



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 06:43 PM UTC

PDB ID : 2A69 / pdb_00002a69
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

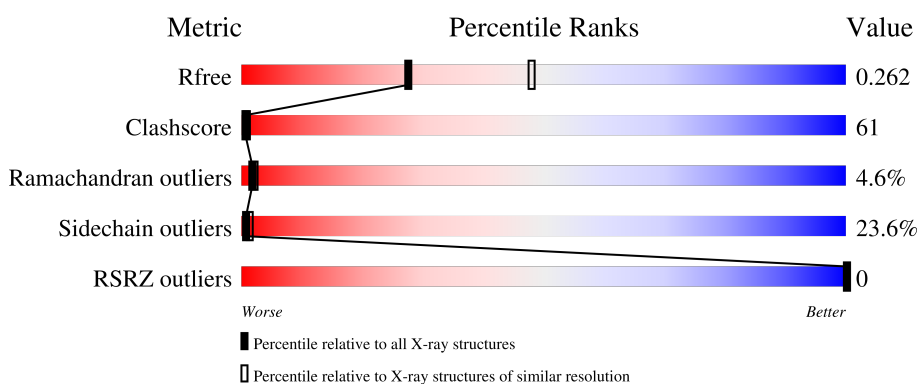
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

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.



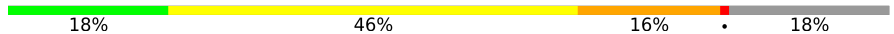
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	
1	B	315	
1	K	315	
1	L	315	
2	C	1119	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	M	1119	 23% 56% 18% .
3	D	1524	 21% 51% 17% . 9%
3	N	1524	 23% 49% 18% . 9%
4	E	99	 27% 45% 23% .
4	O	99	 24% 49% 19% . .
5	F	423	 18% 46% 16% . 18%
5	P	423	 20% 46% 14% . 18%

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			

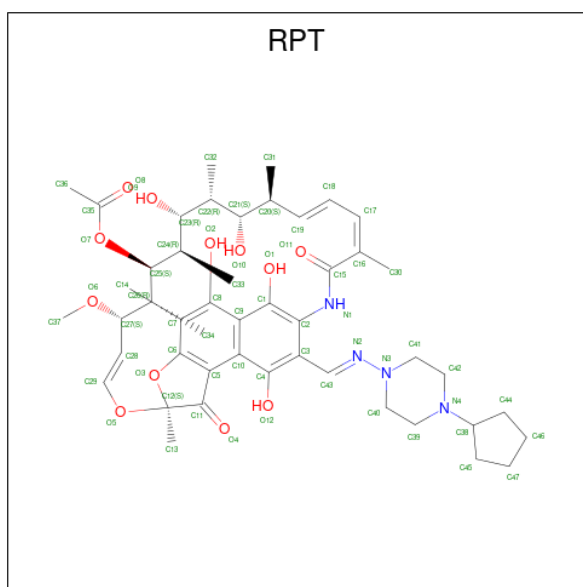
- Molecule 5 is a protein called RNA polymerase sigma factor rpoD.

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

- Molecule 6 is MAGNESIUM ION (CCD ID: 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 (CCD ID: 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 (CCD ID: 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.

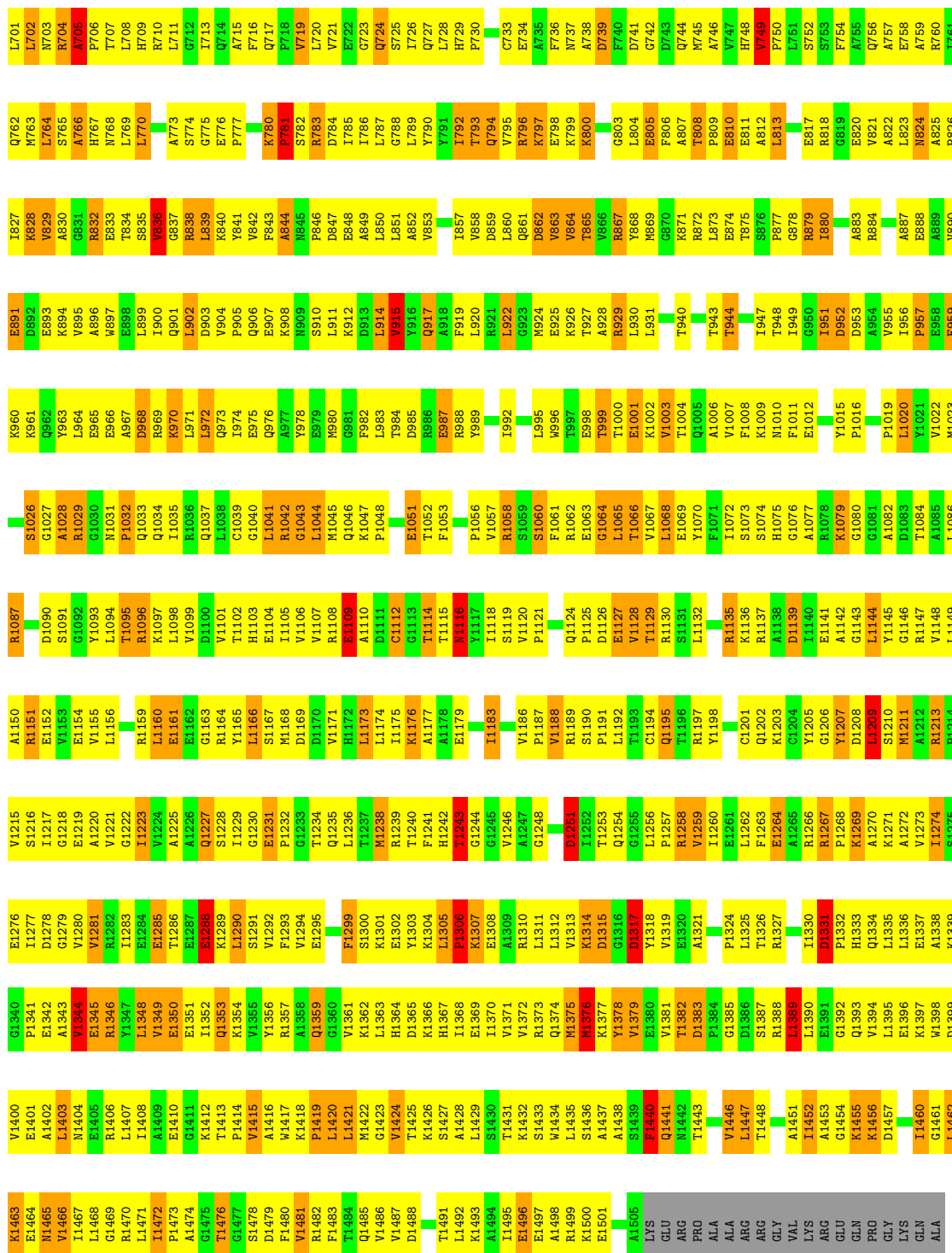
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	239	Total	O	0	0
			239	239		
9	B	258	Total	O	0	0
			258	258		
9	C	979	Total	O	0	0
			979	979		
9	D	1252	Total	O	0	0
			1252	1252		
9	E	117	Total	O	0	0
			117	117		

Continued on next page...

Continued from previous page...

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

H1006	H1007	R1008	S1009	T1010	G1011	P1012	Y1013	S1014	P1015	T1016	K1017	D1018	Q1019	P1020	E1021	G1022	Q1026	F1027	G1029	Y1030	Q1031	G1033	E1034	M1035	E1036	Y1037	W1038	A1039	A1042	Y1043	G1044	A1045	A1046	H1047	T1048	L1049	Q1050	E1051	M1052	L1053	T1054	K1055	M1056	S1057	D1058	D1059	I1060	E1061	G1062	R1063	H1064	M1000	V1001	A1065	A1066	Y1067	E1068	A1069																																																																																																																																																																																																																																																																																																																																																																																																								
R845	E948	K949	L950	G951	L952	V953	L954	P955	K956	K957	L958	Q959	E960	E961	G962	L963	K964	E965	F967	L968	Q969	G970	K971	V972	F906	D907	Y975	A908	K910	R845	E911	F912	G913	E914	P982	L983	E984	G985	P986	L987	V988	G989	T990	Q991	M992	F993	I994	M995	K996	F934	H998	H999	D937	M1000	V1001	E1002	K1003	V943	L944																																																																																																																																																																																																																																																																																																																																																																																																							
P811	G812	W813	K816	P817	G818	W819	R820	L886	L887	H889	L890	G891	L892	L893	F861	K862	F896	L897	G898	Q899	R900	Y901	L902	S903	F904	I905	D907	W975	A908	K910	R845	E911	F912	G913	E914	P982	L983	E984	G985	P986	L987	V988	G989	T990	Q991	M992	F993	I994	M995	K996	F934	H998	H999	D937	M1000	V1001	E1002	K1003	V943	L944																																																																																																																																																																																																																																																																																																																																																																																																						
A747	E748	W749	K750	P751	G752	W753	L754	L755	V756	G757	R758	L759	W760	W761	K762	P767	W768	F769	E770	E771	R772	L773	L774	R775	S776	R777	W778	G779	E780	K781	A782	W783	D784	W785	K786	D787	L788	S789	L790	W791	V792	W793	F794	G795	E796	G797	G798	L799	W800	W801	R802	F803	W804	R805	W806	R808	L809	W810																																																																																																																																																																																																																																																																																																																																																																																																								
G686	A687	W688	L689	P690	S691	E692	E693	L694	L695	G696	R697	D698	F699	Y700	P701	W702	W703	H704	I705	E706	R707	Y708	E709	L710	E711	A712	R713	D714	W715	K716	L717	E720	W721	I722	W723	R724	D725	I726	P727	W728	H729	E730	E731	A732	A733	L734	R735	W736	L737	D738	W739	E740	G741	R805	W806	R808	L809	W810																																																																																																																																																																																																																																																																																																																																																																																																								
R626	A627	F628	W629	R630	S631	M632	Q633	G634	T635	L636	L637	D638	Q639	R640	P641	R642	W643	W644	W645	G646	R647	R648	V649	R650	K651	G652	D653	L654	W655	L656	W657	P658	L659	A660	S661	E662	M663	G664	F665	W666	A667	L668	G669	Q670	N671	V672	L673	W674	L675	L676	M677	F678	F679	E680	D681	D682	W683	W684	E685																																																																																																																																																																																																																																																																																																																																																																																																							
S562	M563	M564	Q565	T566	E567	A568	W569	P570	L571	A572	L573	E511	M512	V513	W514	L555	A556	W557	R558	L583	E584	E585	V586	W587	W588	S589	D590	L591	S592	W593	L594	L595	A596	E597	E598	E599	D600	G601	E602	W603	A604	K605	W606	D607	G608	N609	L610	L611	L612	E613	R614	W615	E616	F617	D618	L619	L620	W621	E622	M623	F684	W685	E686																																																																																																																																																																																																																																																																																																																																																																																																			
B376	P377	L378	E379	A380	A381	L382	R383	D384	D385	D386	D387	R388	G389	Q390	L391	S392	L393	F394	K395	D396	E397	T398	L399	M340	T341	D342	Q343	F344	R345	V346	C347	R348	A349	R350	L351	A352	R353	G354	V355	R356	E357	R358	K359	L360	M361	E362	S363	E364	L365	D366	W367	H368	A369	L418	T419	R420	E421	R422	L423	P415	L414	C414	P415	L418	D481	E482	V483	W484	Y485	A423	H431	R432	T433	F434	H435	Y436	L437	A438	W439	L440	A441	L442	L443	S444	F445	L446	L447	L448	L449	G450	L451	R452	L453	S454	L455	A456	A457	Y458	A459	D460	V461	D462	E463	F464	W465	W466	L467	L468	L469	L470	L471	R472	L473	L474	G475	L476	W477	L478	Y479	T480	D481	E482	V483	W484	Y485	M486	L487	A488	D489	E490	D491	L492	L493	H494	Y495	L496	A497	L498	W499	L500	T501	P502	Q503	E504	M505	L506	E507	L508	F509	L510	E511	L512	L513	L514	L515	L516	L517	L518	L519	L520	L521	L522	L523	L524	L525	L526	L527	L528	L529	L530	L531	L532	L533	L534	L535	L536	L537	L538	L539	L540	L541	L542	L543	L544	L545	L546	L547	L548	L549	L550	L551	L552	L553	L554	L555	L556	L557	L558	L559	L560	L561	L562	L563	L564	L565	L566	L567	L568	L569	L570	L571	L572	L573	L574	L575	L576	L577	L578	L579	L580	L581	L582	L583	L584	L585	L586	L587	L588	L589	L590	L591	L592	L593	L594	L595	L596	L597	L598	L599	L600	L601	L602	L603	L604	L605	L606	L607	L608	L609	L610	L611	L612	L613	L614	L615	L616	L617	L618	L619	L620	L621	L622	L623	L624	L625	L626	L627	L628	L629	L630	L631	L632	L633	L634	L635	L636	L637	L638	L639	L640	L641	L642	L643	L644	L645	L646	L647	L648	L649	L650	L651	L652	L653	L654	L655	L656	L657	L658	L659	L660	L661	L662	L663	L664	L665	L666	L667	L668	L669	L670	L671	L672	L673	L674	L675	L676	L677	L678	L679	L680	L681	L682	L683	L684	L685	L686	L687	L688	L689	L690	L691	L692	L693	L694	L695	L696	L697	L698	L699	L700	L701	L702	L703	L704	L705	L706	L707	L708	L709	L710	L711	L712	L713	L714	L715	L716	L717	L718	L719	L720	L721	L722	L723	L724	L725	L726	L727	L728	L729	L730	L731	L732	L733	L734	L735	L736	L737	L738	L739	L740	L741	L742	L743	L744	L745	L746	L747	L748	L749	L750	L751	L752	L753	L754	L755	L756	L757	L758	L759	L760	L761	L762	L763	L764	L765	L766	L767	L768	L769	L770	L771	L772	L773	L774	L775	L776	L777	L778	L779	L780	L781	L782	L783	L784	L785	L786	L787	L788	L789	L790	L791	L792	L793	L794	L795	L796	L797	L798	L799	L800	L801	L802	L803	L804	L805	L806	L807	L808	L809	L810
V65	L66	D67	F68	L69	E70	Y71	L72	L73	G74	E75	P76	P77	F78	P79	Q80	D81	E82	C83	R84	D87	L88	T89	Y90	Q91	A92	P93	L94	Y95	A96	R97	L98	Q99	L100	I101	H102	K103	D104	T105	G106	L107	I108	K109	E110	D111	E112	F113	L114	L115	G116	H117	I118	P119	S118	M121	T122	V116	K252	D124	G125																																																																																																																																																																																																																																																																																																																																																																																																							
S126	F127	I128	I129	A132	D133	R134	V135	G136	L137	E138	L200	Q139	L140	H141	Q142	S143	P144	G145	V146	Y147	F148	L149	P150	D151	P152	G156	R157	Y158	I159	A160	S161	I162	L163	P164	L165	P166	K167	R168	G169	P170	W171	L172	D173	L174	E175	F176	E177	P178	M179	L180	V181	W182	S183	M184	K185	V186	N187	K188																																																																																																																																																																																																																																																																																																																																																																																																								
R189	K190	P191	F192	L193	V194	L195	L196	L197	R198	G199	P204	R205	L206	A207	Z202	D203	Q204	S205	T206	L207	A208	R209	E210	L211	G212	L213	L214	G215	V218	L219	L220	L221	L222	D223	V226	F227	A228	M229	R230	P231	E232	E233	A234	L235	L236	R237	L238	F239	L240	L241	L242	R243	P244	G245	D246	R250	D251	L252	A253																																																																																																																																																																																																																																																																																																																																																																																																							
V254	A255	Y256	W257	G258	L259	L260	L261	A262	P263	D264	R265	L266	G267	E268	Y269	D268	L269	G270	E271	A272	G273	R274	Y275	K276	E279	K280	L281	G282	L283	R284	L285	S286	G287	R288	T289	L290	A291	R292	F293	G296	E297	F298	K299	D300	E301	L302	F303	L304	P305	T306	L307	R308	P309	S309	L310	F311	A312	L313	T314	A315																																																																																																																																																																																																																																																																																																																																																																																																						
G316	V317	P318	G319	H320	E321	L322	D323	D324	D325	D326	H327	L328	G329	M330	R331	R332	L333	F334	T335	V336	G337	E338	L339	M340	T341	D342	Q343	F344	R345	V346	C347	R348	A349	R350	L351	A352	R353	G354	V355	R356	E357	R358	K359	L360	M361	E362	S363	E364	L365	D366	W367	H368	A369	L418	T419	R420	E421	R422	L423	P415	L414	C414	P415	L418	D481	E482	V483	W484	Y485	A423	H431	R432	T433	F434	H435	Y436	L437	A438	W439	L440	A441	L442	L443	S444	F445	L446	L447	L448	L449	G450	L451	R452	L453	S454	L455	A456	A457	Y458	A459	D460	V461	D462	E463	F464	W465	W466	L467	L468	L469	L470	L471	R472	L473	L474	G475	L476	W477	L478	Y479	T480	D481	E482	V483	W484	Y485	M486	L487	A488	D489	E490	D491	L492	L493	H494	Y495	L496	A497	L498	W499	L500	T501	P502	Q503	E504	M505	L506	E507	L508	F509	L510	E511	L512	L513	L514	L515	L516	L517	L518	L519	L520	L521	L522	L523	L524	L525	L526	L527	L528	L529	L530	L531	L532	L533	L534	L535	L536	L537	L538	L539	L540	L541	L542	L543	L544	L545	L546	L547	L548	L549	L550	L551	L552	L553	L554	L555	L556	L557	L558	L559	L560	L561	L562	L563	L564	L565	L566	L567	L568	L569	L570	L571	L572	L573	L574	L575	L576	L577	L578	L579	L580	L581	L582	L583	L584	L585	L586	L587	L588	L589	L590	L591	L592	L593	L594	L595	L596	L597	L598	L599	L600	L601	L602	L603	L604	L605	L606	L607	L608	L609	L610	L611	L612	L613	L614	L615	L616	L617	L618	L619	L620	L621	L622	L623	L624	L625	L626	L627	L628	L629	L630	L631	L632	L633	L634	L635	L636	L637	L638	L639	L640	L641	L642	L643	L644	L645	L646	L647	L648	L649	L650	L651	L652	L653	L654	L655	L656	L657	L658	L659	L660	L661	L662	L663	L664	L665	L666	L667	L668	L669	L670	L671	L672	L673	L674	L675	L676	L677	L678	L679	L680	L681	L682	L683	L684	L685	L686	L687	L688	L689	L690	L691	L692	L693	L694	L695	L696	L697	L698	L699	L700	L701	L702	L703	L704	L705	L706	L707	L708	L709	L710	L711	L712	L713	L714	L715	L716	L717	L718	L719	L720	L721	L722	L723	L724	L725	L726	L727	L728	L729	L730	L731	L732	L733	L734	L735	L736	L737	L738	L739	L740	L741	L742	L743	L744	L745	L746	L747	L74																																																														



• 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 25.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.50) 92.6 (25.00-2.50)	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 0.227 , 0.262	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 , 77.7	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	0.97	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: ZN, MG, RPT

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	0.90	5/1838 (0.3%)	1.22	9/2498 (0.4%)
1	B	0.77	0/1838	1.08	7/2498 (0.3%)
1	K	0.80	2/1838 (0.1%)	1.17	10/2498 (0.4%)
1	L	0.79	3/1838 (0.2%)	1.10	9/2498 (0.4%)
2	C	0.88	5/8997 (0.1%)	1.28	76/12164 (0.6%)
2	M	0.86	5/8997 (0.1%)	1.26	71/12164 (0.6%)
3	D	0.94	12/10975 (0.1%)	1.33	102/14836 (0.7%)
3	N	0.91	13/10975 (0.1%)	1.31	88/14836 (0.6%)
4	E	0.96	1/783 (0.1%)	1.37	9/1054 (0.9%)
4	O	0.90	0/783	1.38	8/1054 (0.8%)
5	F	0.79	2/2812 (0.1%)	1.21	15/3781 (0.4%)
5	P	0.76	1/2812 (0.0%)	1.18	13/3781 (0.3%)
All	All	0.88	49/54486 (0.1%)	1.27	417/73662 (0.6%)

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	48	ILE	C-N	9.99	1.45	1.33
1	L	172	SER	N-CA	-7.66	1.35	1.46
3	D	82	LYS	CA-C	7.45	1.62	1.52
3	D	53	ILE	CA-CB	7.41	1.63	1.54
3	N	126	VAL	CA-CB	7.40	1.62	1.54

The worst 5 of 417 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	207	PHE	CA-C-N	16.48	140.44	119.84
3	D	207	PHE	C-N-CA	16.48	140.44	119.84
3	N	207	PHE	CA-C-N	16.42	140.37	119.84
3	N	207	PHE	C-N-CA	16.42	140.37	119.84
3	N	508	ARG	CA-C-N	15.57	139.30	119.84

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	238	0
1	B	1806	0	1861	217	0
1	K	1806	0	1861	176	0
1	L	1806	0	1861	186	0
2	C	8829	0	8933	1252	0
2	M	8829	0	8933	1198	0
3	D	10797	0	10873	1532	0
3	N	10797	0	10873	1349	0
4	E	769	0	775	95	0
4	O	769	0	775	99	0
5	F	2771	0	2844	358	0
5	P	2771	0	2844	363	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	5	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	226	0
9	D	1252	0	0	280	0
9	E	117	0	0	28	0

Continued on next page...

Continued from previous page...

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	251	0
9	N	1265	0	0	253	0
9	O	108	0	0	26	0
9	P	361	0	0	79	0
All	All	60572	0	54418	6667	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 61.

The worst 5 of 6667 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%)	5 9
1	B	227/315 (72%)	198 (87%)	23 (10%)	6 (3%)	4 7
1	K	227/315 (72%)	200 (88%)	23 (10%)	4 (2%)	6 12
1	L	227/315 (72%)	203 (89%)	20 (9%)	4 (2%)	6 12

Continued on next page...

Continued from previous page...

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%)	1	1
3	N	1388/1524 (91%)	1105 (80%)	208 (15%)	75 (5%)	1	1
4	E	93/99 (94%)	75 (81%)	15 (16%)	3 (3%)	3	4
4	O	93/99 (94%)	75 (81%)	15 (16%)	3 (3%)	3	4
5	F	341/423 (81%)	285 (84%)	38 (11%)	18 (5%)	1	1
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%)	156 (77%)	46 (23%)	1	1
1	B	202/273 (74%)	163 (81%)	39 (19%)	1	2
1	K	202/273 (74%)	161 (80%)	41 (20%)	1	2
1	L	202/273 (74%)	154 (76%)	48 (24%)	1	1
2	C	941/941 (100%)	708 (75%)	233 (25%)	1	1
2	M	941/941 (100%)	719 (76%)	222 (24%)	1	1
3	D	1123/1279 (88%)	851 (76%)	272 (24%)	1	1
3	N	1123/1279 (88%)	847 (75%)	276 (25%)	1	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	83/87 (95%)	62 (75%)	21 (25%)	0	1
4	O	83/87 (95%)	62 (75%)	21 (25%)	0	1
5	F	295/370 (80%)	228 (77%)	67 (23%)	1	1
5	P	295/370 (80%)	236 (80%)	59 (20%)	1	2
All	All	5692/6446 (88%)	4347 (76%)	1345 (24%)	1	1

5 of 1345 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	755	LEU
3	N	971	LEU
2	M	911	GLU
2	M	754	ILE
3	N	394	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 179 such sidechains are listed below:

Mol	Chain	Res	Type
2	M	663	ASN
3	N	855	HIS
2	M	881	ASN
3	N	507	ASN
3	N	1116	ASN

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

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	2.61	22 (32%)	101,101,101	1.24	10 (9%)
7	RPT	C	8001	-	68,68,68	2.53	23 (33%)	101,101,101	1.24	12 (11%)

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	-	-	22/64/96/96	0/6/6/6
7	RPT	C	8001	-	-	12/64/96/96	0/6/6/6

The worst 5 of 45 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	8002	RPT	C39-N4	6.87	1.59	1.47
7	M	8002	RPT	C42-N4	6.73	1.59	1.47
7	C	8001	RPT	O6-C27	6.22	1.58	1.43
7	C	8001	RPT	O5-C29	6.18	1.55	1.39
7	M	8002	RPT	O5-C29	6.04	1.54	1.39

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	8002	RPT	C24-C23-C22	3.76	121.68	115.41
7	C	8001	RPT	C2-N1-C15	3.35	134.26	124.06
7	C	8001	RPT	C24-C23-C22	3.31	120.92	115.41
7	M	8002	RPT	C20-C21-C22	3.26	121.58	114.97
7	C	8001	RPT	C25-O7-C35	3.22	122.72	117.72

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

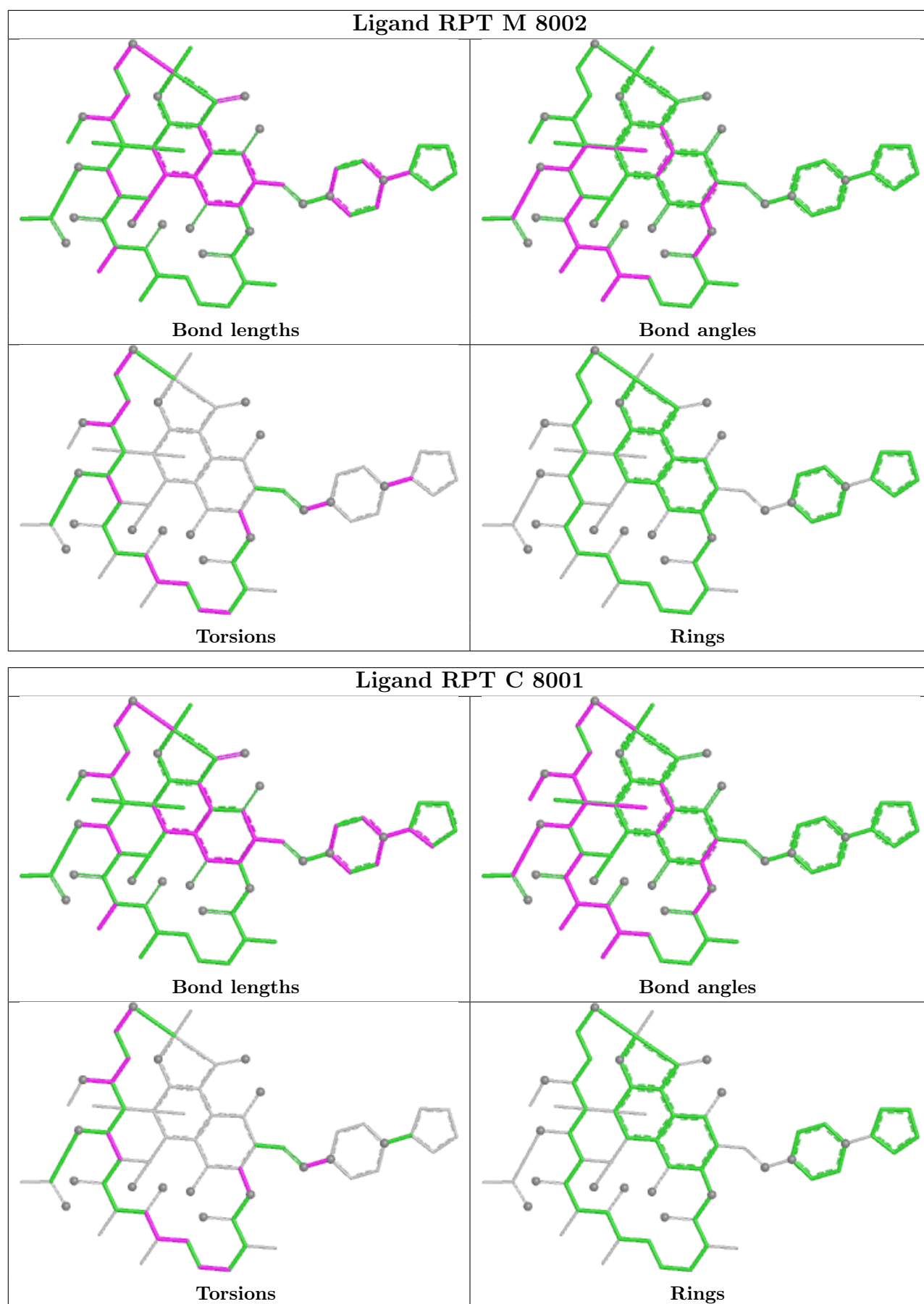
Mol	Chain	Res	Type	Atoms
7	C	8001	RPT	C26-C27-C28-C29
7	C	8001	RPT	C26-C27-O6-C37
7	C	8001	RPT	C28-C27-O6-C37
7	M	8002	RPT	C28-C27-O6-C37
7	M	8002	RPT	C44-C38-N4-C39

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	M	8002	RPT	7	0
7	C	8001	RPT	5	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 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%)	-1.62	0 100 100	27, 63, 91, 115	0
1	B	229/315 (72%)	-1.49	0 100 100	48, 93, 115, 119	0
1	K	229/315 (72%)	-1.62	0 100 100	34, 65, 94, 134	0
1	L	229/315 (72%)	-1.55	0 100 100	52, 92, 110, 131	0
2	C	1119/1119 (100%)	-1.59	0 100 100	21, 75, 106, 118	0
2	M	1119/1119 (100%)	-1.58	0 100 100	25, 79, 109, 122	0
3	D	1392/1524 (91%)	-1.60	0 100 100	24, 65, 112, 132	0
3	N	1392/1524 (91%)	-1.57	0 100 100	25, 69, 117, 138	0
4	E	95/99 (95%)	-1.50	0 100 100	42, 83, 108, 126	0
4	O	95/99 (95%)	-1.56	0 100 100	46, 80, 107, 114	0
5	F	345/423 (81%)	-1.57	0 100 100	49, 84, 110, 127	0
5	P	345/423 (81%)	-1.55	0 100 100	63, 89, 114, 124	0
All	All	6818/7590 (89%)	-1.58	0 100 100	21, 75, 112, 138	0

There are no RSRZ outliers to report.

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 oligosaccharides 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
6	MG	D	9177	1/1	0.98	0.03	64,64,64,64	0
6	MG	A	9043	1/1	0.99	0.01	37,37,37,37	0
6	MG	A	9153	1/1	0.99	0.04	66,66,66,66	0
6	MG	A	9171	1/1	0.99	0.03	58,58,58,58	0
6	MG	A	9380	1/1	0.99	0.03	44,44,44,44	0
6	MG	B	9080	1/1	0.99	0.02	56,56,56,56	0
6	MG	B	9093	1/1	0.99	0.02	40,40,40,40	0
6	MG	C	9021	1/1	0.99	0.04	37,37,37,37	0
6	MG	C	9047	1/1	0.99	0.03	53,53,53,53	0
6	MG	C	9067	1/1	0.99	0.02	57,57,57,57	0
6	MG	C	9112	1/1	0.99	0.03	39,39,39,39	0
6	MG	C	9122	1/1	0.99	0.03	56,56,56,56	0
6	MG	C	9160	1/1	0.99	0.05	44,44,44,44	0
6	MG	C	9175	1/1	0.99	0.02	68,68,68,68	0
6	MG	C	9340	1/1	0.99	0.04	60,60,60,60	0
6	MG	C	9360	1/1	0.99	0.03	53,53,53,53	0
6	MG	C	9362	1/1	0.99	0.02	55,55,55,55	0
6	MG	C	9454	1/1	0.99	0.04	55,55,55,55	0
6	MG	C	9462	1/1	0.99	0.04	43,43,43,43	0
6	MG	C	9463	1/1	0.99	0.02	55,55,55,55	0
6	MG	D	9024	1/1	0.99	0.02	36,36,36,36	0
6	MG	D	9030	1/1	0.99	0.04	48,48,48,48	0
6	MG	D	9082	1/1	0.99	0.02	60,60,60,60	0
6	MG	D	9137	1/1	0.99	0.04	47,47,47,47	0
6	MG	D	9140	1/1	0.99	0.03	40,40,40,40	0
6	MG	D	9152	1/1	0.99	0.03	67,67,67,67	0
6	MG	D	9163	1/1	0.99	0.03	52,52,52,52	0
6	MG	D	9167	1/1	0.99	0.02	49,49,49,49	0
6	MG	D	9173	1/1	0.99	0.04	48,48,48,48	0
6	MG	A	9016	1/1	0.99	0.02	36,36,36,36	0
6	MG	D	9330	1/1	0.99	0.02	39,39,39,39	0
6	MG	D	9348	1/1	0.99	0.02	57,57,57,57	0
6	MG	D	9349	1/1	0.99	0.01	33,33,33,33	0
6	MG	D	9367	1/1	0.99	0.04	31,31,31,31	0
6	MG	D	9459	1/1	0.99	0.04	54,54,54,54	0
6	MG	D	9480	1/1	0.99	0.03	55,55,55,55	0
6	MG	E	9045	1/1	0.99	0.02	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	F	9008	1/1	0.99	0.02	40,40,40,40	0
6	MG	F	9099	1/1	0.99	0.01	56,56,56,56	0
6	MG	F	9148	1/1	0.99	0.02	54,54,54,54	0
6	MG	F	9159	1/1	0.99	0.02	57,57,57,57	0
6	MG	F	9370	1/1	0.99	0.03	46,46,46,46	0
6	MG	F	9389	1/1	0.99	0.04	53,53,53,53	0
6	MG	K	9188	1/1	0.99	0.02	40,40,40,40	0
6	MG	K	9433	1/1	0.99	0.03	50,50,50,50	0
6	MG	L	9245	1/1	0.99	0.02	62,62,62,62	0
6	MG	L	9246	1/1	0.99	0.02	52,52,52,52	0
6	MG	L	9283	1/1	0.99	0.02	59,59,59,59	0
6	MG	L	9289	1/1	0.99	0.02	62,62,62,62	0
6	MG	L	9414	1/1	0.99	0.02	51,51,51,51	0
6	MG	M	9201	1/1	0.99	0.02	45,45,45,45	0
6	MG	M	9210	1/1	0.99	0.02	41,41,41,41	0
6	MG	M	9220	1/1	0.99	0.03	51,51,51,51	0
6	MG	M	9263	1/1	0.99	0.04	56,56,56,56	0
6	MG	M	9272	1/1	0.99	0.02	45,45,45,45	0
6	MG	M	9310	1/1	0.99	0.03	46,46,46,46	0
6	MG	M	9324	1/1	0.99	0.04	41,41,41,41	0
6	MG	M	9406	1/1	0.99	0.03	67,67,67,67	0
6	MG	M	9416	1/1	0.99	0.03	45,45,45,45	0
6	MG	M	9440	1/1	0.99	0.03	50,50,50,50	0
6	MG	M	9442	1/1	0.99	0.04	59,59,59,59	0
6	MG	M	9447	1/1	0.99	0.02	64,64,64,64	0
6	MG	M	9452	1/1	0.99	0.02	42,42,42,42	0
6	MG	M	9475	1/1	0.99	0.04	62,62,62,62	0
6	MG	N	9185	1/1	0.99	0.02	56,56,56,56	0
6	MG	N	9200	1/1	0.99	0.02	38,38,38,38	0
6	MG	N	9207	1/1	0.99	0.02	41,41,41,41	0
6	MG	N	9211	1/1	0.99	0.02	44,44,44,44	0
6	MG	N	9217	1/1	0.99	0.02	48,48,48,48	0
6	MG	N	9238	1/1	0.99	0.07	43,43,43,43	0
6	MG	N	9253	1/1	0.99	0.02	42,42,42,42	0
6	MG	N	9308	1/1	0.99	0.02	55,55,55,55	0
6	MG	N	9313	1/1	0.99	0.04	43,43,43,43	0
6	MG	N	9317	1/1	0.99	0.03	43,43,43,43	0
6	MG	N	9425	1/1	0.99	0.02	46,46,46,46	0
6	MG	N	9426	1/1	0.99	0.04	41,41,41,41	0
6	MG	N	9427	1/1	0.99	0.02	58,58,58,58	0
6	MG	N	9445	1/1	0.99	0.03	51,51,51,51	0
6	MG	N	9449	1/1	0.99	0.03	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	N	9465	1/1	0.99	0.03	49,49,49,49	0
6	MG	N	9476	1/1	0.99	0.03	54,54,54,54	0
6	MG	P	9226	1/1	0.99	0.05	43,43,43,43	0
6	MG	P	9228	1/1	0.99	0.03	43,43,43,43	0
6	MG	P	9280	1/1	0.99	0.02	51,51,51,51	0
6	MG	P	9282	1/1	0.99	0.03	56,56,56,56	0
6	MG	P	9325	1/1	0.99	0.02	49,49,49,49	0
6	MG	P	9436	1/1	0.99	0.02	49,49,49,49	0
6	MG	C	9119	1/1	1.00	0.02	43,43,43,43	0
6	MG	A	9081	1/1	1.00	0.03	40,40,40,40	0
6	MG	C	9126	1/1	1.00	0.03	46,46,46,46	0
6	MG	C	9128	1/1	1.00	0.02	52,52,52,52	0
6	MG	C	9138	1/1	1.00	0.03	43,43,43,43	0
6	MG	C	9142	1/1	1.00	0.02	48,48,48,48	0
6	MG	C	9143	1/1	1.00	0.01	35,35,35,35	0
6	MG	C	9145	1/1	1.00	0.01	66,66,66,66	0
6	MG	C	9149	1/1	1.00	0.02	48,48,48,48	0
6	MG	C	9154	1/1	1.00	0.04	43,43,43,43	0
6	MG	A	9088	1/1	1.00	0.02	36,36,36,36	0
6	MG	C	9162	1/1	1.00	0.03	50,50,50,50	0
6	MG	C	9164	1/1	1.00	0.01	49,49,49,49	0
6	MG	C	9168	1/1	1.00	0.03	45,45,45,45	0
6	MG	C	9169	1/1	1.00	0.02	42,42,42,42	0
6	MG	C	9170	1/1	1.00	0.03	41,41,41,41	0
6	MG	A	9097	1/1	1.00	0.01	34,34,34,34	0
6	MG	C	9176	1/1	1.00	0.03	28,28,28,28	0
6	MG	C	9178	1/1	1.00	0.03	39,39,39,39	0
6	MG	A	9106	1/1	1.00	0.01	38,38,38,38	0
6	MG	C	9350	1/1	1.00	0.01	60,60,60,60	0
6	MG	C	9353	1/1	1.00	0.01	48,48,48,48	0
6	MG	C	9355	1/1	1.00	0.02	58,58,58,58	0
6	MG	A	9111	1/1	1.00	0.03	35,35,35,35	0
6	MG	C	9361	1/1	1.00	0.03	41,41,41,41	0
6	MG	A	9124	1/1	1.00	0.02	39,39,39,39	0
6	MG	C	9366	1/1	1.00	0.01	41,41,41,41	0
6	MG	C	9371	1/1	1.00	0.01	54,54,54,54	0
6	MG	C	9372	1/1	1.00	0.06	61,61,61,61	0
6	MG	C	9377	1/1	1.00	0.02	44,44,44,44	0
6	MG	C	9381	1/1	1.00	0.01	53,53,53,53	0
6	MG	C	9391	1/1	1.00	0.04	60,60,60,60	0
6	MG	C	9394	1/1	1.00	0.03	33,33,33,33	0
6	MG	A	9125	1/1	1.00	0.01	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	C	9455	1/1	1.00	0.03	40,40,40,40	0
6	MG	C	9461	1/1	1.00	0.04	50,50,50,50	0
6	MG	A	9012	1/1	1.00	0.03	47,47,47,47	0
6	MG	A	9156	1/1	1.00	0.02	43,43,43,43	0
6	MG	C	9464	1/1	1.00	0.02	48,48,48,48	0
6	MG	C	9487	1/1	1.00	0.02	32,32,32,32	0
6	MG	D	9001	1/1	1.00	0.03	36,36,36,36	0
6	MG	D	9005	1/1	1.00	0.02	40,40,40,40	0
6	MG	D	9006	1/1	1.00	0.02	40,40,40,40	0
6	MG	D	9009	1/1	1.00	0.01	43,43,43,43	0
6	MG	D	9011	1/1	1.00	0.01	33,33,33,33	0
6	MG	D	9014	1/1	1.00	0.01	41,41,41,41	0
6	MG	D	9017	1/1	1.00	0.02	42,42,42,42	0
6	MG	D	9018	1/1	1.00	0.01	39,39,39,39	0
6	MG	D	9023	1/1	1.00	0.01	34,34,34,34	0
6	MG	A	9013	1/1	1.00	0.01	44,44,44,44	0
6	MG	D	9028	1/1	1.00	0.01	34,34,34,34	0
6	MG	D	9029	1/1	1.00	0.01	33,33,33,33	0
6	MG	A	9332	1/1	1.00	0.02	35,35,35,35	0
6	MG	D	9034	1/1	1.00	0.01	41,41,41,41	0
6	MG	D	9036	1/1	1.00	0.01	44,44,44,44	0
6	MG	D	9038	1/1	1.00	0.04	39,39,39,39	0
6	MG	D	9039	1/1	1.00	0.02	44,44,44,44	0
6	MG	D	9041	1/1	1.00	0.01	47,47,47,47	0
6	MG	D	9052	1/1	1.00	0.01	65,65,65,65	0
6	MG	D	9054	1/1	1.00	0.01	44,44,44,44	0
6	MG	D	9058	1/1	1.00	0.02	38,38,38,38	0
6	MG	D	9062	1/1	1.00	0.02	47,47,47,47	0
6	MG	D	9063	1/1	1.00	0.04	33,33,33,33	0
6	MG	D	9064	1/1	1.00	0.01	44,44,44,44	0
6	MG	D	9069	1/1	1.00	0.01	48,48,48,48	0
6	MG	D	9070	1/1	1.00	0.03	33,33,33,33	0
6	MG	D	9072	1/1	1.00	0.02	32,32,32,32	0
6	MG	D	9073	1/1	1.00	0.03	34,34,34,34	0
6	MG	D	9077	1/1	1.00	0.03	35,35,35,35	0
6	MG	A	9342	1/1	1.00	0.01	39,39,39,39	0
6	MG	D	9084	1/1	1.00	0.01	37,37,37,37	0
6	MG	D	9085	1/1	1.00	0.02	49,49,49,49	0
6	MG	D	9087	1/1	1.00	0.05	43,43,43,43	0
6	MG	D	9089	1/1	1.00	0.04	36,36,36,36	0
6	MG	D	9091	1/1	1.00	0.03	27,27,27,27	0
6	MG	D	9095	1/1	1.00	0.03	30,30,30,30	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	D	9096	1/1	1.00	0.02	60,60,60,60	0
6	MG	D	9100	1/1	1.00	0.05	43,43,43,43	0
6	MG	D	9102	1/1	1.00	0.03	44,44,44,44	0
6	MG	D	9108	1/1	1.00	0.01	51,51,51,51	0
6	MG	D	9113	1/1	1.00	0.02	34,34,34,34	0
6	MG	D	9117	1/1	1.00	0.02	48,48,48,48	0
6	MG	D	9118	1/1	1.00	0.02	44,44,44,44	0
6	MG	D	9120	1/1	1.00	0.03	31,31,31,31	0
6	MG	D	9121	1/1	1.00	0.01	35,35,35,35	0
6	MG	D	9127	1/1	1.00	0.01	48,48,48,48	0
6	MG	D	9129	1/1	1.00	0.01	42,42,42,42	0
6	MG	D	9130	1/1	1.00	0.01	51,51,51,51	0
6	MG	D	9132	1/1	1.00	0.02	43,43,43,43	0
6	MG	D	9133	1/1	1.00	0.02	42,42,42,42	0
6	MG	D	9134	1/1	1.00	0.02	47,47,47,47	0
6	MG	D	9135	1/1	1.00	0.02	50,50,50,50	0
6	MG	A	9345	1/1	1.00	0.02	41,41,41,41	0
6	MG	A	9352	1/1	1.00	0.01	46,46,46,46	0
6	MG	D	9141	1/1	1.00	0.03	50,50,50,50	0
6	MG	D	9144	1/1	1.00	0.03	39,39,39,39	0
6	MG	D	9146	1/1	1.00	0.02	31,31,31,31	0
6	MG	D	9147	1/1	1.00	0.02	41,41,41,41	0
6	MG	D	9150	1/1	1.00	0.01	31,31,31,31	0
6	MG	D	9151	1/1	1.00	0.01	57,57,57,57	0
6	MG	A	9354	1/1	1.00	0.02	37,37,37,37	0
6	MG	D	9158	1/1	1.00	0.04	60,60,60,60	0
6	MG	D	9161	1/1	1.00	0.02	57,57,57,57	0
6	MG	A	9357	1/1	1.00	0.02	54,54,54,54	0
6	MG	D	9165	1/1	1.00	0.04	32,32,32,32	0
6	MG	D	9166	1/1	1.00	0.02	40,40,40,40	0
6	MG	A	9368	1/1	1.00	0.02	43,43,43,43	0
6	MG	A	9002	1/1	1.00	0.01	31,31,31,31	0
6	MG	D	9174	1/1	1.00	0.02	47,47,47,47	0
6	MG	A	9384	1/1	1.00	0.02	39,39,39,39	0
6	MG	D	9328	1/1	1.00	0.03	30,30,30,30	0
6	MG	D	9329	1/1	1.00	0.02	33,33,33,33	0
6	MG	A	9395	1/1	1.00	0.03	50,50,50,50	0
6	MG	D	9331	1/1	1.00	0.01	43,43,43,43	0
6	MG	D	9333	1/1	1.00	0.05	33,33,33,33	0
6	MG	D	9334	1/1	1.00	0.01	54,54,54,54	0
6	MG	D	9335	1/1	1.00	0.02	52,52,52,52	0
6	MG	D	9336	1/1	1.00	0.02	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	D	9337	1/1	1.00	0.02	53,53,53,53	0
6	MG	D	9338	1/1	1.00	0.02	42,42,42,42	0
6	MG	D	9339	1/1	1.00	0.01	37,37,37,37	0
6	MG	D	9341	1/1	1.00	0.02	41,41,41,41	0
6	MG	D	9343	1/1	1.00	0.03	59,59,59,59	0
6	MG	D	9344	1/1	1.00	0.03	55,55,55,55	0
6	MG	D	9346	1/1	1.00	0.02	47,47,47,47	0
6	MG	D	9347	1/1	1.00	0.01	49,49,49,49	0
6	MG	A	9460	1/1	1.00	0.03	55,55,55,55	0
6	MG	A	9477	1/1	1.00	0.02	52,52,52,52	0
6	MG	D	9351	1/1	1.00	0.01	43,43,43,43	0
6	MG	D	9364	1/1	1.00	0.02	47,47,47,47	0
6	MG	D	9365	1/1	1.00	0.02	41,41,41,41	0
6	MG	B	9032	1/1	1.00	0.05	34,34,34,34	0
6	MG	D	9369	1/1	1.00	0.01	49,49,49,49	0
6	MG	D	9373	1/1	1.00	0.03	51,51,51,51	0
6	MG	D	9374	1/1	1.00	0.02	41,41,41,41	0
6	MG	D	9379	1/1	1.00	0.03	47,47,47,47	0
6	MG	D	9385	1/1	1.00	0.01	35,35,35,35	0
6	MG	D	9386	1/1	1.00	0.03	40,40,40,40	0
6	MG	D	9388	1/1	1.00	0.01	37,37,37,37	0
6	MG	D	9392	1/1	1.00	0.02	52,52,52,52	0
6	MG	D	9396	1/1	1.00	0.04	62,62,62,62	0
6	MG	D	9397	1/1	1.00	0.02	51,51,51,51	0
6	MG	D	9453	1/1	1.00	0.02	38,38,38,38	0
6	MG	D	9456	1/1	1.00	0.02	55,55,55,55	0
6	MG	B	9033	1/1	1.00	0.01	33,33,33,33	0
6	MG	B	9040	1/1	1.00	0.01	36,36,36,36	0
6	MG	E	9007	1/1	1.00	0.01	40,40,40,40	0
6	MG	B	9056	1/1	1.00	0.01	43,43,43,43	0
6	MG	E	9074	1/1	1.00	0.01	59,59,59,59	0
6	MG	E	9155	1/1	1.00	0.02	44,44,44,44	0
6	MG	E	9479	1/1	1.00	0.01	62,62,62,62	0
6	MG	B	9059	1/1	1.00	0.03	48,48,48,48	0
6	MG	F	9035	1/1	1.00	0.01	40,40,40,40	0
6	MG	F	9048	1/1	1.00	0.02	41,41,41,41	0
6	MG	F	9057	1/1	1.00	0.03	30,30,30,30	0
6	MG	F	9060	1/1	1.00	0.02	41,41,41,41	0
6	MG	F	9098	1/1	1.00	0.02	54,54,54,54	0
6	MG	A	9027	1/1	1.00	0.04	37,37,37,37	0
6	MG	F	9101	1/1	1.00	0.03	44,44,44,44	0
6	MG	F	9105	1/1	1.00	0.01	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	F	9109	1/1	1.00	0.02	60,60,60,60	0
6	MG	F	9123	1/1	1.00	0.03	37,37,37,37	0
6	MG	F	9139	1/1	1.00	0.02	38,38,38,38	0
6	MG	B	9083	1/1	1.00	0.01	40,40,40,40	0
6	MG	F	9157	1/1	1.00	0.02	42,42,42,42	0
6	MG	A	9010	1/1	1.00	0.01	30,30,30,30	0
6	MG	F	9172	1/1	1.00	0.01	51,51,51,51	0
6	MG	F	9356	1/1	1.00	0.01	37,37,37,37	0
6	MG	F	9363	1/1	1.00	0.02	53,53,53,53	0
6	MG	B	9094	1/1	1.00	0.02	38,38,38,38	0
6	MG	F	9375	1/1	1.00	0.01	36,36,36,36	0
6	MG	F	9376	1/1	1.00	0.02	62,62,62,62	0
6	MG	F	9382	1/1	1.00	0.03	40,40,40,40	0
6	MG	F	9383	1/1	1.00	0.04	48,48,48,48	0
6	MG	F	9387	1/1	1.00	0.03	53,53,53,53	0
6	MG	B	9103	1/1	1.00	0.01	43,43,43,43	0
6	MG	F	9390	1/1	1.00	0.02	46,46,46,46	0
6	MG	F	9393	1/1	1.00	0.01	38,38,38,38	0
6	MG	F	9481	1/1	1.00	0.03	57,57,57,57	0
6	MG	K	9180	1/1	1.00	0.04	42,42,42,42	0
6	MG	B	9104	1/1	1.00	0.02	45,45,45,45	0
6	MG	K	9191	1/1	1.00	0.01	32,32,32,32	0
6	MG	K	9213	1/1	1.00	0.01	43,43,43,43	0
6	MG	K	9223	1/1	1.00	0.03	32,32,32,32	0
6	MG	K	9244	1/1	1.00	0.03	44,44,44,44	0
6	MG	K	9251	1/1	1.00	0.02	43,43,43,43	0
6	MG	K	9257	1/1	1.00	0.03	58,58,58,58	0
6	MG	K	9264	1/1	1.00	0.02	42,42,42,42	0
6	MG	K	9290	1/1	1.00	0.01	51,51,51,51	0
6	MG	K	9301	1/1	1.00	0.02	43,43,43,43	0
6	MG	K	9405	1/1	1.00	0.01	56,56,56,56	0
6	MG	K	9410	1/1	1.00	0.11	36,36,36,36	0
6	MG	K	9413	1/1	1.00	0.02	54,54,54,54	0
6	MG	K	9432	1/1	1.00	0.02	49,49,49,49	0
6	MG	B	9110	1/1	1.00	0.02	49,49,49,49	0
6	MG	K	9438	1/1	1.00	0.01	52,52,52,52	0
6	MG	K	9469	1/1	1.00	0.01	50,50,50,50	0
6	MG	K	9470	1/1	1.00	0.04	55,55,55,55	0
6	MG	L	9182	1/1	1.00	0.02	47,47,47,47	0
6	MG	L	9183	1/1	1.00	0.01	37,37,37,37	0
6	MG	L	9218	1/1	1.00	0.03	33,33,33,33	0
6	MG	B	9116	1/1	1.00	0.03	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MG	B	9131	1/1	1.00	0.04	33,33,33,33	0
6	MG	L	9252	1/1	1.00	0.01	45,45,45,45	0
6	MG	L	9278	1/1	1.00	0.01	44,44,44,44	0
6	MG	B	9136	1/1	1.00	0.03	47,47,47,47	0
6	MG	B	9358	1/1	1.00	0.04	39,39,39,39	0
6	MG	L	9306	1/1	1.00	0.02	57,57,57,57	0
6	MG	L	9307	1/1	1.00	0.02	35,35,35,35	0
6	MG	L	9309	1/1	1.00	0.01	49,49,49,49	0
6	MG	L	9314	1/1	1.00	0.01	56,56,56,56	0
6	MG	B	9359	1/1	1.00	0.04	52,52,52,52	0
6	MG	L	9421	1/1	1.00	0.02	53,53,53,53	0
6	MG	L	9437	1/1	1.00	0.04	40,40,40,40	0
6	MG	L	9466	1/1	1.00	0.02	49,49,49,49	0
6	MG	M	9190	1/1	1.00	0.01	29,29,29,29	0
6	MG	M	9195	1/1	1.00	0.03	34,34,34,34	0
6	MG	M	9196	1/1	1.00	0.02	42,42,42,42	0
6	MG	B	9378	1/1	1.00	0.01	47,47,47,47	0
6	MG	M	9203	1/1	1.00	0.01	32,32,32,32	0
6	MG	M	9205	1/1	1.00	0.04	38,38,38,38	0
6	MG	M	9208	1/1	1.00	0.03	39,39,39,39	0
6	MG	B	9457	1/1	1.00	0.04	43,43,43,43	0
6	MG	M	9212	1/1	1.00	0.02	32,32,32,32	0
6	MG	M	9219	1/1	1.00	0.03	47,47,47,47	0
6	MG	B	9458	1/1	1.00	0.03	44,44,44,44	0
6	MG	M	9222	1/1	1.00	0.03	35,35,35,35	0
6	MG	M	9224	1/1	1.00	0.01	40,40,40,40	0
6	MG	M	9225	1/1	1.00	0.02	56,56,56,56	0
6	MG	M	9227	1/1	1.00	0.01	35,35,35,35	0
6	MG	M	9230	1/1	1.00	0.01	50,50,50,50	0
6	MG	M	9234	1/1	1.00	0.02	53,53,53,53	0
6	MG	M	9237	1/1	1.00	0.02	52,52,52,52	0
6	MG	M	9239	1/1	1.00	0.03	34,34,34,34	0
6	MG	M	9241	1/1	1.00	0.03	36,36,36,36	0
6	MG	M	9242	1/1	1.00	0.03	35,35,35,35	0
6	MG	M	9247	1/1	1.00	0.04	51,51,51,51	0
6	MG	M	9248	1/1	1.00	0.02	48,48,48,48	0
6	MG	M	9250	1/1	1.00	0.01	38,38,38,38	0
6	MG	M	9256	1/1	1.00	0.02	56,56,56,56	0
6	MG	M	9260	1/1	1.00	0.02	36,36,36,36	0
6	MG	M	9261	1/1	1.00	0.01	47,47,47,47	0
6	MG	B	9478	1/1	1.00	0.01	61,61,61,61	0
6	MG	M	9268	1/1	1.00	0.02	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	C	9003	1/1	1.00	0.02	38,38,38,38	0
6	MG	M	9273	1/1	1.00	0.03	44,44,44,44	0
6	MG	M	9275	1/1	1.00	0.01	55,55,55,55	0
6	MG	M	9281	1/1	1.00	0.01	49,49,49,49	0
6	MG	M	9284	1/1	1.00	0.01	54,54,54,54	0
6	MG	M	9294	1/1	1.00	0.05	52,52,52,52	0
6	MG	M	9295	1/1	1.00	0.01	42,42,42,42	0
6	MG	M	9299	1/1	1.00	0.04	43,43,43,43	0
6	MG	M	9300	1/1	1.00	0.01	39,39,39,39	0
6	MG	M	9305	1/1	1.00	0.02	46,46,46,46	0
6	MG	C	9004	1/1	1.00	0.02	39,39,39,39	0
6	MG	M	9312	1/1	1.00	0.01	37,37,37,37	0
6	MG	M	9319	1/1	1.00	0.01	41,41,41,41	0
6	MG	M	9320	1/1	1.00	0.04	34,34,34,34	0
6	MG	M	9321	1/1	1.00	0.02	41,41,41,41	0
6	MG	C	9015	1/1	1.00	0.03	38,38,38,38	0
6	MG	M	9400	1/1	1.00	0.01	40,40,40,40	0
6	MG	M	9401	1/1	1.00	0.02	37,37,37,37	0
6	MG	C	9019	1/1	1.00	0.01	57,57,57,57	0
6	MG	M	9407	1/1	1.00	0.02	35,35,35,35	0
6	MG	M	9409	1/1	1.00	0.02	36,36,36,36	0
6	MG	M	9411	1/1	1.00	0.02	47,47,47,47	0
6	MG	M	9412	1/1	1.00	0.02	43,43,43,43	0
6	MG	C	9020	1/1	1.00	0.01	34,34,34,34	0
6	MG	M	9424	1/1	1.00	0.02	34,34,34,34	0
6	MG	M	9434	1/1	1.00	0.03	34,34,34,34	0
6	MG	A	9066	1/1	1.00	0.01	47,47,47,47	0
6	MG	M	9441	1/1	1.00	0.03	45,45,45,45	0
6	MG	C	9022	1/1	1.00	0.01	37,37,37,37	0
6	MG	C	9025	1/1	1.00	0.02	39,39,39,39	0
6	MG	C	9026	1/1	1.00	0.01	42,42,42,42	0
6	MG	M	9471	1/1	1.00	0.03	47,47,47,47	0
6	MG	M	9474	1/1	1.00	0.04	49,49,49,49	0
6	MG	C	9031	1/1	1.00	0.03	40,40,40,40	0
6	MG	M	9485	1/1	1.00	0.04	54,54,54,54	0
6	MG	M	9486	1/1	1.00	0.05	48,48,48,48	0
6	MG	N	9179	1/1	1.00	0.02	33,33,33,33	0
6	MG	N	9181	1/1	1.00	0.01	47,47,47,47	0
6	MG	N	9184	1/1	1.00	0.01	29,29,29,29	0
6	MG	C	9037	1/1	1.00	0.01	51,51,51,51	0
6	MG	N	9186	1/1	1.00	0.01	49,49,49,49	0
6	MG	N	9187	1/1	1.00	0.01	33,33,33,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	N	9192	1/1	1.00	0.01	62,62,62,62	0
6	MG	N	9193	1/1	1.00	0.01	34,34,34,34	0
6	MG	N	9194	1/1	1.00	0.01	51,51,51,51	0
6	MG	N	9199	1/1	1.00	0.01	35,35,35,35	0
6	MG	C	9042	1/1	1.00	0.01	47,47,47,47	0
6	MG	N	9204	1/1	1.00	0.01	44,44,44,44	0
6	MG	N	9206	1/1	1.00	0.01	31,31,31,31	0
6	MG	C	9044	1/1	1.00	0.01	34,34,34,34	0
6	MG	C	9046	1/1	1.00	0.02	38,38,38,38	0
6	MG	N	9214	1/1	1.00	0.03	33,33,33,33	0
6	MG	N	9215	1/1	1.00	0.02	32,32,32,32	0
6	MG	A	9068	1/1	1.00	0.03	39,39,39,39	0
6	MG	N	9221	1/1	1.00	0.01	44,44,44,44	0
6	MG	N	9229	1/1	1.00	0.03	41,41,41,41	0
6	MG	N	9231	1/1	1.00	0.01	52,52,52,52	0
6	MG	N	9232	1/1	1.00	0.02	47,47,47,47	0
6	MG	N	9233	1/1	1.00	0.03	62,62,62,62	0
6	MG	N	9236	1/1	1.00	0.02	39,39,39,39	0
6	MG	C	9049	1/1	1.00	0.01	46,46,46,46	0
6	MG	N	9240	1/1	1.00	0.02	46,46,46,46	0
6	MG	N	9243	1/1	1.00	0.01	35,35,35,35	0
6	MG	N	9249	1/1	1.00	0.02	45,45,45,45	0
6	MG	C	9050	1/1	1.00	0.01	37,37,37,37	0
6	MG	N	9259	1/1	1.00	0.01	34,34,34,34	0
6	MG	N	9262	1/1	1.00	0.03	51,51,51,51	0
6	MG	N	9265	1/1	1.00	0.02	61,61,61,61	0
6	MG	N	9267	1/1	1.00	0.01	42,42,42,42	0
6	MG	N	9269	1/1	1.00	0.04	42,42,42,42	0
6	MG	N	9270	1/1	1.00	0.02	39,39,39,39	0
6	MG	N	9271	1/1	1.00	0.03	43,43,43,43	0
6	MG	N	9274	1/1	1.00	0.01	40,40,40,40	0
6	MG	N	9276	1/1	1.00	0.02	61,61,61,61	0
6	MG	N	9279	1/1	1.00	0.02	54,54,54,54	0
6	MG	N	9286	1/1	1.00	0.01	31,31,31,31	0
6	MG	N	9287	1/1	1.00	0.02	53,53,53,53	0
6	MG	N	9288	1/1	1.00	0.04	49,49,49,49	0
6	MG	N	9291	1/1	1.00	0.02	64,64,64,64	0
6	MG	N	9292	1/1	1.00	0.02	56,56,56,56	0
6	MG	N	9293	1/1	1.00	0.01	42,42,42,42	0
6	MG	N	9298	1/1	1.00	0.02	55,55,55,55	0
6	MG	N	9302	1/1	1.00	0.01	31,31,31,31	0
6	MG	N	9303	1/1	1.00	0.03	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	N	9304	1/1	1.00	0.01	47,47,47,47	0
6	MG	C	9051	1/1	1.00	0.03	37,37,37,37	0
6	MG	N	9311	1/1	1.00	0.02	39,39,39,39	0
6	MG	C	9053	1/1	1.00	0.02	30,30,30,30	0
6	MG	N	9316	1/1	1.00	0.04	37,37,37,37	0
6	MG	C	9055	1/1	1.00	0.03	38,38,38,38	0
6	MG	N	9318	1/1	1.00	0.04	34,34,34,34	0
6	MG	N	9322	1/1	1.00	0.02	54,54,54,54	0
6	MG	N	9323	1/1	1.00	0.04	38,38,38,38	0
6	MG	N	9326	1/1	1.00	0.02	62,62,62,62	0
6	MG	N	9327	1/1	1.00	0.02	40,40,40,40	0
6	MG	N	9398	1/1	1.00	0.02	48,48,48,48	0
6	MG	N	9402	1/1	1.00	0.02	45,45,45,45	0
6	MG	N	9403	1/1	1.00	0.01	34,34,34,34	0
6	MG	N	9404	1/1	1.00	0.01	55,55,55,55	0
6	MG	N	9408	1/1	1.00	0.02	45,45,45,45	0
6	MG	N	9415	1/1	1.00	0.02	42,42,42,42	0
6	MG	N	9417	1/1	1.00	0.02	39,39,39,39	0
6	MG	N	9418	1/1	1.00	0.01	49,49,49,49	0
6	MG	N	9419	1/1	1.00	0.02	51,51,51,51	0
6	MG	N	9422	1/1	1.00	0.02	56,56,56,56	0
6	MG	N	9423	1/1	1.00	0.02	58,58,58,58	0
6	MG	C	9061	1/1	1.00	0.02	34,34,34,34	0
6	MG	C	9065	1/1	1.00	0.01	37,37,37,37	0
6	MG	A	9075	1/1	1.00	0.03	36,36,36,36	0
6	MG	N	9428	1/1	1.00	0.01	42,42,42,42	0
6	MG	N	9429	1/1	1.00	0.03	45,45,45,45	0
6	MG	N	9430	1/1	1.00	0.05	57,57,57,57	0
6	MG	N	9431	1/1	1.00	0.03	39,39,39,39	0
6	MG	N	9435	1/1	1.00	0.01	53,53,53,53	0
6	MG	N	9443	1/1	1.00	0.01	54,54,54,54	0
6	MG	N	9444	1/1	1.00	0.02	49,49,49,49	0
6	MG	C	9071	1/1	1.00	0.02	42,42,42,42	0
6	MG	N	9448	1/1	1.00	0.02	51,51,51,51	0
6	MG	C	9076	1/1	1.00	0.03	33,33,33,33	0
6	MG	N	9450	1/1	1.00	0.02	48,48,48,48	0
6	MG	N	9451	1/1	1.00	0.05	41,41,41,41	0
6	MG	C	9079	1/1	1.00	0.03	38,38,38,38	0
6	MG	N	9467	1/1	1.00	0.09	35,35,35,35	0
6	MG	N	9468	1/1	1.00	0.03	55,55,55,55	0
6	MG	N	9472	1/1	1.00	0.01	56,56,56,56	0
6	MG	N	9473	1/1	1.00	0.02	51,51,51,51	0

Continued on next page...

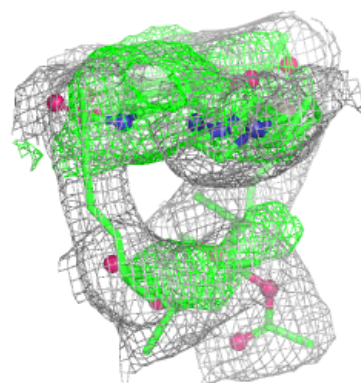
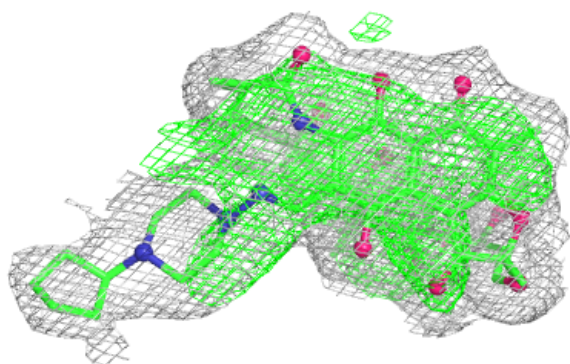
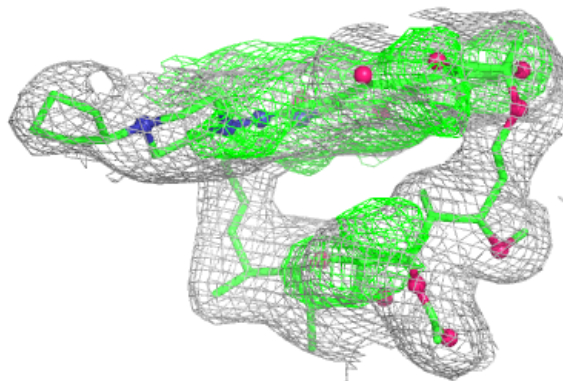
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	C	9086	1/1	1.00	0.02	39,39,39,39	0
6	MG	N	9484	1/1	1.00	0.02	37,37,37,37	0
6	MG	O	9197	1/1	1.00	0.04	57,57,57,57	0
6	MG	O	9198	1/1	1.00	0.01	36,36,36,36	0
6	MG	O	9254	1/1	1.00	0.02	39,39,39,39	0
6	MG	O	9266	1/1	1.00	0.01	47,47,47,47	0
6	MG	O	9296	1/1	1.00	0.03	42,42,42,42	0
6	MG	O	9420	1/1	1.00	0.05	51,51,51,51	0
6	MG	O	9439	1/1	1.00	0.01	56,56,56,56	0
6	MG	O	9483	1/1	1.00	0.03	63,63,63,63	0
6	MG	P	9189	1/1	1.00	0.05	49,49,49,49	0
6	MG	P	9202	1/1	1.00	0.02	49,49,49,49	0
6	MG	P	9209	1/1	1.00	0.02	46,46,46,46	0
6	MG	P	9216	1/1	1.00	0.01	48,48,48,48	0
6	MG	C	9090	1/1	1.00	0.03	47,47,47,47	0
6	MG	C	9092	1/1	1.00	0.03	44,44,44,44	0
6	MG	P	9235	1/1	1.00	0.01	40,40,40,40	0
6	MG	P	9255	1/1	1.00	0.04	34,34,34,34	0
6	MG	P	9258	1/1	1.00	0.01	51,51,51,51	0
6	MG	P	9277	1/1	1.00	0.03	41,41,41,41	0
6	MG	C	9107	1/1	1.00	0.01	42,42,42,42	0
6	MG	A	9078	1/1	1.00	0.04	66,66,66,66	0
6	MG	P	9285	1/1	1.00	0.02	56,56,56,56	0
6	MG	P	9297	1/1	1.00	0.01	45,45,45,45	0
6	MG	P	9315	1/1	1.00	0.03	35,35,35,35	0
6	MG	C	9114	1/1	1.00	0.04	30,30,30,30	0
6	MG	P	9399	1/1	1.00	0.01	34,34,34,34	0
6	MG	C	9115	1/1	1.00	0.01	36,36,36,36	0
6	MG	P	9446	1/1	1.00	0.01	34,34,34,34	0
6	MG	P	9482	1/1	1.00	0.02	48,48,48,48	0
7	RPT	C	8001	63/63	1.00	0.04	26,40,66,82	0
7	RPT	M	8002	63/63	1.00	0.03	33,45,55,57	0
8	ZN	D	7058	1/1	1.00	0.02	106,106,106,106	0
8	ZN	D	7112	1/1	1.00	0.03	80,80,80,80	0
8	ZN	N	7059	1/1	1.00	0.01	93,93,93,93	0
8	ZN	N	7113	1/1	1.00	0.01	84,84,84,84	0

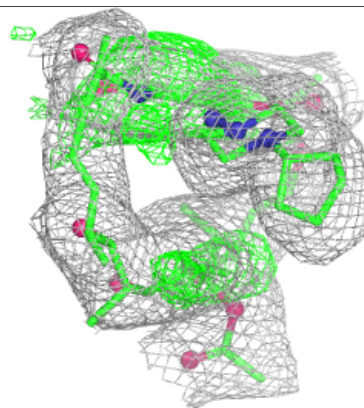
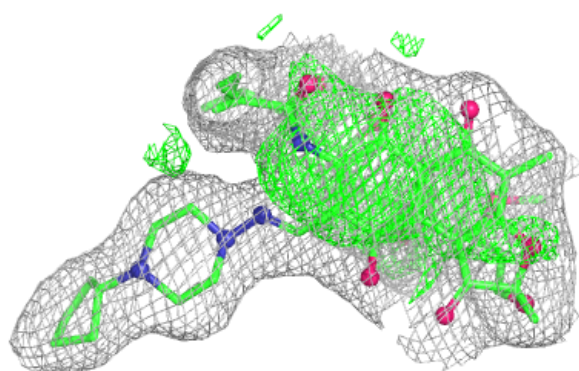
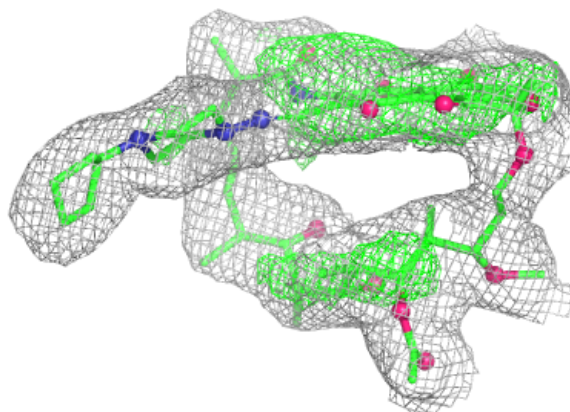
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around RPT C 8001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around RPT M 8002:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.