276	E277	K280	L281	Y214	L283	L285	S286	G287	R288	T289	L290	A291	R292	F293	G296	E297	F298	K299	D300	E301	V302	F303	L304	P305	T306	L307	R308	Y309	D310	L311	A312	L313	T314												
P318	G319	H320	E321	V322	D323	D324	I325	F326	H327	L328	G329	N330	R331	R332	R333	R334	T335	V336	G337	E338	L339	M340	T341	Q343	F344	R345	G346	R347	L348	A349	R350	L351	A352	R353	G354	V355	R356	E357	R358	M359	L360	M361	G362	E363	E364	D365	L366	T367	T368	P369	K370	G371	G372	V373	N374	S375	L376	P377								
L378	E379	A380	G381	L382	R383	E384	F385	F386	G387	R388	G389	Q390	L391	S392	Q393	F394	K395	D396	E397	T398	N399	P400	S403	L404	H405	H406	R407	R408	R409	I410	A411	A412	L413	G414	P415	T419	R420	E421	R422	A423	G424	F425	D426	V427	H431	R432	T433	H434	Y435	G436	R437	L438	C439	F440	L441	E442										
T443	P444	G445	G446	A447	N448	I449	G450	R451	V452	I453	S454	L455	A456	A457	Y458	L459	R460	V461	D462	T463	L464	G465	I467	R468	T469	P470	Y471	R472	R473	V474	V475	V476	V477	T480	M481	E482	V483	Y484	Y485	M486	T487	A488	T489	E490	E491	D492	R493	Y494	T495	L496	A497	Q498	A499	G500	L501	P502	L503	E504								
G505	N506	I507	I508	A509	A510	E511	R512	V513	V514	A515	R516	R517	K518	G519	E520	R521	R522	I523	V524	S525	D526	E527	E528	E529	E530	F531	D532	D533	V534	S535	N536	Q538	S541	V542	N543	T544	I547	P548	F549	L550	E551	H552	D553	D554	A555	N556	R557	A558	E559	L559	M560	G561	R562	N563	L564	Q565	T566									
Q567	A568	V569	P570	L571	I572	Q575	A576	P577	V578	R579	M580	L583	E584	E585	R586	E587	V588	R589	D589	S591	L592	A593	A594	L595	Y596	E597	E598	E599	D600	G601	Q602	V603	R610	L611	V612	V613	R614	Y615	E616	F617	R618	E619	D620	B621	E622	N623	F624	L625	R626	D627	F628	Y629	S631													
M632	Q633	T634	P635	A636	L637	D638	Q639	R640	P641	R642	V643	V644	V645	Q646	E647	R648	V649	R650	K651	R652	D653	L654	A655	D656	G658	P659	A660	S661	E662	M663	G664	F665	L666	A667	K668	G669	Q670	M671	V672	L673	P674	M675	P676	F677	D678	L679	E679	E680	L681	L682	L683	L684	L685	L686	L687	L688	V689	L690	S691							
E692	E693	L694	L695	K696	R697	D698	F699	Y700	T701	S702	I703	H704	I705	O706	R707	O708	Y709	I710	E711	R712	R713	D714	T715	K716	L717	E720	I721	I722	I723	R724	D725	V726	H727	H728	L729	S730	E731	A732	D733	L734	R735	D736	L737	D738	E739	E740	G741	V742	V743	R744	F745	G746	P747	A748	R749	L750	P751	G752								
L755	G756	R757	R758	Y759	S760	F761	S765	R766	T767	T768	P769	E770	E771	D772	L773	L774	R775	R776	I777	F778	H779	G784	E780	K781	A782	V783	D784	V785	L788	S789	L790	R791	M792	P793	P794	G795	E796	G797	G798	L799	T800	R801	D802	D803	V804	R805	R806	R807	D808	G809	D810	P811	S812	V813	K816	R817	L818	L819	G820							
V819	R820	E821	V825	R826	V827	A828	R829	R830	R831	L832	L833	Q834	R835	G836	D837	K838	L839	R840	R841	R842	R843	G844	R845	K846	V849	L852	L853	R854	V855	E856	D857	M858	R859	H860	L861	P862	D863	G864	T865	P866	V867	D868	V869	L870	R871	R872	L873	L874	G875	V876	P877	S878	R879	K880	M881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892
O884	L885	L886	P889	L890	G891	L892	A893	F896	L897	G898	Q899	R900	Y901	S902	S903	P904	L905	F906	D907	G908	G909	A910	E911	F912	E913	L914	K915	E916	L917	L918	A919	E923	G924	Y924	Y925	F926	G927	K930	G931	F934	D937	K938	R939	E940	Y943	L944	R945	S878	S879	K949	L950	G951	L952													
V953	T954	P955	G956	K957	T958	E961	K964	E965	L966	F967	L968	Q969	G970	R971	G972	V973	L974	Y975	D976	G977	G978	A909	E911	F912	E913	L914	K915	E916	L917	L918	A919	E923	G924	Y924	Y925	F926	G927	K930	G931	F934	D937	K938	R939	E940	Y943	L944	R945	S878	S879	K949	L950	G951	L952													



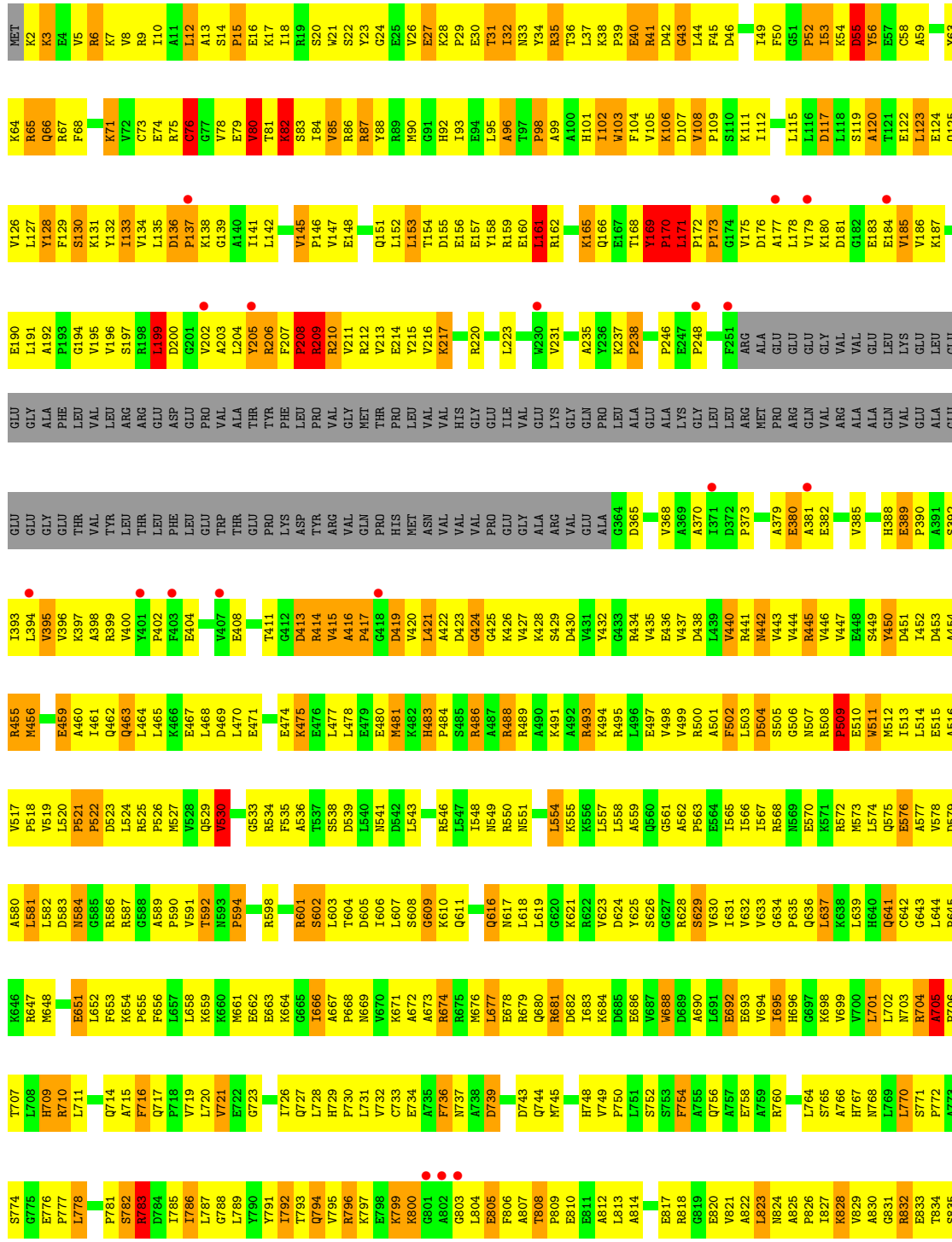
● Molecule 2: DNA-directed RNA polymerase beta chain

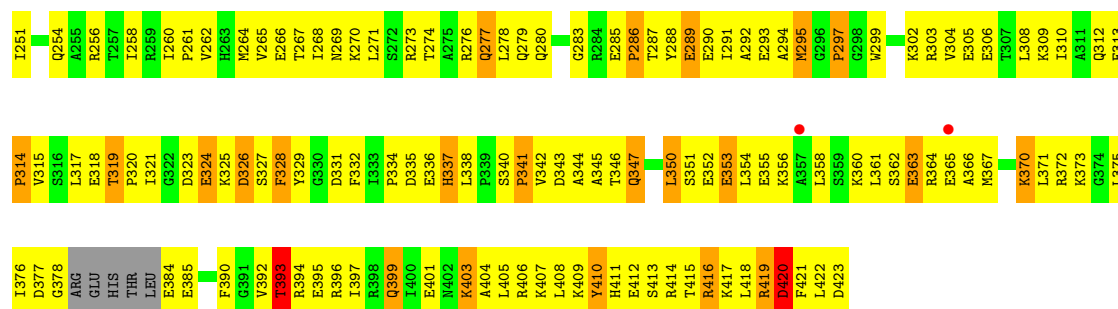


V1404	E1405	R1406	L1407	A1408	I1409	E1410	G1411	K1412	T1413	P1414	V1415	W1416	W1417	K1418	P1419	L1420	L1421	W1422	V1423	V1424	K1425	K1426	S1427	L1428	S1430	T1431	K1432	K1433	K1434	L1435	S1436	A1437	A1438	S1439	F1440	Q1441	R1442	T1443	V1446	L1447	T1448	I1452	G1453	G1454	K1455	K1456	D1457	I1460	G1461	L1462	K1463	E1464	V1465	A1466	I1467								
V1344	E1345	R1346	L1347	L1348	E1349	E1350	E1351	L1352	Q1353	K1354	L1355	V1356	R1357	A1358	Q1359	G1360	V1361	K1362	L1363	H1364	D1365	K1366	H1367	L1368	E1369	I1370	V1371	V1372	R1373	K1374	Q1375	M1376	K1377	V1378	V1379	E1380	V1381	D1382	P1383	L1384	L1385	S1386	R1387	R1388	L1389	E1390	D1391	L1392	L1393	D1394	L1395	E1396	K1397	L1398	D1399	V1400	E1401	A1402	L1403				
E1219	A1220	V1221	G1222	I1223	E1224	A1225	A1226	Q1227	S1228	L1229	G1230	E1231	P1232	G1233	T1234	Q1235	L1236	T1237	M1238	L1239	T1240	F1241	H1242	H1243	G1244	I1245	A1246	G1247	G1248	D1249	F1250	T1251	G1252	L1253	G1254	L1255	L1256	P1257	R1258	V1259	I1260	E1261	L1262	F1263	E1264	A1265	R1266	R1267	P1268	K1269	K1270	A1271	M1272	V1273	V1274	L1275	L1276	L1277	D1278	G1279			
V1280	V1281	R1282	I1283	E1284	E1285	T1286	E1287	E1288	K1289	L1290	S1291	V1292	F1293	E1294	Q1295	G1296	F1299	K1300	E1301	E1302	Y1303	K1304	L1305	P1306	K1307	A1308	A1309	L1310	L1311	L1312	V1313	K1314	D1315	G1316	D1317	L1318	V1319	E1320	A1321	P1324	L1325	T1326	R1327	I1330	D1331	E1332	H1333	Q1334	L1335	L1336	E1337	L1338	A1339	H1340	E1341	L1342	G1343	V1400	E1401	A1402	L1403		
V1344	E1345	R1346	L1347	L1348	E1349	E1350	E1351	L1352	Q1353	K1354	L1355	V1356	R1357	A1358	Q1359	G1360	V1361	K1362	L1363	H1364	D1365	K1366	H1367	L1368	E1369	I1370	V1371	V1372	R1373	K1374	Q1375	M1376	K1377	V1378	V1379	E1380	V1381	D1382	P1383	L1384	L1385	S1386	R1387	R1388	L1389	E1390	D1391	L1392	L1393	D1394	L1395	E1396	K1397	L1398	D1399	V1400	E1401	A1402	L1403				
E1513	L514	E515	A516	V517	P518	V519	L520	P521	P522	D523	L524	R525	P526	M527	V528	Q529	V530	D531	G532	G533	F534	F535	A536	T537	S538	L539	D540	N541	L542	L543	Y544	R545	R546	L547	I548	A549	R550	N551	N552	L553	L554	K555	L556	A557	Q558	Q559	G560	G561	V623	D624	Y625	E564	L565	S629	V630	I631	R632	N633	E570	K571	V699	P655	M573
L574	Q575	E576	A577	V578	D579	L580	L581	L582	D583	N584	G585	R586	R587	G588	V589	P590	V591	T592	N593	P594	D597	R598	L600	R601	L602	L603	L604	A605	L606	L607	S608	G609	K610	Q611	A612	A613	F614	R615	Q616	N617	L618	L619	G620	K621	R622	V623	D624	Y625	R628	S629	V630	I631	R632	N633	E570	K571	V699	P655	M573				
L637	K638	L639	H640	Q641	C642	G643	L644	P645	K646	R710	M648	M649	L650	G651	L652	F653	K654	P655	F656	L657	D658	L659	K660	E662	E663	L664	L665	A666	L667	M668	N669	V670	K671	F736	N737	A672	A673	R674	R675	M676	L677	E678	R679	G680	R681	D682	I683	K684	D685	F686	V687	W688	V689	L690	V700								
L701	L702	R703	R704	A705	P706	T707	L708	H709	K710	L711	G712	I713	Q714	A715	F716	E717	F718	P719	L720	V721	G722	G723	Q724	A725	I726	Q727	L728	H729	P730	C733	E734	A735	F736	N737	A672	A673	D739	F740	D741	G742	L743	Q744	M745	A746	D682	I683	K684	D685	F686	V687	W688	V689	L690	V700									
Q762	M763	R764	S765	H766	M767	N768	L769	L770	A773	G774	S775	E776	F777	K780	L781	R782	L783	D784	L785	I786	T787	L788	V789	Y790	Y791	L792	T793	Q794	V795	R796	L797	K798	L799	E800	K801	A802	L803	L804	E805	F806	A807	T808	P809	I810	E811	A812	L813	E814	R815	L816	L817	L818	L819	L820	L821	L822	L823	A825					
R826	L827	K828	H829	A830	R831	R832	E833	T834	R835	V836	C837	R838	L839	R840	H841	W842	F843	A844	R845	R846	D847	E848	A849	L850	L851	A852	Y853	L857	R858	L859	R860	D862	E798	V863	W864	T865	Y866	R867	Y868	L869	M869	L870	E871	T872	E873	L874	E875	R876	S877	C878	R879	L880	A881	R882	A883	R884	A887	E888	A889				
V890	E891	D892	E893	K894	W895	A896	M897	E898	L899	R900	L901	L902	D903	V904	E905	W906	E907	F908	K909	S910	R911	L912	D913	K914	V915	V916	Q917	R918	Y919	R920	R921	L922	G923	E925	K926	T927	A928	R929	L930	L931	T940	T943	L944	K1008	K1009	M1010	F1011	E1012	Y1015	E1016	D952	A953	V955	V956	P957	E958							
E959	K960	Y963	E964	E965	E966	A967	R968	Q1033	L1034	I1035	L1036	Q1037	L1038	C1039	G1040	L1041	R1042	G1043	L1044	M1045	Q1046	K1047	P1048	E1051	F1052	F1053	P1056	R988	Y989	L992	L995	W996	E997	K926	T927	I1000	E1001	K1002	L1003	T1004	A1006	V1007	F1008	K1009	M1010	F1011	E1012	Y1015	E1016	D952	A953	V955	V956	P957	E958								
S1026	G1027	A1028	R1029	G1030	H1031	P1032	Q1033	L1034	I1035	L1036	Q1037	L1038	C1039	G1040	L1041	R1042	G1043	L1044	M1045	Q1046	K1047	P1048	E1051	F1052	F1053	P1056	R988	Y989	L992	L995	W996	E997	K926	T927	I1000	E1001	K1002	L1003	T1004	A1006	V1007	F1008	K1009	M1010	F1011	E1012	Y1015	E1016	D952	A953	V955	V956	P957	E958									
R1087	D1090	S1091	G1092	Y1093	L1094	T1095	R1096	Q1163	K1097	L1098	V1099	D1100	V1101	H1102	H1103	E1104	I1105	V1106	R1107	R1108	E1109	G1112	T1114	H1115	M1116	Y1117	P1118	S1119	V1120	P1121	Q1124	E1127	L1128	T1129	R1130	R1135	K1136	L1137	A1138	D1139	I1140	E1141	A1142	G1143	L1144	Y1145	G1146	R1147	V1148	L1149	A1150	R1151	E1152	V1153									
E1154	V1155	L1156	L1157	L1158	E1159	E1160	E1161	E1162	R1163	R1164	L1165	S1166	M1167	D1169	D1170	V1171	H1172	L1173	L1174	L1175	K1176	A1177	A1178	E1179	I1183	V1186	P1187	V1188	L1189	S1190	L1191	L1192	L1193	C1194	Q1195	L1196	R1197	Y1198	C1201	Q1202	K1203	C1204	Y1205	L1206	A1207	P1208	L1209	S1210	M1211	A1212	R1213	P1214	V1215	S1216	G1218								
E1219	A1220	V1221	G1222	I1223	E1224	A1225	A1226	Q1227	S1228	L1229	G1230	E1231	P1232	G1233	T1234	Q1235	L1236	T1237	M1238	L1239	T1240	F1241	H1242	H1243	G1244	I1245	A1246	G1247	G1248	D1249	F1250	T1251	G1252	L1253	G1254	L1255	L1256	P1257	R1258	V1259	I1260	E1261	L1262	F1263	E1264	A1265	R1266	R1267	P1268	K1269	K1270	A1271	M1272	V1273	V1274	L1275	L1276	L1277	D1278	G1279			
V1280	V1281	R1282	I1283	E1284	E1285	T1286	E1287	E1288	K1289	L1290	S1291	V1292	F1293	E1294	Q1295	G1296	F1299	K1300	E1301	E1302	Y1303	K1304	L1305	P1306	K1307	A1308	A1309	L1310	L1311	L1312	V1313	K1314	D1315	G1316	D1317	L1318	V1319	E1320	A1321	P1324	L1325	T1326	R1327	I1330	D1331	E1332	H1333	Q1334	L1335	L1336	E1337	L1338	A1339	H1340	E1341	L1342	G1343	V1400	E1401	A1402	L1403		
V1344	E1345	R1346	L1347	L1348	E1349	E1350	E1351	L1352	Q1353	K1354	L1355	V1356	R1357	A1358	Q1359	G1360	V1361	K1362	L1363	H1364	D1365	K1366	H1367	L1368	E1369	I1370	V1371	V1372	R1373	K1374	Q1375	M1376	K1377	V1378	V1379	E1380	V1381	D1382	P1383	L1384	L1385	S1386	R1387	R1388	L1389	E1390	D1391	L1392	L1393	D1394	L1395	E1396	K1397	L1398	D1399	V1400	E1401	A1402	L1403				



● Molecule 3: DNA-directed RNA polymerase beta' chain





4 Data and refinement statistics i

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	239.50Å 239.50Å 253.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.50 24.85 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.50) 92.5 (24.85-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.50Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.230 , 0.267 0.228 , 0.264	Depositor DCC
R_{free} test set	29710 reflections (5.75%)	wwPDB-VP
Wilson B-factor (Å ²)	47.8	Xtrriage
Anisotropy	0.214	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 76.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtrriage
Estimated twinning fraction	0.499 for -h,-k,l 0.076 for h,-h-k,-l 0.076 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	60572	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

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

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	0.81	1/1838 (0.1%)	0.88	4/2498 (0.2%)
1	B	0.74	0/1838	0.81	2/2498 (0.1%)
1	K	0.75	0/1838	0.86	3/2498 (0.1%)
1	L	0.73	1/1838 (0.1%)	0.80	2/2498 (0.1%)
2	C	0.83	2/8997 (0.0%)	0.89	7/12164 (0.1%)
2	M	0.81	0/8997	0.88	8/12164 (0.1%)
3	D	0.84	0/10975	0.94	20/14836 (0.1%)
3	N	0.82	0/10975	0.92	17/14836 (0.1%)
4	E	0.84	0/783	0.94	0/1054
4	O	0.82	0/783	0.96	2/1054 (0.2%)
5	F	0.74	0/2812	0.82	4/3781 (0.1%)
5	P	0.71	0/2812	0.80	1/3781 (0.0%)
All	All	0.81	4/54486 (0.0%)	0.89	70/73662 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	48	ILE	C-N	6.06	1.45	1.34
1	L	172	SER	N-CA	-5.43	1.35	1.46
2	C	792	VAL	CB-CG1	-5.28	1.41	1.52
2	C	393	GLN	CD-OE1	5.25	1.35	1.24

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1389	LEU	CA-CB-CG	8.13	133.99	115.30
1	K	211	LEU	CA-CB-CG	8.11	133.95	115.30
1	B	138	LEU	CA-CB-CG	7.70	133.00	115.30
1	A	192	LEU	CA-CB-CG	7.60	132.79	115.30
3	D	199	LEU	CA-CB-CG	-7.59	97.84	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1806	0	1861	232	0
1	B	1806	0	1861	216	0
1	K	1806	0	1861	173	0
1	L	1806	0	1861	186	0
2	C	8829	0	8933	1215	0
2	M	8829	0	8933	1174	0
3	D	10797	0	10873	1490	0
3	N	10797	0	10873	1288	0
4	E	769	0	775	89	0
4	O	769	0	775	95	0
5	F	2771	0	2844	346	0
5	P	2771	0	2844	352	0
6	A	33	0	0	0	0
6	B	21	0	0	0	0
6	C	73	0	0	0	0
6	D	106	0	0	0	0
6	E	5	0	0	0	0
6	F	28	0	0	0	0
6	K	19	0	0	0	0
6	L	17	0	0	0	0
6	M	65	0	0	0	0
6	N	92	0	0	0	0
6	O	8	0	0	0	0
6	P	20	0	0	0	0
7	C	63	0	62	6	0
7	M	63	0	62	7	0
8	D	2	0	0	0	0
8	N	2	0	0	0	0
9	A	239	0	0	50	0
9	B	258	0	0	46	0
9	C	979	0	0	224	0
9	D	1252	0	0	277	0
9	E	117	0	0	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	F	420	0	0	94	0
9	K	183	0	0	39	0
9	L	219	0	0	46	0
9	M	998	0	0	249	0
9	N	1265	0	0	250	0
9	O	108	0	0	26	0
9	P	361	0	0	78	0
All	All	60572	0	54418	6470	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 60.

The worst 5 of 6470 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:GLN:HA	1:A:146:ARG:HH12	1.07	1.11
2:M:952:LEU:HD12	2:M:969:GLN:HE22	1.13	1.11
3:D:1087:ARG:HG2	3:D:1234:THR:HA	1.27	1.07
1:B:152:PRO:HD2	1:B:155:LYS:HD3	1.36	1.05
2:M:605:LYS:HB2	2:M:610:ARG:HH12	1.16	1.05

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	227/315 (72%)	201 (88%)	21 (9%)	5 (2%)	6 10
1	B	227/315 (72%)	198 (87%)	23 (10%)	6 (3%)	5 8
1	K	227/315 (72%)	200 (88%)	23 (10%)	4 (2%)	8 14
1	L	227/315 (72%)	203 (89%)	20 (9%)	4 (2%)	8 14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	1117/1119 (100%)	907 (81%)	157 (14%)	53 (5%)	2	2
2	M	1117/1119 (100%)	906 (81%)	158 (14%)	53 (5%)	2	2
3	D	1388/1524 (91%)	1108 (80%)	207 (15%)	73 (5%)	2	2
3	N	1388/1524 (91%)	1105 (80%)	208 (15%)	75 (5%)	2	2
4	E	93/99 (94%)	75 (81%)	15 (16%)	3 (3%)	4	5
4	O	93/99 (94%)	75 (81%)	15 (16%)	3 (3%)	4	5
5	F	341/423 (81%)	285 (84%)	38 (11%)	18 (5%)	2	2
5	P	341/423 (81%)	287 (84%)	38 (11%)	16 (5%)	2	2
All	All	6786/7590 (89%)	5550 (82%)	923 (14%)	313 (5%)	2	2

5 of 313 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	B	29	GLU
1	B	48	ILE
2	C	152	PRO
2	C	178	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	202/273 (74%)	159 (79%)	43 (21%)	1	2
1	B	202/273 (74%)	161 (80%)	41 (20%)	1	2
1	K	202/273 (74%)	158 (78%)	44 (22%)	1	1
1	L	202/273 (74%)	160 (79%)	42 (21%)	1	2
2	C	941/941 (100%)	714 (76%)	227 (24%)	0	1
2	M	941/941 (100%)	738 (78%)	203 (22%)	1	1
3	D	1123/1279 (88%)	868 (77%)	255 (23%)	1	1
3	N	1123/1279 (88%)	871 (78%)	252 (22%)	1	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	83/87 (95%)	62 (75%)	21 (25%)	0	1
4	O	83/87 (95%)	65 (78%)	18 (22%)	1	1
5	F	295/370 (80%)	233 (79%)	62 (21%)	1	2
5	P	295/370 (80%)	246 (83%)	49 (17%)	2	4
All	All	5692/6446 (88%)	4435 (78%)	1257 (22%)	1	1

5 of 1257 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	1074	GLU
3	N	1306	PRO
3	N	66	GLN
2	M	1060	ILE
3	N	704	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 169 such sidechains are listed below:

Mol	Chain	Res	Type
2	M	920	GLN
3	N	1242	HIS
3	N	101	HIS
3	N	748	HIS
3	N	1441	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 493 ligands modelled in this entry, 491 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	RPT	M	8002	-	68,68,68	2.52	22 (32%)	101,101,101	1.22	9 (8%)
7	RPT	C	8001	-	68,68,68	2.45	22 (32%)	101,101,101	1.23	11 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	RPT	M	8002	-	-	20/64/96/96	0/6/6/6
7	RPT	C	8001	-	-	12/64/96/96	0/6/6/6

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	8002	RPT	C39-N4	6.55	1.59	1.47
7	M	8002	RPT	C42-N4	6.42	1.59	1.47
7	C	8001	RPT	O6-C27	6.22	1.58	1.43
7	C	8001	RPT	O5-C29	6.12	1.55	1.39
7	M	8002	RPT	O5-C29	5.98	1.54	1.39

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	8002	RPT	C24-C23-C22	3.73	121.68	115.43
7	C	8001	RPT	C24-C23-C22	3.28	120.92	115.43
7	M	8002	RPT	C20-C21-C22	3.25	121.58	114.96
7	C	8001	RPT	C25-O7-C35	3.23	122.72	117.72
7	C	8001	RPT	C2-N1-C15	3.10	134.26	124.11

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	8001	RPT	C26-C27-C28-C29
7	C	8001	RPT	C26-C27-O6-C37
7	C	8001	RPT	C28-C27-O6-C37
7	M	8002	RPT	C28-C27-O6-C37
7	M	8002	RPT	C44-C38-N4-C39

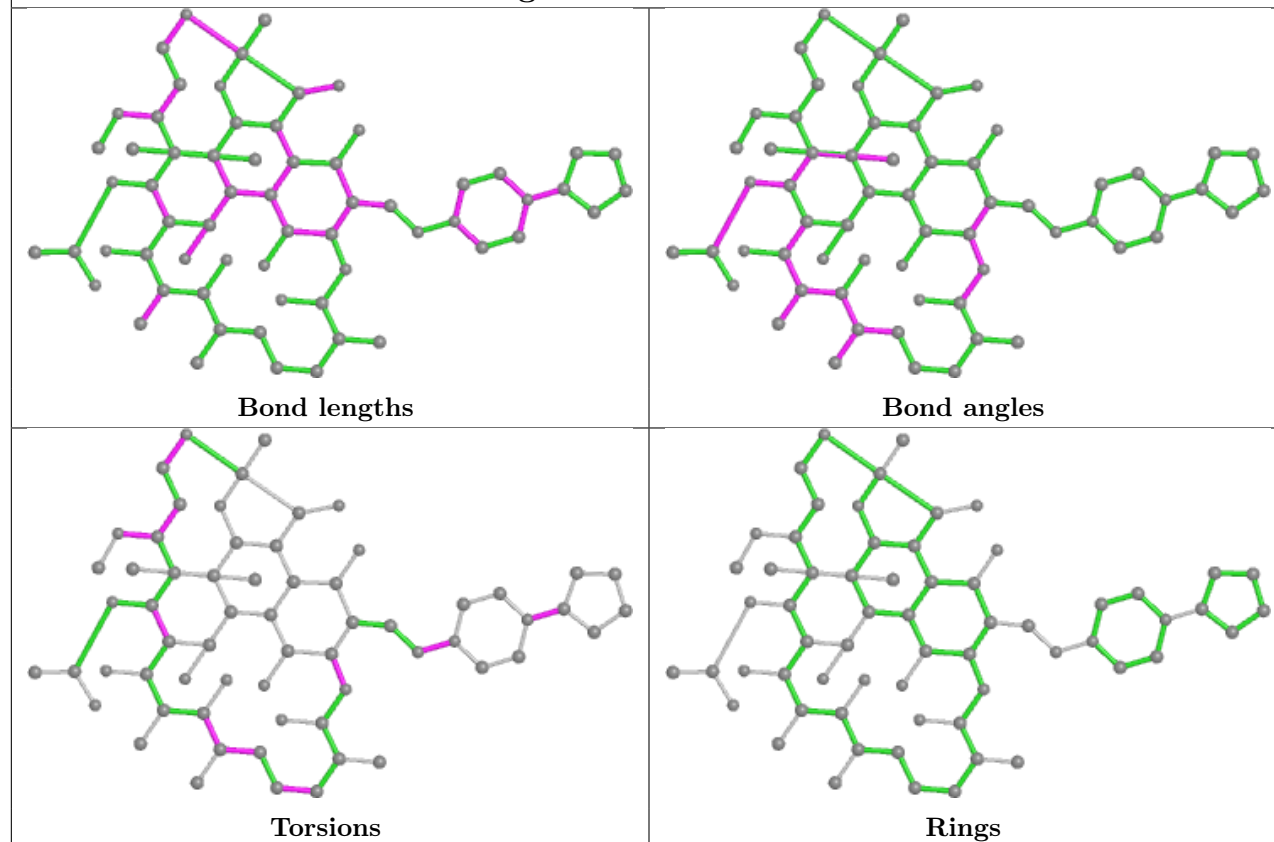
There are no ring outliers.

2 monomers are involved in 13 short contacts:

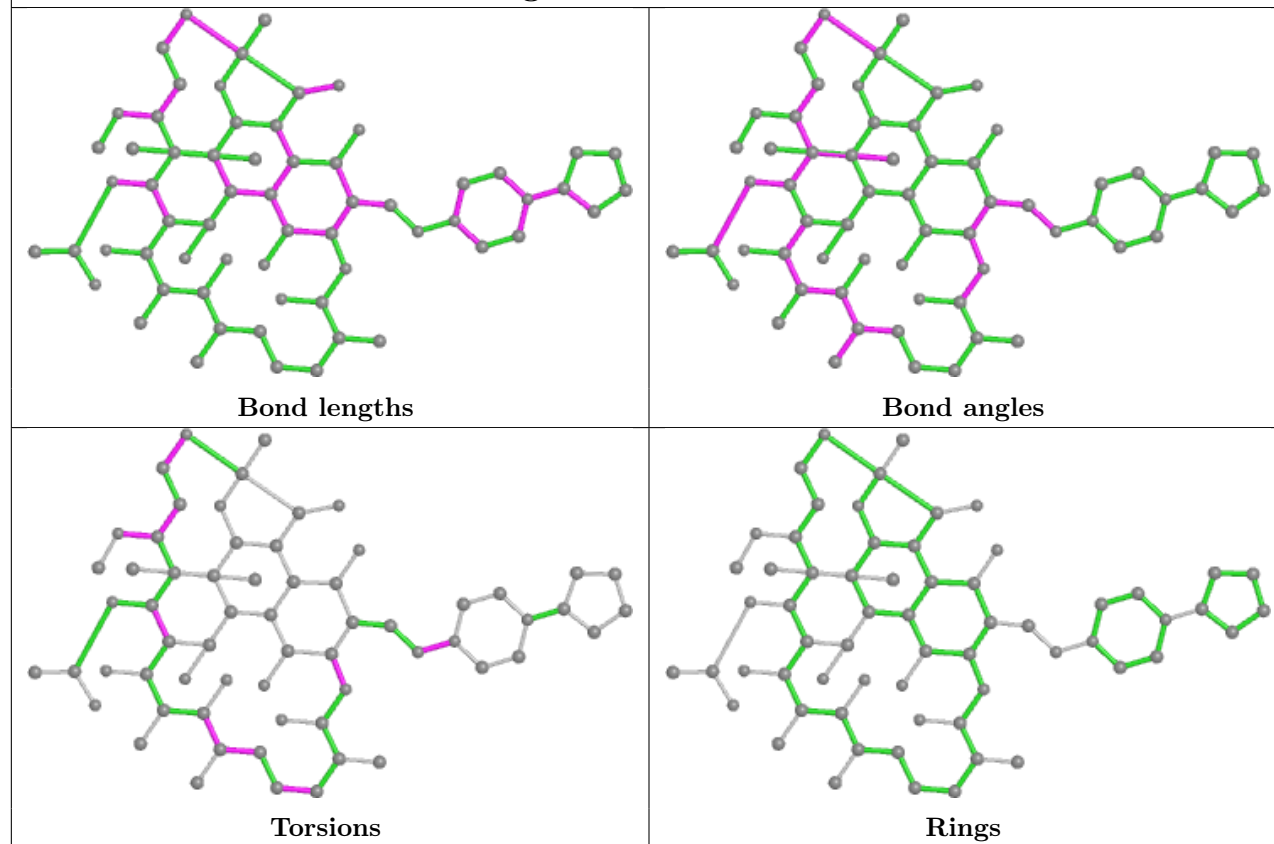
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	M	8002	RPT	7	0
7	C	8001	RPT	6	0

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

Ligand RPT M 8002



Ligand RPT C 8001



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	229/315 (72%)	-0.31	1 (0%) 92 93	27, 63, 91, 115	0
1	B	229/315 (72%)	-0.11	12 (5%) 27 29	48, 93, 115, 119	0
1	K	229/315 (72%)	-0.30	2 (0%) 84 86	34, 65, 94, 134	0
1	L	229/315 (72%)	-0.21	6 (2%) 56 59	52, 92, 110, 131	0
2	C	1119/1119 (100%)	-0.34	14 (1%) 77 79	21, 75, 106, 118	0
2	M	1119/1119 (100%)	-0.31	15 (1%) 77 79	25, 79, 109, 122	0
3	D	1392/1524 (91%)	-0.27	24 (1%) 70 72	24, 65, 112, 132	0
3	N	1392/1524 (91%)	-0.25	31 (2%) 62 65	25, 69, 117, 138	0
4	E	95/99 (95%)	-0.27	5 (5%) 26 28	42, 83, 108, 126	0
4	O	95/99 (95%)	-0.39	1 (1%) 80 82	46, 80, 107, 114	0
5	F	345/423 (81%)	-0.36	6 (1%) 70 72	49, 84, 110, 127	0
5	P	345/423 (81%)	-0.28	6 (1%) 70 72	63, 89, 114, 124	0
All	All	6818/7590 (89%)	-0.29	123 (1%) 68 71	21, 75, 112, 138	0

The worst 5 of 123 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	802	ALA	7.6
3	D	1240	THR	5.8
3	N	1249	ALA	5.5
2	C	180	GLY	5.3
3	D	1245	GLY	5.3

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	ZN	D	7058	1/1	0.87	0.07	106,106,106,106	0
6	MG	M	9256	1/1	0.89	0.17	56,56,56,56	0
6	MG	C	9362	1/1	0.90	0.15	55,55,55,55	0
6	MG	K	9470	1/1	0.91	0.13	55,55,55,55	0
6	MG	C	9168	1/1	0.91	0.10	45,45,45,45	0
6	MG	N	9192	1/1	0.91	0.12	62,62,62,62	0
6	MG	D	9161	1/1	0.91	0.09	57,57,57,57	0
6	MG	N	9221	1/1	0.92	0.13	44,44,44,44	0
6	MG	D	9330	1/1	0.92	0.14	39,39,39,39	0
6	MG	C	9350	1/1	0.93	0.07	60,60,60,60	0
6	MG	A	9078	1/1	0.93	0.13	66,66,66,66	0
6	MG	F	9390	1/1	0.93	0.07	46,46,46,46	0
6	MG	P	9226	1/1	0.93	0.08	43,43,43,43	0
6	MG	D	9001	1/1	0.93	0.10	36,36,36,36	0
6	MG	C	9149	1/1	0.94	0.16	48,48,48,48	0
6	MG	L	9182	1/1	0.94	0.05	47,47,47,47	0
6	MG	L	9414	1/1	0.94	0.13	51,51,51,51	0
6	MG	D	9102	1/1	0.94	0.13	44,44,44,44	0
6	MG	M	9263	1/1	0.94	0.10	56,56,56,56	0
6	MG	M	9411	1/1	0.94	0.09	47,47,47,47	0
6	MG	M	9447	1/1	0.94	0.07	64,64,64,64	0
6	MG	A	9357	1/1	0.94	0.11	54,54,54,54	0
6	MG	N	9194	1/1	0.94	0.12	51,51,51,51	0
6	MG	C	9049	1/1	0.94	0.10	46,46,46,46	0
6	MG	N	9313	1/1	0.94	0.10	43,43,43,43	0
6	MG	N	9427	1/1	0.94	0.14	58,58,58,58	0
6	MG	N	9449	1/1	0.94	0.09	51,51,51,51	0
6	MG	O	9420	1/1	0.94	0.10	51,51,51,51	0
6	MG	P	9202	1/1	0.94	0.10	49,49,49,49	0
6	MG	F	9109	1/1	0.94	0.11	60,60,60,60	0
6	MG	C	9067	1/1	0.94	0.17	57,57,57,57	0
6	MG	N	9217	1/1	0.95	0.15	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	C	9162	1/1	0.95	0.12	50,50,50,50	0
6	MG	N	9233	1/1	0.95	0.14	62,62,62,62	0
6	MG	N	9291	1/1	0.95	0.12	64,64,64,64	0
6	MG	M	9324	1/1	0.95	0.08	41,41,41,41	0
6	MG	N	9327	1/1	0.95	0.07	40,40,40,40	0
6	MG	D	9014	1/1	0.95	0.10	41,41,41,41	0
6	MG	D	9036	1/1	0.95	0.09	44,44,44,44	0
6	MG	M	9471	1/1	0.95	0.08	47,47,47,47	0
6	MG	D	9082	1/1	0.95	0.14	60,60,60,60	0
6	MG	F	9148	1/1	0.95	0.08	54,54,54,54	0
6	MG	P	9297	1/1	0.95	0.09	45,45,45,45	0
6	MG	N	9200	1/1	0.95	0.10	38,38,38,38	0
6	MG	M	9210	1/1	0.96	0.13	41,41,41,41	0
6	MG	M	9225	1/1	0.96	0.14	56,56,56,56	0
6	MG	M	9234	1/1	0.96	0.12	53,53,53,53	0
6	MG	B	9059	1/1	0.96	0.07	48,48,48,48	0
6	MG	M	9261	1/1	0.96	0.11	47,47,47,47	0
6	MG	B	9359	1/1	0.96	0.10	52,52,52,52	0
6	MG	M	9294	1/1	0.96	0.09	52,52,52,52	0
6	MG	D	9054	1/1	0.96	0.08	44,44,44,44	0
6	MG	M	9406	1/1	0.96	0.15	67,67,67,67	0
6	MG	D	9062	1/1	0.96	0.08	47,47,47,47	0
6	MG	C	9019	1/1	0.96	0.13	57,57,57,57	0
6	MG	D	9096	1/1	0.96	0.15	60,60,60,60	0
6	MG	C	9175	1/1	0.96	0.14	68,68,68,68	0
6	MG	C	9047	1/1	0.96	0.12	53,53,53,53	0
6	MG	C	9355	1/1	0.96	0.12	58,58,58,58	0
6	MG	D	9365	1/1	0.96	0.06	41,41,41,41	0
6	MG	D	9453	1/1	0.96	0.11	38,38,38,38	0
6	MG	E	9074	1/1	0.96	0.09	59,59,59,59	0
6	MG	A	9081	1/1	0.96	0.08	40,40,40,40	0
6	MG	N	9292	1/1	0.96	0.12	56,56,56,56	0
6	MG	C	9372	1/1	0.96	0.09	61,61,61,61	0
6	MG	N	9326	1/1	0.96	0.14	62,62,62,62	0
6	MG	F	9172	1/1	0.96	0.11	51,51,51,51	0
6	MG	N	9426	1/1	0.96	0.09	41,41,41,41	0
6	MG	F	9370	1/1	0.96	0.09	46,46,46,46	0
6	MG	C	9381	1/1	0.96	0.08	53,53,53,53	0
6	MG	O	9198	1/1	0.96	0.12	36,36,36,36	0
6	MG	C	9391	1/1	0.96	0.06	60,60,60,60	0
6	MG	A	9013	1/1	0.96	0.12	44,44,44,44	0
6	MG	P	9209	1/1	0.96	0.15	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	L	9218	1/1	0.96	0.09	33,33,33,33	0
6	MG	L	9278	1/1	0.96	0.11	44,44,44,44	0
7	RPT	C	8001	63/63	0.96	0.23	26,40,66,82	0
7	RPT	M	8002	63/63	0.96	0.22	33,45,55,57	0
6	MG	D	9009	1/1	0.96	0.09	43,43,43,43	0
6	MG	K	9188	1/1	0.97	0.12	40,40,40,40	0
6	MG	K	9251	1/1	0.97	0.11	43,43,43,43	0
6	MG	K	9257	1/1	0.97	0.10	58,58,58,58	0
6	MG	K	9410	1/1	0.97	0.15	36,36,36,36	0
6	MG	K	9433	1/1	0.97	0.07	50,50,50,50	0
6	MG	C	9122	1/1	0.97	0.10	56,56,56,56	0
6	MG	D	9017	1/1	0.97	0.10	42,42,42,42	0
6	MG	D	9030	1/1	0.97	0.09	48,48,48,48	0
6	MG	L	9245	1/1	0.97	0.09	62,62,62,62	0
6	MG	L	9252	1/1	0.97	0.09	45,45,45,45	0
6	MG	A	9125	1/1	0.97	0.12	36,36,36,36	0
6	MG	L	9289	1/1	0.97	0.14	62,62,62,62	0
6	MG	D	9041	1/1	0.97	0.13	47,47,47,47	0
6	MG	M	9196	1/1	0.97	0.09	42,42,42,42	0
6	MG	M	9201	1/1	0.97	0.10	45,45,45,45	0
6	MG	C	9160	1/1	0.97	0.09	44,44,44,44	0
6	MG	M	9219	1/1	0.97	0.09	47,47,47,47	0
6	MG	B	9103	1/1	0.97	0.12	43,43,43,43	0
6	MG	D	9073	1/1	0.97	0.12	34,34,34,34	0
6	MG	M	9237	1/1	0.97	0.15	52,52,52,52	0
6	MG	B	9104	1/1	0.97	0.10	45,45,45,45	0
6	MG	D	9087	1/1	0.97	0.07	43,43,43,43	0
6	MG	D	9095	1/1	0.97	0.15	30,30,30,30	0
6	MG	M	9273	1/1	0.97	0.12	44,44,44,44	0
6	MG	M	9275	1/1	0.97	0.12	55,55,55,55	0
6	MG	A	9153	1/1	0.97	0.15	66,66,66,66	0
6	MG	C	9178	1/1	0.97	0.09	39,39,39,39	0
6	MG	D	9127	1/1	0.97	0.14	48,48,48,48	0
6	MG	D	9158	1/1	0.97	0.12	60,60,60,60	0
6	MG	M	9412	1/1	0.97	0.14	43,43,43,43	0
6	MG	B	9458	1/1	0.97	0.08	44,44,44,44	0
6	MG	D	9165	1/1	0.97	0.07	32,32,32,32	0
6	MG	M	9475	1/1	0.97	0.05	62,62,62,62	0
6	MG	D	9166	1/1	0.97	0.09	40,40,40,40	0
6	MG	D	9167	1/1	0.97	0.12	49,49,49,49	0
6	MG	D	9174	1/1	0.97	0.12	47,47,47,47	0
6	MG	N	9211	1/1	0.97	0.10	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	D	9177	1/1	0.97	0.13	64,64,64,64	0
6	MG	A	9156	1/1	0.97	0.08	43,43,43,43	0
6	MG	N	9232	1/1	0.97	0.08	47,47,47,47	0
6	MG	D	9346	1/1	0.97	0.07	47,47,47,47	0
6	MG	N	9276	1/1	0.97	0.08	61,61,61,61	0
6	MG	D	9348	1/1	0.97	0.14	57,57,57,57	0
6	MG	C	9360	1/1	0.97	0.13	53,53,53,53	0
6	MG	D	9367	1/1	0.97	0.06	31,31,31,31	0
6	MG	D	9373	1/1	0.97	0.12	51,51,51,51	0
6	MG	D	9388	1/1	0.97	0.09	37,37,37,37	0
6	MG	N	9422	1/1	0.97	0.14	56,56,56,56	0
6	MG	N	9425	1/1	0.97	0.12	46,46,46,46	0
6	MG	C	9022	1/1	0.97	0.12	37,37,37,37	0
6	MG	A	9171	1/1	0.97	0.11	58,58,58,58	0
6	MG	F	9060	1/1	0.97	0.10	41,41,41,41	0
6	MG	N	9450	1/1	0.97	0.10	48,48,48,48	0
6	MG	N	9473	1/1	0.97	0.12	51,51,51,51	0
6	MG	F	9099	1/1	0.97	0.13	56,56,56,56	0
6	MG	A	9352	1/1	0.97	0.10	46,46,46,46	0
6	MG	P	9189	1/1	0.97	0.11	49,49,49,49	0
6	MG	F	9123	1/1	0.97	0.09	37,37,37,37	0
6	MG	A	9066	1/1	0.97	0.14	47,47,47,47	0
6	MG	P	9216	1/1	0.97	0.13	48,48,48,48	0
6	MG	C	9107	1/1	0.97	0.09	42,42,42,42	0
6	MG	D	9006	1/1	0.97	0.12	40,40,40,40	0
6	MG	P	9325	1/1	0.97	0.12	49,49,49,49	0
6	MG	F	9376	1/1	0.97	0.19	62,62,62,62	0
6	MG	F	9389	1/1	0.97	0.11	53,53,53,53	0
6	MG	C	9119	1/1	0.97	0.07	43,43,43,43	0
6	MG	F	9387	1/1	0.98	0.10	53,53,53,53	0
6	MG	C	9112	1/1	0.98	0.11	39,39,39,39	0
6	MG	D	9052	1/1	0.98	0.07	65,65,65,65	0
6	MG	B	9080	1/1	0.98	0.10	56,56,56,56	0
6	MG	K	9191	1/1	0.98	0.15	32,32,32,32	0
6	MG	K	9213	1/1	0.98	0.11	43,43,43,43	0
6	MG	B	9093	1/1	0.98	0.15	40,40,40,40	0
6	MG	D	9063	1/1	0.98	0.08	33,33,33,33	0
6	MG	K	9264	1/1	0.98	0.08	42,42,42,42	0
6	MG	K	9290	1/1	0.98	0.12	51,51,51,51	0
6	MG	K	9301	1/1	0.98	0.12	43,43,43,43	0
6	MG	K	9405	1/1	0.98	0.11	56,56,56,56	0
6	MG	D	9064	1/1	0.98	0.14	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	D	9069	1/1	0.98	0.12	48,48,48,48	0
6	MG	K	9438	1/1	0.98	0.10	52,52,52,52	0
6	MG	C	9128	1/1	0.98	0.12	52,52,52,52	0
6	MG	C	9138	1/1	0.98	0.08	43,43,43,43	0
6	MG	C	9142	1/1	0.98	0.15	48,48,48,48	0
6	MG	A	9012	1/1	0.98	0.10	47,47,47,47	0
6	MG	L	9246	1/1	0.98	0.12	52,52,52,52	0
6	MG	C	9154	1/1	0.98	0.07	43,43,43,43	0
6	MG	A	9068	1/1	0.98	0.12	39,39,39,39	0
6	MG	L	9283	1/1	0.98	0.12	59,59,59,59	0
6	MG	D	9108	1/1	0.98	0.15	51,51,51,51	0
6	MG	L	9309	1/1	0.98	0.13	49,49,49,49	0
6	MG	L	9314	1/1	0.98	0.07	56,56,56,56	0
6	MG	D	9113	1/1	0.98	0.11	34,34,34,34	0
6	MG	L	9421	1/1	0.98	0.12	53,53,53,53	0
6	MG	D	9118	1/1	0.98	0.11	44,44,44,44	0
6	MG	D	9121	1/1	0.98	0.09	35,35,35,35	0
6	MG	M	9205	1/1	0.98	0.11	38,38,38,38	0
6	MG	A	9010	1/1	0.98	0.12	30,30,30,30	0
6	MG	M	9212	1/1	0.98	0.08	32,32,32,32	0
6	MG	D	9132	1/1	0.98	0.10	43,43,43,43	0
6	MG	D	9135	1/1	0.98	0.14	50,50,50,50	0
6	MG	D	9137	1/1	0.98	0.08	47,47,47,47	0
6	MG	D	9152	1/1	0.98	0.12	67,67,67,67	0
6	MG	M	9239	1/1	0.98	0.07	34,34,34,34	0
6	MG	M	9241	1/1	0.98	0.11	36,36,36,36	0
6	MG	M	9247	1/1	0.98	0.07	51,51,51,51	0
6	MG	M	9250	1/1	0.98	0.07	38,38,38,38	0
6	MG	B	9457	1/1	0.98	0.07	43,43,43,43	0
6	MG	A	9016	1/1	0.98	0.14	36,36,36,36	0
6	MG	D	9163	1/1	0.98	0.14	52,52,52,52	0
6	MG	B	9478	1/1	0.98	0.12	61,61,61,61	0
6	MG	C	9340	1/1	0.98	0.09	60,60,60,60	0
6	MG	M	9284	1/1	0.98	0.14	54,54,54,54	0
6	MG	C	9004	1/1	0.98	0.10	39,39,39,39	0
6	MG	M	9305	1/1	0.98	0.09	46,46,46,46	0
6	MG	M	9310	1/1	0.98	0.07	46,46,46,46	0
6	MG	D	9173	1/1	0.98	0.07	48,48,48,48	0
6	MG	C	9015	1/1	0.98	0.09	38,38,38,38	0
6	MG	M	9407	1/1	0.98	0.14	35,35,35,35	0
6	MG	A	9111	1/1	0.98	0.09	35,35,35,35	0
6	MG	C	9021	1/1	0.98	0.09	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	M	9424	1/1	0.98	0.13	34,34,34,34	0
6	MG	M	9434	1/1	0.98	0.11	34,34,34,34	0
6	MG	M	9440	1/1	0.98	0.10	50,50,50,50	0
6	MG	M	9441	1/1	0.98	0.07	45,45,45,45	0
6	MG	D	9338	1/1	0.98	0.10	42,42,42,42	0
6	MG	M	9452	1/1	0.98	0.13	42,42,42,42	0
6	MG	D	9344	1/1	0.98	0.11	55,55,55,55	0
6	MG	A	9384	1/1	0.98	0.14	39,39,39,39	0
6	MG	N	9181	1/1	0.98	0.16	47,47,47,47	0
6	MG	N	9184	1/1	0.98	0.10	29,29,29,29	0
6	MG	N	9185	1/1	0.98	0.14	56,56,56,56	0
6	MG	C	9025	1/1	0.98	0.14	39,39,39,39	0
6	MG	D	9349	1/1	0.98	0.13	33,33,33,33	0
6	MG	C	9037	1/1	0.98	0.16	51,51,51,51	0
6	MG	N	9204	1/1	0.98	0.19	44,44,44,44	0
6	MG	C	9394	1/1	0.98	0.09	33,33,33,33	0
6	MG	N	9214	1/1	0.98	0.10	33,33,33,33	0
6	MG	N	9215	1/1	0.98	0.12	32,32,32,32	0
6	MG	D	9369	1/1	0.98	0.10	49,49,49,49	0
6	MG	C	9461	1/1	0.98	0.07	50,50,50,50	0
6	MG	N	9231	1/1	0.98	0.11	52,52,52,52	0
6	MG	D	9374	1/1	0.98	0.10	41,41,41,41	0
6	MG	D	9379	1/1	0.98	0.11	47,47,47,47	0
6	MG	N	9236	1/1	0.98	0.10	39,39,39,39	0
6	MG	N	9243	1/1	0.98	0.09	35,35,35,35	0
6	MG	N	9253	1/1	0.98	0.12	42,42,42,42	0
6	MG	N	9259	1/1	0.98	0.15	34,34,34,34	0
6	MG	N	9265	1/1	0.98	0.14	61,61,61,61	0
6	MG	N	9267	1/1	0.98	0.12	42,42,42,42	0
6	MG	N	9270	1/1	0.98	0.05	39,39,39,39	0
6	MG	C	9464	1/1	0.98	0.06	48,48,48,48	0
6	MG	N	9286	1/1	0.98	0.14	31,31,31,31	0
6	MG	N	9287	1/1	0.98	0.09	53,53,53,53	0
6	MG	D	9392	1/1	0.98	0.12	52,52,52,52	0
6	MG	D	9397	1/1	0.98	0.12	51,51,51,51	0
6	MG	N	9293	1/1	0.98	0.15	42,42,42,42	0
6	MG	N	9298	1/1	0.98	0.05	55,55,55,55	0
6	MG	A	9460	1/1	0.98	0.07	55,55,55,55	0
6	MG	N	9322	1/1	0.98	0.10	54,54,54,54	0
6	MG	D	9459	1/1	0.98	0.05	54,54,54,54	0
6	MG	E	9007	1/1	0.98	0.11	40,40,40,40	0
6	MG	N	9404	1/1	0.98	0.12	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	N	9415	1/1	0.98	0.07	42,42,42,42	0
6	MG	N	9419	1/1	0.98	0.11	51,51,51,51	0
6	MG	E	9045	1/1	0.98	0.12	61,61,61,61	0
6	MG	N	9423	1/1	0.98	0.17	58,58,58,58	0
6	MG	A	9477	1/1	0.98	0.18	52,52,52,52	0
6	MG	E	9479	1/1	0.98	0.10	62,62,62,62	0
6	MG	F	9008	1/1	0.98	0.09	40,40,40,40	0
6	MG	N	9428	1/1	0.98	0.10	42,42,42,42	0
6	MG	N	9429	1/1	0.98	0.10	45,45,45,45	0
6	MG	N	9435	1/1	0.98	0.23	53,53,53,53	0
6	MG	N	9445	1/1	0.98	0.10	51,51,51,51	0
6	MG	C	9065	1/1	0.98	0.10	37,37,37,37	0
6	MG	F	9098	1/1	0.98	0.11	54,54,54,54	0
6	MG	N	9465	1/1	0.98	0.08	49,49,49,49	0
6	MG	B	9056	1/1	0.98	0.13	43,43,43,43	0
6	MG	O	9197	1/1	0.98	0.04	57,57,57,57	0
6	MG	F	9105	1/1	0.98	0.14	36,36,36,36	0
6	MG	O	9296	1/1	0.98	0.11	42,42,42,42	0
6	MG	C	9090	1/1	0.98	0.10	47,47,47,47	0
6	MG	O	9439	1/1	0.98	0.16	56,56,56,56	0
6	MG	D	9018	1/1	0.98	0.11	39,39,39,39	0
6	MG	D	9024	1/1	0.98	0.14	36,36,36,36	0
6	MG	F	9159	1/1	0.98	0.15	57,57,57,57	0
6	MG	D	9028	1/1	0.98	0.13	34,34,34,34	0
6	MG	F	9356	1/1	0.98	0.14	37,37,37,37	0
6	MG	P	9228	1/1	0.98	0.09	43,43,43,43	0
6	MG	P	9235	1/1	0.98	0.16	40,40,40,40	0
6	MG	P	9280	1/1	0.98	0.10	51,51,51,51	0
6	MG	P	9282	1/1	0.98	0.09	56,56,56,56	0
6	MG	P	9285	1/1	0.98	0.09	56,56,56,56	0
6	MG	F	9363	1/1	0.98	0.12	53,53,53,53	0
6	MG	C	9092	1/1	0.98	0.06	44,44,44,44	0
6	MG	F	9375	1/1	0.98	0.13	36,36,36,36	0
6	MG	A	9027	1/1	0.98	0.08	37,37,37,37	0
6	MG	F	9383	1/1	0.98	0.11	48,48,48,48	0
6	MG	B	9131	1/1	0.99	0.08	33,33,33,33	0
6	MG	L	9183	1/1	0.99	0.13	37,37,37,37	0
6	MG	B	9136	1/1	0.99	0.10	47,47,47,47	0
6	MG	B	9358	1/1	0.99	0.07	39,39,39,39	0
6	MG	C	9143	1/1	0.99	0.10	35,35,35,35	0
6	MG	D	9120	1/1	0.99	0.08	31,31,31,31	0
6	MG	C	9145	1/1	0.99	0.13	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	A	9354	1/1	0.99	0.09	37,37,37,37	0
6	MG	D	9129	1/1	0.99	0.14	42,42,42,42	0
6	MG	L	9306	1/1	0.99	0.11	57,57,57,57	0
6	MG	L	9307	1/1	0.99	0.10	35,35,35,35	0
6	MG	D	9130	1/1	0.99	0.09	51,51,51,51	0
6	MG	B	9378	1/1	0.99	0.13	47,47,47,47	0
6	MG	D	9133	1/1	0.99	0.13	42,42,42,42	0
6	MG	D	9134	1/1	0.99	0.13	47,47,47,47	0
6	MG	L	9437	1/1	0.99	0.06	40,40,40,40	0
6	MG	L	9466	1/1	0.99	0.10	49,49,49,49	0
6	MG	M	9190	1/1	0.99	0.16	29,29,29,29	0
6	MG	M	9195	1/1	0.99	0.08	34,34,34,34	0
6	MG	A	9075	1/1	0.99	0.10	36,36,36,36	0
6	MG	A	9368	1/1	0.99	0.13	43,43,43,43	0
6	MG	M	9203	1/1	0.99	0.11	32,32,32,32	0
6	MG	D	9140	1/1	0.99	0.13	40,40,40,40	0
6	MG	M	9208	1/1	0.99	0.10	39,39,39,39	0
6	MG	D	9141	1/1	0.99	0.06	50,50,50,50	0
6	MG	D	9144	1/1	0.99	0.12	39,39,39,39	0
6	MG	D	9146	1/1	0.99	0.10	31,31,31,31	0
6	MG	M	9220	1/1	0.99	0.11	51,51,51,51	0
6	MG	M	9222	1/1	0.99	0.10	35,35,35,35	0
6	MG	M	9224	1/1	0.99	0.13	40,40,40,40	0
6	MG	D	9147	1/1	0.99	0.10	41,41,41,41	0
6	MG	M	9227	1/1	0.99	0.12	35,35,35,35	0
6	MG	D	9150	1/1	0.99	0.14	31,31,31,31	0
6	MG	D	9151	1/1	0.99	0.15	57,57,57,57	0
6	MG	C	9164	1/1	0.99	0.10	49,49,49,49	0
6	MG	A	9380	1/1	0.99	0.11	44,44,44,44	0
6	MG	M	9242	1/1	0.99	0.11	35,35,35,35	0
6	MG	C	9169	1/1	0.99	0.13	42,42,42,42	0
6	MG	C	9170	1/1	0.99	0.06	41,41,41,41	0
6	MG	C	9003	1/1	0.99	0.13	38,38,38,38	0
6	MG	M	9260	1/1	0.99	0.12	36,36,36,36	0
6	MG	C	9176	1/1	0.99	0.09	28,28,28,28	0
6	MG	A	9124	1/1	0.99	0.12	39,39,39,39	0
6	MG	M	9268	1/1	0.99	0.09	32,32,32,32	0
6	MG	M	9272	1/1	0.99	0.17	45,45,45,45	0
6	MG	A	9395	1/1	0.99	0.14	50,50,50,50	0
6	MG	A	9002	1/1	0.99	0.17	31,31,31,31	0
6	MG	M	9281	1/1	0.99	0.11	49,49,49,49	0
6	MG	C	9353	1/1	0.99	0.10	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	D	9328	1/1	0.99	0.12	30,30,30,30	0
6	MG	M	9295	1/1	0.99	0.08	42,42,42,42	0
6	MG	M	9299	1/1	0.99	0.09	43,43,43,43	0
6	MG	M	9300	1/1	0.99	0.09	39,39,39,39	0
6	MG	D	9329	1/1	0.99	0.12	33,33,33,33	0
6	MG	C	9020	1/1	0.99	0.10	34,34,34,34	0
6	MG	M	9312	1/1	0.99	0.12	37,37,37,37	0
6	MG	D	9331	1/1	0.99	0.18	43,43,43,43	0
6	MG	M	9400	1/1	0.99	0.12	40,40,40,40	0
6	MG	D	9333	1/1	0.99	0.07	33,33,33,33	0
6	MG	D	9334	1/1	0.99	0.10	54,54,54,54	0
6	MG	M	9409	1/1	0.99	0.10	36,36,36,36	0
6	MG	D	9335	1/1	0.99	0.06	52,52,52,52	0
6	MG	D	9336	1/1	0.99	0.10	53,53,53,53	0
6	MG	M	9416	1/1	0.99	0.11	45,45,45,45	0
6	MG	D	9337	1/1	0.99	0.15	53,53,53,53	0
6	MG	A	9043	1/1	0.99	0.17	37,37,37,37	0
6	MG	D	9339	1/1	0.99	0.14	37,37,37,37	0
6	MG	D	9341	1/1	0.99	0.10	41,41,41,41	0
6	MG	M	9442	1/1	0.99	0.07	59,59,59,59	0
6	MG	D	9343	1/1	0.99	0.10	59,59,59,59	0
6	MG	B	9032	1/1	0.99	0.06	34,34,34,34	0
6	MG	C	9366	1/1	0.99	0.14	41,41,41,41	0
6	MG	M	9474	1/1	0.99	0.14	49,49,49,49	0
6	MG	D	9347	1/1	0.99	0.09	49,49,49,49	0
6	MG	M	9486	1/1	0.99	0.07	48,48,48,48	0
6	MG	N	9179	1/1	0.99	0.12	33,33,33,33	0
6	MG	C	9371	1/1	0.99	0.15	54,54,54,54	0
6	MG	B	9033	1/1	0.99	0.14	33,33,33,33	0
6	MG	D	9351	1/1	0.99	0.06	43,43,43,43	0
6	MG	N	9186	1/1	0.99	0.12	49,49,49,49	0
6	MG	N	9187	1/1	0.99	0.18	33,33,33,33	0
6	MG	D	9364	1/1	0.99	0.12	47,47,47,47	0
6	MG	C	9377	1/1	0.99	0.09	44,44,44,44	0
6	MG	N	9199	1/1	0.99	0.11	35,35,35,35	0
6	MG	C	9026	1/1	0.99	0.13	42,42,42,42	0
6	MG	C	9031	1/1	0.99	0.10	40,40,40,40	0
6	MG	N	9206	1/1	0.99	0.16	31,31,31,31	0
6	MG	N	9207	1/1	0.99	0.13	41,41,41,41	0
6	MG	B	9040	1/1	0.99	0.16	36,36,36,36	0
6	MG	C	9454	1/1	0.99	0.09	55,55,55,55	0
6	MG	C	9455	1/1	0.99	0.11	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	D	9385	1/1	0.99	0.13	35,35,35,35	0
6	MG	D	9386	1/1	0.99	0.11	40,40,40,40	0
6	MG	N	9229	1/1	0.99	0.07	41,41,41,41	0
6	MG	C	9042	1/1	0.99	0.07	47,47,47,47	0
6	MG	C	9462	1/1	0.99	0.08	43,43,43,43	0
6	MG	D	9396	1/1	0.99	0.10	62,62,62,62	0
6	MG	C	9463	1/1	0.99	0.09	55,55,55,55	0
6	MG	N	9238	1/1	0.99	0.11	43,43,43,43	0
6	MG	N	9240	1/1	0.99	0.14	46,46,46,46	0
6	MG	C	9044	1/1	0.99	0.14	34,34,34,34	0
6	MG	D	9456	1/1	0.99	0.10	55,55,55,55	0
6	MG	C	9046	1/1	0.99	0.11	38,38,38,38	0
6	MG	N	9262	1/1	0.99	0.09	51,51,51,51	0
6	MG	D	9480	1/1	0.99	0.10	55,55,55,55	0
6	MG	D	9005	1/1	0.99	0.11	40,40,40,40	0
6	MG	N	9269	1/1	0.99	0.07	42,42,42,42	0
6	MG	A	9088	1/1	0.99	0.07	36,36,36,36	0
6	MG	N	9274	1/1	0.99	0.18	40,40,40,40	0
6	MG	A	9097	1/1	0.99	0.16	34,34,34,34	0
6	MG	N	9279	1/1	0.99	0.11	54,54,54,54	0
6	MG	E	9155	1/1	0.99	0.14	44,44,44,44	0
6	MG	D	9011	1/1	0.99	0.12	33,33,33,33	0
6	MG	N	9288	1/1	0.99	0.09	49,49,49,49	0
6	MG	C	9050	1/1	0.99	0.15	37,37,37,37	0
6	MG	F	9035	1/1	0.99	0.10	40,40,40,40	0
6	MG	F	9048	1/1	0.99	0.10	41,41,41,41	0
6	MG	C	9051	1/1	0.99	0.12	37,37,37,37	0
6	MG	N	9302	1/1	0.99	0.10	31,31,31,31	0
6	MG	N	9303	1/1	0.99	0.08	54,54,54,54	0
6	MG	N	9304	1/1	0.99	0.11	47,47,47,47	0
6	MG	N	9308	1/1	0.99	0.15	55,55,55,55	0
6	MG	C	9053	1/1	0.99	0.12	30,30,30,30	0
6	MG	N	9316	1/1	0.99	0.08	37,37,37,37	0
6	MG	N	9317	1/1	0.99	0.09	43,43,43,43	0
6	MG	N	9318	1/1	0.99	0.11	34,34,34,34	0
6	MG	D	9023	1/1	0.99	0.14	34,34,34,34	0
6	MG	N	9323	1/1	0.99	0.09	38,38,38,38	0
6	MG	C	9055	1/1	0.99	0.11	38,38,38,38	0
6	MG	C	9061	1/1	0.99	0.07	34,34,34,34	0
6	MG	N	9398	1/1	0.99	0.15	48,48,48,48	0
6	MG	N	9402	1/1	0.99	0.07	45,45,45,45	0
6	MG	N	9403	1/1	0.99	0.12	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	D	9029	1/1	0.99	0.12	33,33,33,33	0
6	MG	F	9139	1/1	0.99	0.10	38,38,38,38	0
6	MG	N	9417	1/1	0.99	0.09	39,39,39,39	0
6	MG	N	9418	1/1	0.99	0.10	49,49,49,49	0
6	MG	A	9332	1/1	0.99	0.06	35,35,35,35	0
6	MG	F	9157	1/1	0.99	0.11	42,42,42,42	0
6	MG	D	9034	1/1	0.99	0.08	41,41,41,41	0
6	MG	B	9083	1/1	0.99	0.13	40,40,40,40	0
6	MG	D	9038	1/1	0.99	0.14	39,39,39,39	0
6	MG	D	9039	1/1	0.99	0.12	44,44,44,44	0
6	MG	C	9071	1/1	0.99	0.11	42,42,42,42	0
6	MG	C	9079	1/1	0.99	0.11	38,38,38,38	0
6	MG	N	9430	1/1	0.99	0.08	57,57,57,57	0
6	MG	N	9431	1/1	0.99	0.12	39,39,39,39	0
6	MG	C	9086	1/1	0.99	0.14	39,39,39,39	0
6	MG	N	9443	1/1	0.99	0.13	54,54,54,54	0
6	MG	N	9444	1/1	0.99	0.15	49,49,49,49	0
6	MG	F	9382	1/1	0.99	0.09	40,40,40,40	0
6	MG	N	9448	1/1	0.99	0.09	51,51,51,51	0
6	MG	D	9058	1/1	0.99	0.08	38,38,38,38	0
6	MG	A	9342	1/1	0.99	0.12	39,39,39,39	0
6	MG	N	9451	1/1	0.99	0.06	41,41,41,41	0
6	MG	B	9094	1/1	0.99	0.15	38,38,38,38	0
6	MG	N	9467	1/1	0.99	0.12	35,35,35,35	0
6	MG	N	9468	1/1	0.99	0.10	55,55,55,55	0
6	MG	N	9472	1/1	0.99	0.15	56,56,56,56	0
6	MG	A	9345	1/1	0.99	0.12	41,41,41,41	0
6	MG	N	9476	1/1	0.99	0.09	54,54,54,54	0
6	MG	N	9484	1/1	0.99	0.07	37,37,37,37	0
6	MG	F	9393	1/1	0.99	0.12	38,38,38,38	0
6	MG	F	9481	1/1	0.99	0.08	57,57,57,57	0
6	MG	O	9254	1/1	0.99	0.08	39,39,39,39	0
6	MG	A	9106	1/1	0.99	0.12	38,38,38,38	0
6	MG	D	9070	1/1	0.99	0.07	33,33,33,33	0
6	MG	D	9072	1/1	0.99	0.14	32,32,32,32	0
6	MG	O	9483	1/1	0.99	0.09	63,63,63,63	0
6	MG	K	9223	1/1	0.99	0.09	32,32,32,32	0
6	MG	K	9244	1/1	0.99	0.07	44,44,44,44	0
6	MG	C	9114	1/1	0.99	0.09	30,30,30,30	0
6	MG	D	9077	1/1	0.99	0.11	35,35,35,35	0
6	MG	C	9115	1/1	0.99	0.11	36,36,36,36	0
6	MG	D	9084	1/1	0.99	0.11	37,37,37,37	0

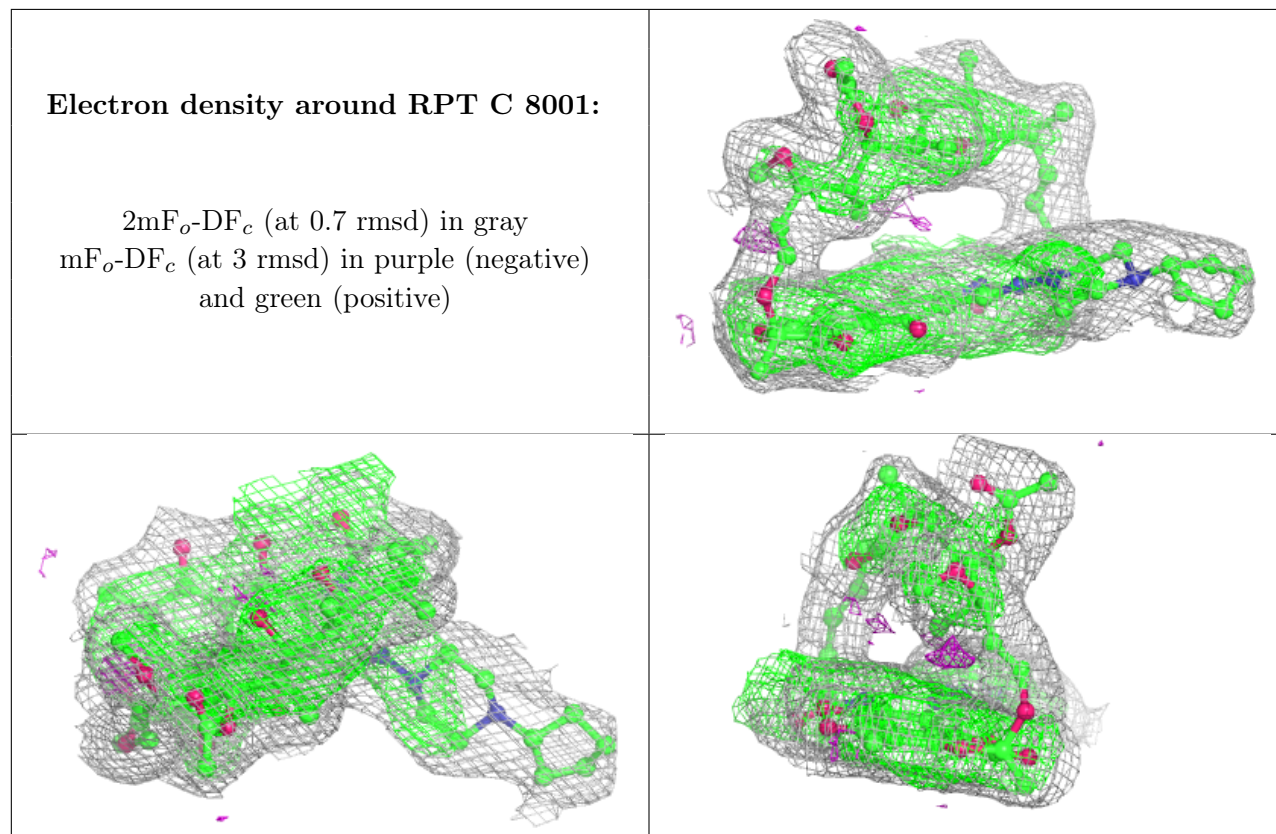
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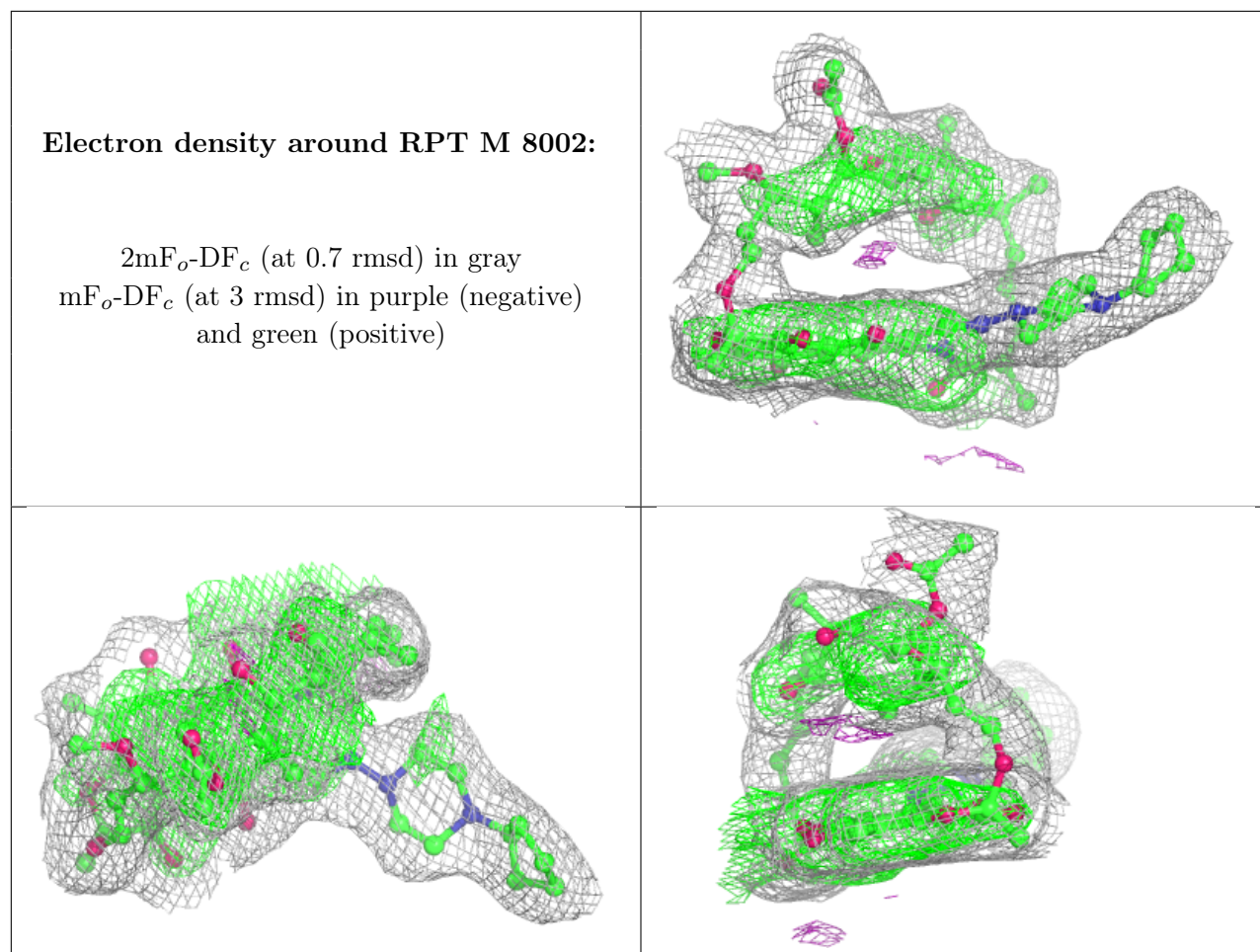
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	D	9085	1/1	0.99	0.18	49,49,49,49	0
6	MG	P	9255	1/1	0.99	0.12	34,34,34,34	0
6	MG	P	9277	1/1	0.99	0.09	41,41,41,41	0
6	MG	B	9110	1/1	0.99	0.12	49,49,49,49	0
6	MG	D	9089	1/1	0.99	0.09	36,36,36,36	0
6	MG	K	9413	1/1	0.99	0.10	54,54,54,54	0
6	MG	K	9432	1/1	0.99	0.13	49,49,49,49	0
6	MG	P	9315	1/1	0.99	0.08	35,35,35,35	0
6	MG	B	9116	1/1	0.99	0.09	38,38,38,38	0
6	MG	P	9399	1/1	0.99	0.11	34,34,34,34	0
6	MG	P	9436	1/1	0.99	0.11	49,49,49,49	0
6	MG	P	9446	1/1	0.99	0.13	34,34,34,34	0
6	MG	C	9126	1/1	0.99	0.10	46,46,46,46	0
6	MG	K	9469	1/1	0.99	0.12	50,50,50,50	0
6	MG	D	9100	1/1	0.99	0.08	43,43,43,43	0
8	ZN	D	7112	1/1	0.99	0.10	80,80,80,80	0
8	ZN	N	7059	1/1	0.99	0.12	93,93,93,93	0
8	ZN	N	7113	1/1	0.99	0.13	84,84,84,84	0
6	MG	K	9180	1/1	1.00	0.11	42,42,42,42	0
6	MG	N	9408	1/1	1.00	0.14	45,45,45,45	0
6	MG	M	9248	1/1	1.00	0.08	48,48,48,48	0
6	MG	N	9249	1/1	1.00	0.10	45,45,45,45	0
6	MG	M	9401	1/1	1.00	0.10	37,37,37,37	0
6	MG	P	9258	1/1	1.00	0.14	51,51,51,51	0
6	MG	F	9101	1/1	1.00	0.12	44,44,44,44	0
6	MG	C	9076	1/1	1.00	0.12	33,33,33,33	0
6	MG	M	9485	1/1	1.00	0.07	54,54,54,54	0
6	MG	N	9311	1/1	1.00	0.10	39,39,39,39	0
6	MG	M	9230	1/1	1.00	0.11	50,50,50,50	0
6	MG	D	9091	1/1	1.00	0.13	27,27,27,27	0
6	MG	F	9057	1/1	1.00	0.09	30,30,30,30	0
6	MG	N	9271	1/1	1.00	0.07	43,43,43,43	0
6	MG	O	9266	1/1	1.00	0.08	47,47,47,47	0
6	MG	C	9361	1/1	1.00	0.10	41,41,41,41	0
6	MG	P	9482	1/1	1.00	0.11	48,48,48,48	0
6	MG	C	9487	1/1	1.00	0.11	32,32,32,32	0
6	MG	D	9117	1/1	1.00	0.13	48,48,48,48	0
6	MG	M	9319	1/1	1.00	0.12	41,41,41,41	0
6	MG	M	9320	1/1	1.00	0.11	34,34,34,34	0
6	MG	N	9193	1/1	1.00	0.15	34,34,34,34	0
6	MG	M	9321	1/1	1.00	0.12	41,41,41,41	0

The following is a graphical depiction of the model fit to experimental electron density of all

instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers [i](#)

There are no such residues in this entry.