



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 01:35 PM UTC

PDB ID : 1WDM / pdb_00001wdm
Title : fatty acid beta-oxidation multienzyme complex from *Pseudomonas fragi*, form I (native3)
Authors : Ishikawa, M.; Tsuchiya, D.; Oyama, T.; Tsunaka, Y.; Morikawa, K.
Deposited on : 2004-05-17
Resolution : 3.80 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (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

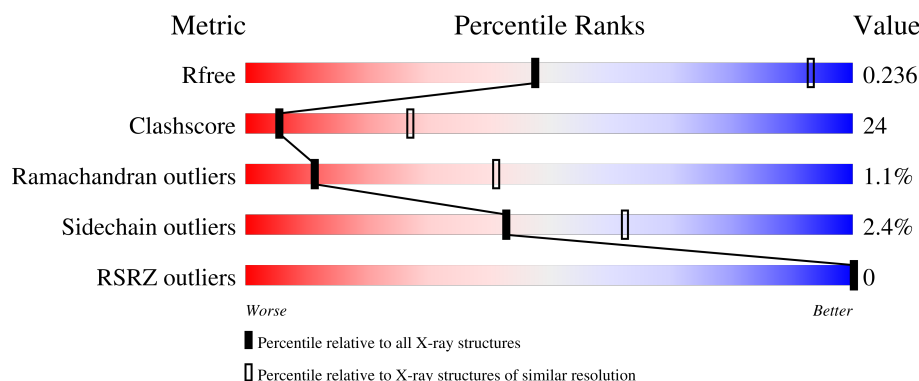
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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	715	 60% 38% ..
1	B	715	 58% 40% ..
2	C	390	 55% 43% .
2	D	390	 54% 43% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16541 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 Fatty oxidation complex alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	707	Total	C	N	O	S	0	0	0
			5257	3355	878	997	27			
1	B	710	Total	C	N	O	S	0	0	0
			5302	3383	889	1003	27			

- Molecule 2 is a protein called 3-ketoacyl-CoA thiolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	390	Total	C	N	O	S	0	0	0
			2871	1786	508	548	29			
2	D	390	Total	C	N	O	S	0	0	0
			2869	1785	510	545	29			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

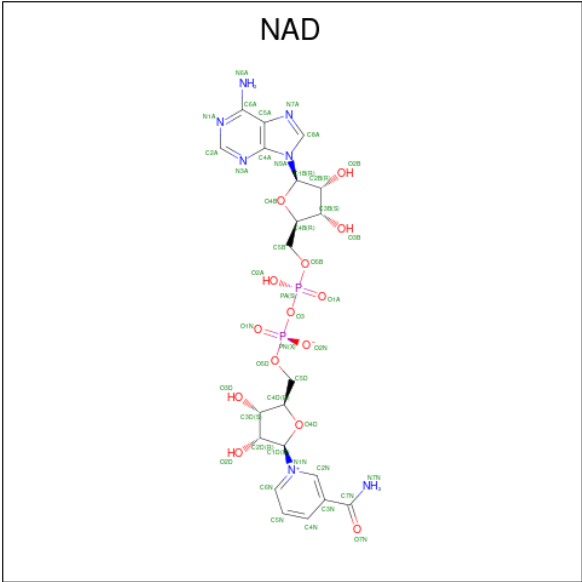
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is ACETYL COENZYME *A (CCD ID: ACO) (formula: C₂₃H₃₈N₇O₁₇P₃S).



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

- Molecule 5 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).

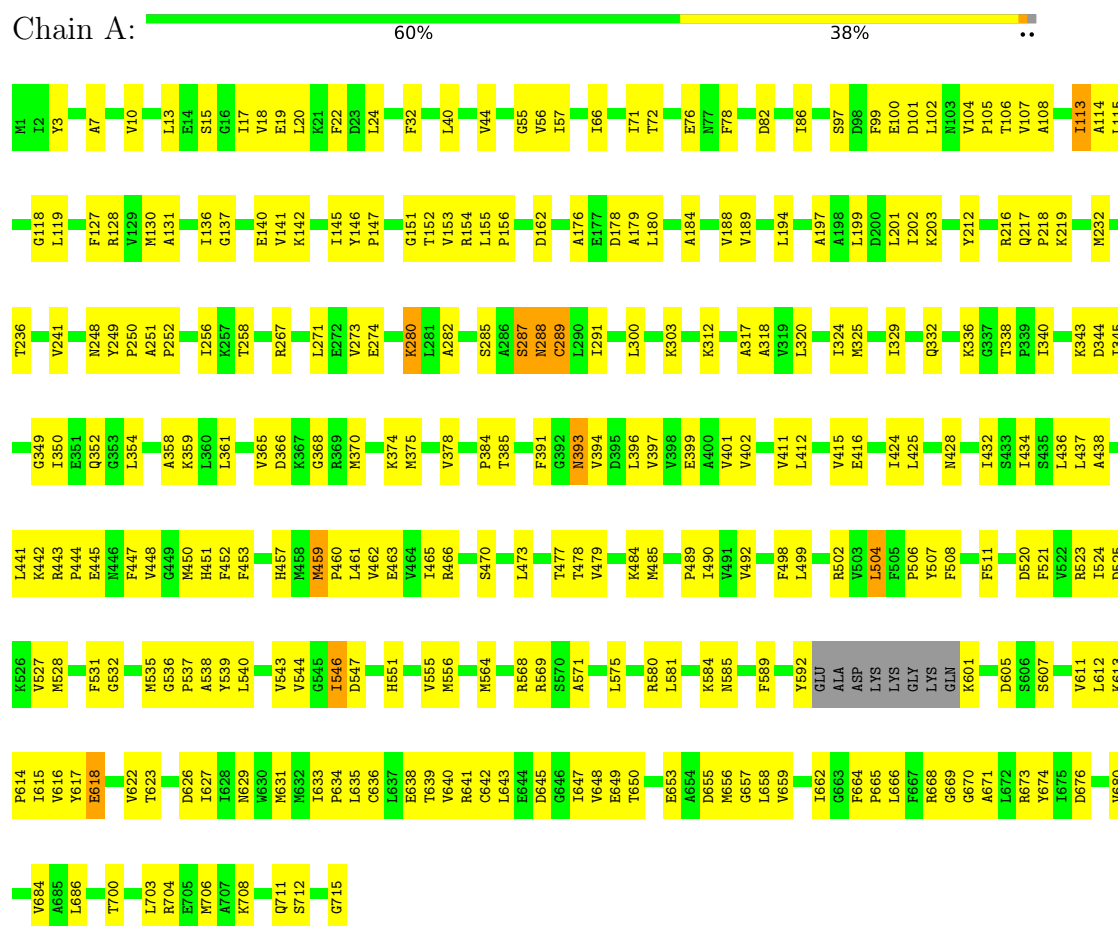


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
5	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

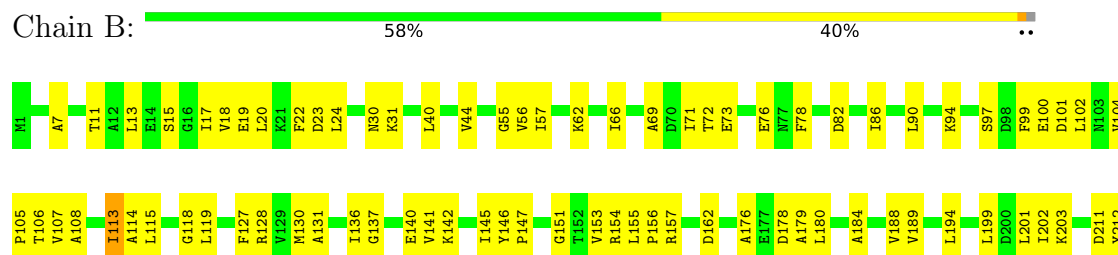
3 Residue-property plots

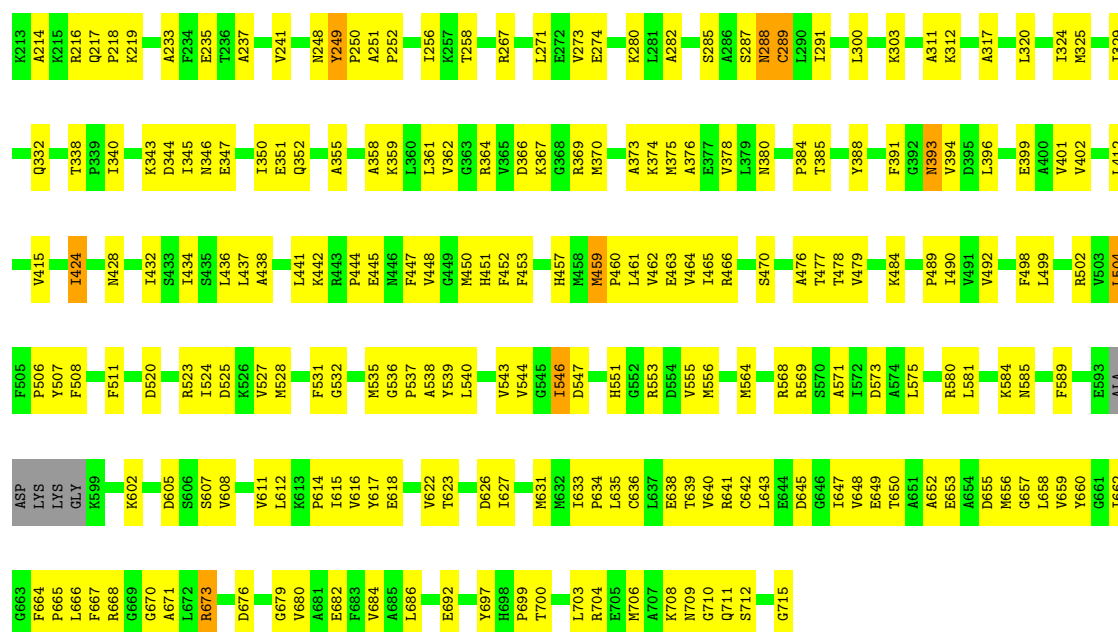
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Fatty oxidation complex alpha subunit



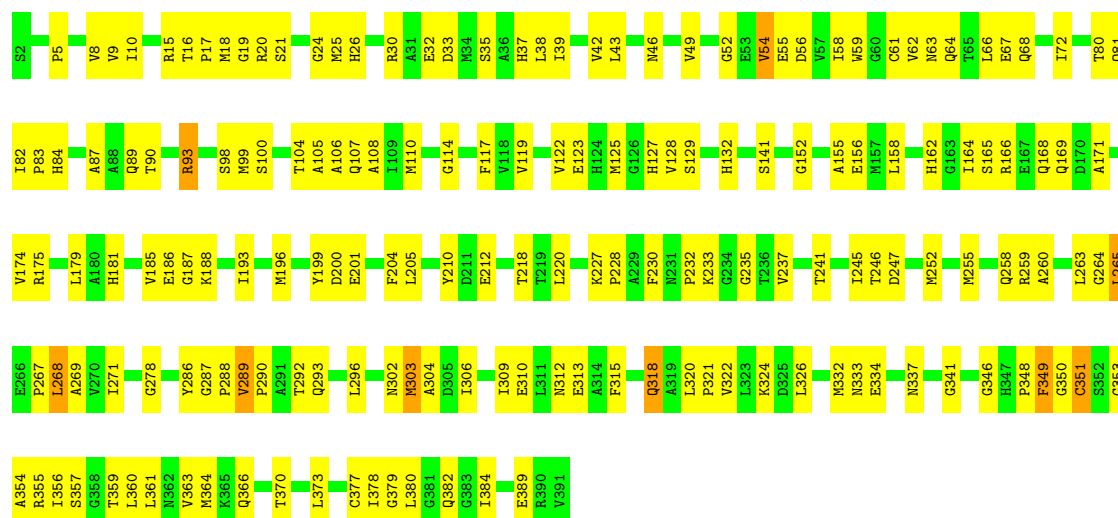
• Molecule 1: Fatty oxidation complex alpha subunit





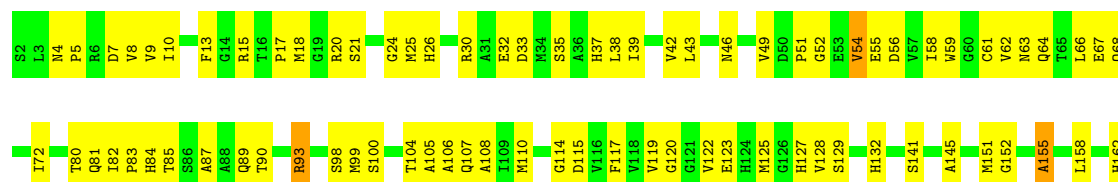
• Molecule 2: 3-ketoacyl-CoA thiolase

Chain C: 55% 43% .



• Molecule 2: 3-ketoacyl-CoA thiolase

Chain D: 54% 43% .



G163	L285	G350	G168	L286	G353	G169	L288	G354	L289	G355	G170	L270	A269	G356	G171	G278	V174	M284	G357	G276	E186	G285	G358	G286	G359	G287	G360	G288	G361	G289	G362	G290	G363	G291	G364	G292	G365	G293	G366	G294	G367	G295	G368	G296	G369	G297	G370	G298	G371	G299	G372	G300	G373	G301	G374	G302	G375	G303	G376	G304	G377	G305	G378	G306	G379	G307	G380	G308	G381	G309	G382	G310	G383	G311	G384	G312	G385	G313	G386	G314	G387	G315	G388	G316	G389	G317	G390	G318	G391	G319	G392	G320	G393	G321	G394	G322	G395	G323	G396	G324	G397	G325	G398	G326	G399	G327	G400	G328	G401	G329	G402	G330	G403	G331	G404	G332	G405	G333	G406	G334	G407	G335	G408	G336	G409	G337	G410	G338	G411	G339	G412	G340	G413	G341	G414	G342	G415	G343	G416	G344	G417	G345	G418	G346	G419	G347	G420	G348	G421	G349	G422	G350	G423	G351	G424	G352	G425	G353	G426	G354	G427	G355	G428	G356	G429	G357	G430	G358	G431	G359	G432	G360	G433	G361	G434	G362	G435	G363	G436	G364	G437	G365	G438	G366	G439	G367	G440	G368	G441	G369	G442	G370	G443	G371	G444	G372	G445	G373	G446	G374	G447	G375	G448	G376	G449	G377	G450	G378	G451	G379	G452	G380	G453	G381	G454	G382	G455	G383	G456	G384	G457	G385	G458	G386	G459	G387	G460	G388	G461	G389	G462	G390	G463	G391	G464	G392	G465	G393	G466	G394	G467	G395	G468	G396	G469	G397	G470	G398	G471	G399	G472	G400	G473	G401	G474	G402	G475	G403	G476	G404	G477	G405	G478	G406	G479	G407	G480	G408	G481	G409	G482	G410	G483	G411	G484	G412	G485	G413	G486	G414	G487	G415	G488	G416	G489	G417	G490	G418	G491	G419	G492	G420	G493	G421	G494	G422	G495	G423	G496	G424	G497	G425	G498	G426	G499	G427	G500	G428	G501	G429	G502	G430	G503	G431	G504	G432	G505	G433	G506	G434	G507	G435	G508	G436	G509	G437	G510	G438	G511	G439	G512	G440	G513	G441	G514	G442	G515	G443	G516	G444	G517	G445	G518	G446	G519	G447	G520	G448	G521	G449	G522	G450	G523	G451	G524	G452	G525	G453	G526	G454	G527	G455	G528	G456	G529	G457	G530	G458	G531	G459	G532	G460	G533	G461	G534	G462	G535	G463	G536	G464	G537	G465	G538	G466	G539	G467	G540	G468	G541	G469	G542	G470	G543	G471	G544	G472	G545	G473	G546	G474	G547	G475	G548	G476	G549	G477	G550	G478	G551	G479	G552	G480	G553	G481	G554	G482	G555	G483	G556	G484	G557	G485	G558	G486	G559	G487	G560	G488	G561	G489	G562	G490	G563	G491	G564	G492	G565	G493	G566	G494	G567	G495	G568	G496	G569	G497	G570	G498	G571	G499	G572	G500	G573	G501	G574	G502	G575	G503	G576	G504	G577	G505	G578	G506	G579	G507	G580	G508	G581	G509	G582	G510	G583	G511	G584	G512	G585	G513	G586	G514	G587	G515	G588	G516	G589	G517	G590	G518	G591	G519	G592	G520	G593	G521	G594	G522	G595	G523	G596	G524	G597	G525	G598	G526	G599	G527	G600	G528	G601	G529	G602	G530	G603	G531	G604	G532	G605	G533	G606	G534	G607	G535	G608	G536	G609	G537	G610	G538	G611	G539	G612	G540	G613	G541	G614	G542	G615	G543	G616	G544	G617	G545	G618	G546	G619	G547	G620	G548	G621	G549	G622	G550	G623	G551	G624	G552	G625	G553	G626	G554	G627	G555	G628	G556	G629	G557	G630	G558	G631	G559	G632	G560	G633	G561	G634	G562	G635	G563	G636	G564	G637	G565	G638	G566	G639	G567	G640	G568	G641	G569	G642	G570	G643	G571	G644	G572	G645	G573	G646	G574	G647	G575	G648	G576	G649	G577	G650	G578	G651	G579	G652	G580	G653	G581	G654	G582	G655	G583	G656	G584	G657	G585	G658	G586	G659	G587	G660	G588	G661	G589	G662	G590	G663	G591	G664	G592	G665	G593	G666	G594	G667	G595	G668	G596	G669	G597	G670	G598	G671	G599	G672	G600	G673	G601	G674	G602	G675	G603	G676	G604	G677	G605	G678	G606	G679	G607	G680	G608	G681	G609	G682	G610	G683	G611	G684	G612	G685	G613	G686	G614	G687	G615	G688	G616	G689	G617	G690	G618	G691	G619	G692	G620	G693	G621	G694	G622	G695	G623	G696	G624	G697	G625	G698	G626	G699	G627	G700	G628	G701	G629	G702	G630	G703	G631	G704	G632	G705	G633	G706	G634	G707	G635	G708	G636	G709	G637	G710	G638	G711	G639	G712	G640	G713	G641	G714	G642	G715	G643	G716	G644	G717	G645	G718	G646	G719	G647	G720	G648	G721	G649	G722	G650	G723	G651	G724	G652	G725	G653	G726	G654	G727	G655	G728	G656	G729	G657	G730	G658	G731	G659	G732	G660	G733	G661	G734	G662	G735	G663	G736	G664	G737	G665	G738	G666	G739	G667	G740	G668	G741	G669	G742	G670	G743	G671	G744	G672	G745	G673	G746	G674	G747	G675	G748	G676	G749	G677	G750	G678	G751	G679	G752	G680	G753	G681	G754	G682	G755	G683	G756	G684	G757	G685	G758	G686	G759	G687	G760	G688	G761	G689	G762	G690	G763	G691	G764	G692	G765	G693	G766	G694	G767	G695	G768	G696	G769	G697	G770	G698	G771	G699	G772	G700	G773	G701	G774	G702	G775	G703	G776	G704	G777	G705	G778	G706	G779	G707	G780	G708	G781	G709	G782	G710	G783	G711	G784	G712	G785	G713	G786	G714	G787	G715	G788	G716	G789	G717	G790	G718	G791	G719	G792	G720	G793	G721	G794	G722	G795	G723	G796	G724	G797	G725	G798	G726	G799	G727	G800	G728	G801	G729	G802	G730	G803	G731	G804	G732	G805	G733	G806	G734	G807	G735	G808	G736	G809	G737	G810	G738	G811	G739	G812	G740	G813	G741	G814	G742	G815	G743	G816	G744	G817	G745	G818	G746	G819	G747	G820	G748	G821	G749	G822	G750	G823	G751	G824	G752	G825	G753	G826	G754	G827	G755	G828	G756	G829	G757	G830	G758	G831	G759	G832	G760	G833	G761	G834	G762	G835	G763	G836	G764	G837	G765	G838	G766	G839	G767	G840	G768	G841	G769	G842	G770	G843	G771	G844	G772	G845	G773	G846	G774	G847	G775	G848	G776	G849	G777	G850	G778	G851	G779	G852	G780	G853	G781	G854	G782	G855	G783	G856	G784	G857	G785	G858	G786	G859	G787	G860	G788	G861	G789	G862	G790	G863	G791	G864	G792	G865	G793	G866	G794	G867	G795	G868	G796	G869	G797	G870	G798	G871	G799	G872	G800	G873	G801	G874	G802	G875	G803	G876	G804	G877	G805	G878	G806	G879	G807	G880	G808	G881	G809	G882	G810	G883	G811	G884	G812	G885	G813	G886	G814	G887	G815	G888	G816	G889	G817	G890	G818	G891	G819	G892	G820	G893	G821	G894	G822	G895	G823	G896	G824	G897	G825	G898	G826	G899	G827	G900	G828	G901	G829	G902	G830	G903	G831	G904	G832	G905	G833	G906	G834	G907	G835	G908	G836	G909	G837	G910	G838	G911	G839	G912	G840	G913	G841	G914	G842	G915	G843	G916	G844	G917	G845	G918	G846	G919	G847	G920	G848	G921	G849	G922	G850	G923	G851	G924	G852	G925	G853	G926	G854	G927	G855	G928	G856	G929	G857	G930	G858	G931	G859	G932	G860	G933	G861	G934	G862	G935	G863	G936	G864	G937	G865	G938	G866	G939	G867	G940	G868	G941	G869	G942	G870	G943	G871	G944	G872	G945	G873	G946	G874	G947	G875	G948	G876	G949	G877	G950	G878	G951	G879	G952	G880	G953	G881	G954	G882	G955	G883	G956	G884	G957	G885	G958	G886	G959	G887	G960	G888	G961	G889	G962	G890	G963	G891	G964	G892	G965	G893	G966	G894	G967	G895	G968	G896	G969	G897	G970	G898	G971	G899	G972	G900	G973	G901	G974	G902	G975	G903	G976	G904	G977	G905	G978	G906	G979	G907	G980	G908	G981	G909	G982	G910	G983	G911	G984	G912	G985	G913	G986	G914	G987	G915	G988	G916	G989	G917	G990	G918	G991	G919	G992	G920	G993	G921	G994	G922	G995	G923	G996	G924	G997	G925	G998	G926	G999	G927	G1000	G928	G1001	G929	G1002	G930	G1003	G931	G1004	G932	G1005	G933	G1006	G934	G1007	G935	G1008	G936	G1009	G937	G1010	G938	G1011	G939	G1012	G940	G1013	G941	G1014	G942	G1015	G943	G1016	G944	G1017	G945	G1018	G946	G1019	G947	G1020	G948	G1021	G949	G1022	G950	G1023	G951	G1024	G952	G1025	G953	G1026	G954	G1027	G955	G1028	G956	G1029	G957	G1030	G958	G1031	G959	G1032	G960	G1033	G961	G1034	G962	G1035	G963	G1036	G964	G1037	G965	G1038	G966	G1039	G967	G1040	G968	G1041	G969	G1042	G970	G1043	G971	G1044	G972	G1045	G973	G1046	G974	G1047	G975	G1048	G976	G1049	G977	G1050	G978	G1051	G979	G1052	G980	G1053	G981	G1054	G982	G1055	G983	G1056	G984	G1057	G985	G1058	G986	G1059	G987	G1060	G988	G1061	G989	G1062	G990	G1063	G991	G1064	G992	G1065	G993	G1066	G994	G1067	G995	G1068	G996	G1069	G997	G1070	G998	G1071	G999	G1072	G1000	G1073	G1001	G1074	G1002	G1075	G1003	G1076	G1004	G1077	G1005	G1078	G1006	G1079	G1007	G1080	G1008	G1081	G1009	G1082	G1010	G1083	G1011	G1084	G1012	G1085	G1013	G1086	G1014	G1087	G1015	G1088	G1016	G1089	G1017	G1090	G1018	G1091	G1019	G1092	G1020	G1093	G1021	G1094	G1022	G1095	G1023	G1096	G1024	G1097	G1025	G1098	G1026	G1099	G1027	G1100	G1028	G1101	G1029	G1102	G1030	G1103	G1031	G1104	G1032	G1105	G1033	G1106	G1034	G1107	G1035	G1108	G1036	G1109	G1037	G1110	G1038</
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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	181.45Å 95.46Å 161.32Å 90.00° 111.79° 90.00°	Depositor
Resolution (Å)	20.00 – 3.80 20.00 – 3.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-3.80) 97.7 (20.00-3.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.39 (at 3.82Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.214 , 0.262 0.194 , 0.236	Depositor DCC
R_{free} test set	1710 reflections (6.87%)	wwPDB-VP
Wilson B-factor (Å ²)	63.5	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 23.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16541	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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, NAD, ACO

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	0.35	0/5343	0.85	7/7237 (0.1%)
1	B	0.35	0/5388	0.84	6/7291 (0.1%)
2	C	0.38	0/2919	0.84	3/3944 (0.1%)
2	D	0.38	1/2917 (0.0%)	0.84	6/3941 (0.2%)
All	All	0.36	1/16567 (0.0%)	0.84	22/22413 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	289	VAL	CA-CB	5.07	1.57	1.54

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	TYR	CA-C-N	7.23	126.73	118.85
1	A	249	TYR	C-N-CA	7.23	126.73	118.85
1	B	249	TYR	CA-C-N	7.16	126.65	118.85
1	B	249	TYR	C-N-CA	7.16	126.65	118.85
2	C	93	ARG	N-CA-C	-6.19	102.87	110.61

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5257	0	5243	230	0
1	B	5302	0	5314	248	0
2	C	2871	0	2848	154	0
2	D	2869	0	2849	165	0
3	A	1	0	0	0	0
4	A	51	0	34	2	0
4	C	51	0	34	0	0
4	D	51	0	34	0	0
5	A	44	0	26	1	0
5	B	44	0	26	1	0
All	All	16541	0	16408	776	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 24.

The worst 5 of 776 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:525:ASP:HB2	1:A:536:GLY:HA3	1.34	1.09
1:B:525:ASP:HB2	1:B:536:GLY:HA3	1.36	1.07
2:D:17:PRO:HB2	2:D:25:MET:HE1	1.54	0.89
2:D:289:VAL:HG13	2:D:290:PRO:HD3	1.55	0.87
2:C:125:MET:HE2	2:C:348:PRO:HA	1.58	0.85

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	703/715 (98%)	632 (90%)	66 (9%)	5 (1%)	18 51
1	B	706/715 (99%)	628 (89%)	73 (10%)	5 (1%)	18 51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	388/390 (100%)	343 (88%)	37 (10%)	8 (2%)	5	31
2	D	388/390 (100%)	346 (89%)	35 (9%)	7 (2%)	6	33
All	All	2185/2210 (99%)	1949 (89%)	211 (10%)	25 (1%)	11	41

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	324	ILE
2	C	332	MET
2	C	349	PHE
2	D	332	MET
2	D	349	PHE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	532/562 (95%)	521 (98%)	11 (2%)	47	64
1	B	539/562 (96%)	526 (98%)	13 (2%)	43	62
2	C	302/307 (98%)	294 (97%)	8 (3%)	40	60
2	D	301/307 (98%)	293 (97%)	8 (3%)	39	59
All	All	1674/1738 (96%)	1634 (98%)	40 (2%)	43	62

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	318	GLN
2	D	265	LEU
2	C	324	LYS
2	D	115	ASP
2	D	318	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	362	ASN
2	D	231	ASN
2	D	4	ASN
2	D	132	HIS
2	D	362	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 [i](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	$\# Z > 2$
5	NAD	B	2001	-	46,48,48	1.50	5 (10%)	64,73,73	1.34	4 (6%)
4	ACO	A	1002	-	51,53,53	0.80	1 (1%)	73,79,79	0.66	1 (1%)
5	NAD	A	1001	-	46,48,48	1.49	4 (8%)	64,73,73	1.35	4 (6%)
4	ACO	C	3001	-	51,53,53	0.96	3 (5%)	73,79,79	0.69	1 (1%)
4	ACO	D	4001	-	51,53,53	0.71	0	73,79,79	0.65	1 (1%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAD	B	2001	-	-	5/30/62/62	0/5/5/5
4	ACO	A	1002	-	-	10/51/67/67	0/3/3/3
5	NAD	A	1001	-	-	8/30/62/62	0/5/5/5
4	ACO	C	3001	-	-	7/51/67/67	0/3/3/3
4	ACO	D	4001	-	-	13/51/67/67	0/3/3/3

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1001	NAD	C3N-C7N	5.40	1.58	1.50
5	B	2001	NAD	C3N-C7N	5.14	1.58	1.50
5	B	2001	NAD	C2N-N1N	4.74	1.40	1.35
5	A	1001	NAD	C2N-N1N	4.69	1.40	1.35
5	B	2001	NAD	C4N-C3N	3.58	1.44	1.39

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1001	NAD	C5N-C4N-C3N	-6.90	113.58	120.36
5	B	2001	NAD	C5N-C4N-C3N	-6.68	113.80	120.36
5	A	1001	NAD	C6N-C5N-C4N	5.51	127.39	119.45
5	B	2001	NAD	C6N-C5N-C4N	5.46	127.32	119.45
4	A	1002	ACO	C2P-S1P-C	3.89	120.15	101.42

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

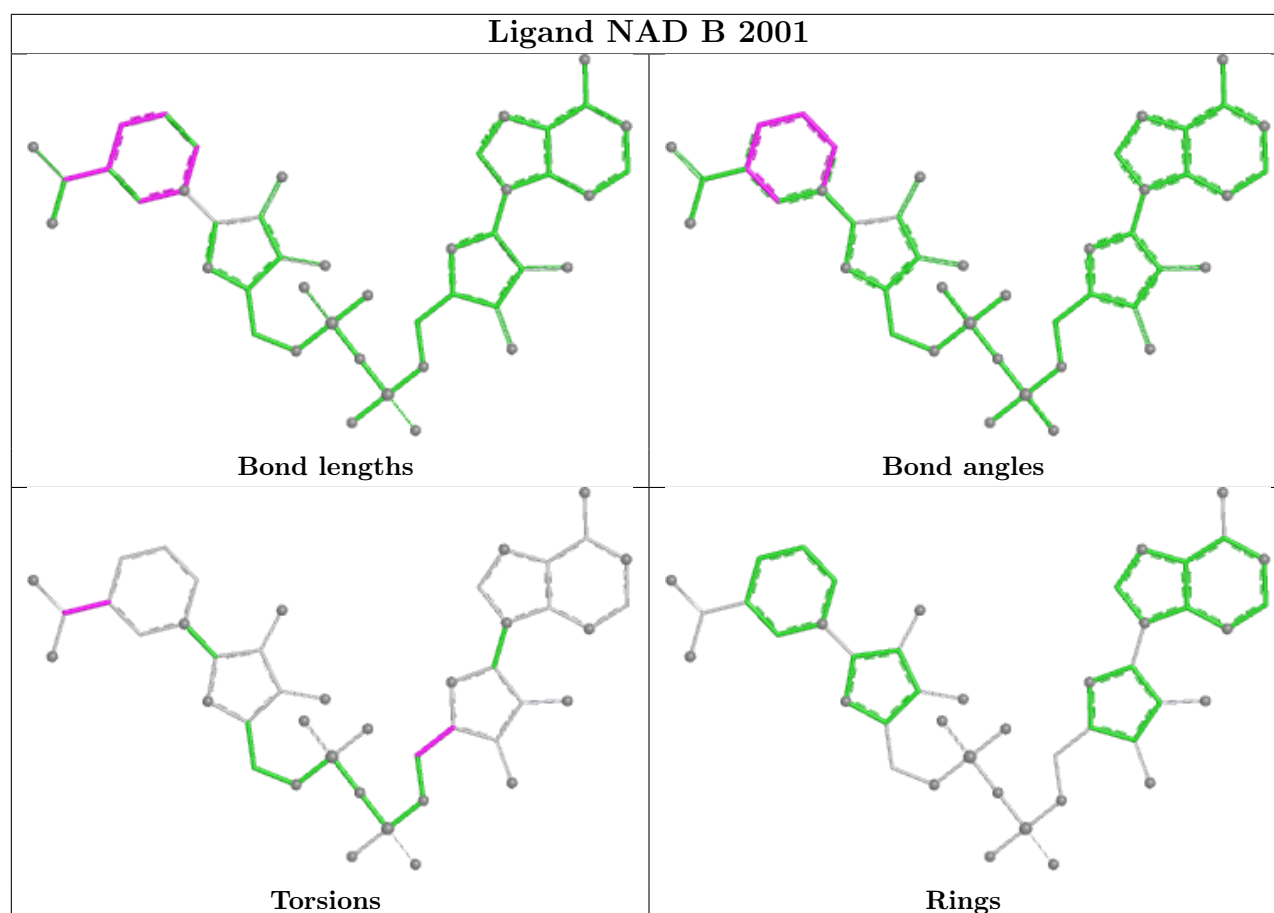
Mol	Chain	Res	Type	Atoms
4	A	1002	ACO	C5B-O5B-P1A-O2A
4	A	1002	ACO	C5B-O5B-P1A-O3A
4	A	1002	ACO	C3P-C2P-S1P-C
4	A	1002	ACO	O-C-S1P-C2P
4	A	1002	ACO	CH3-C-S1P-C2P

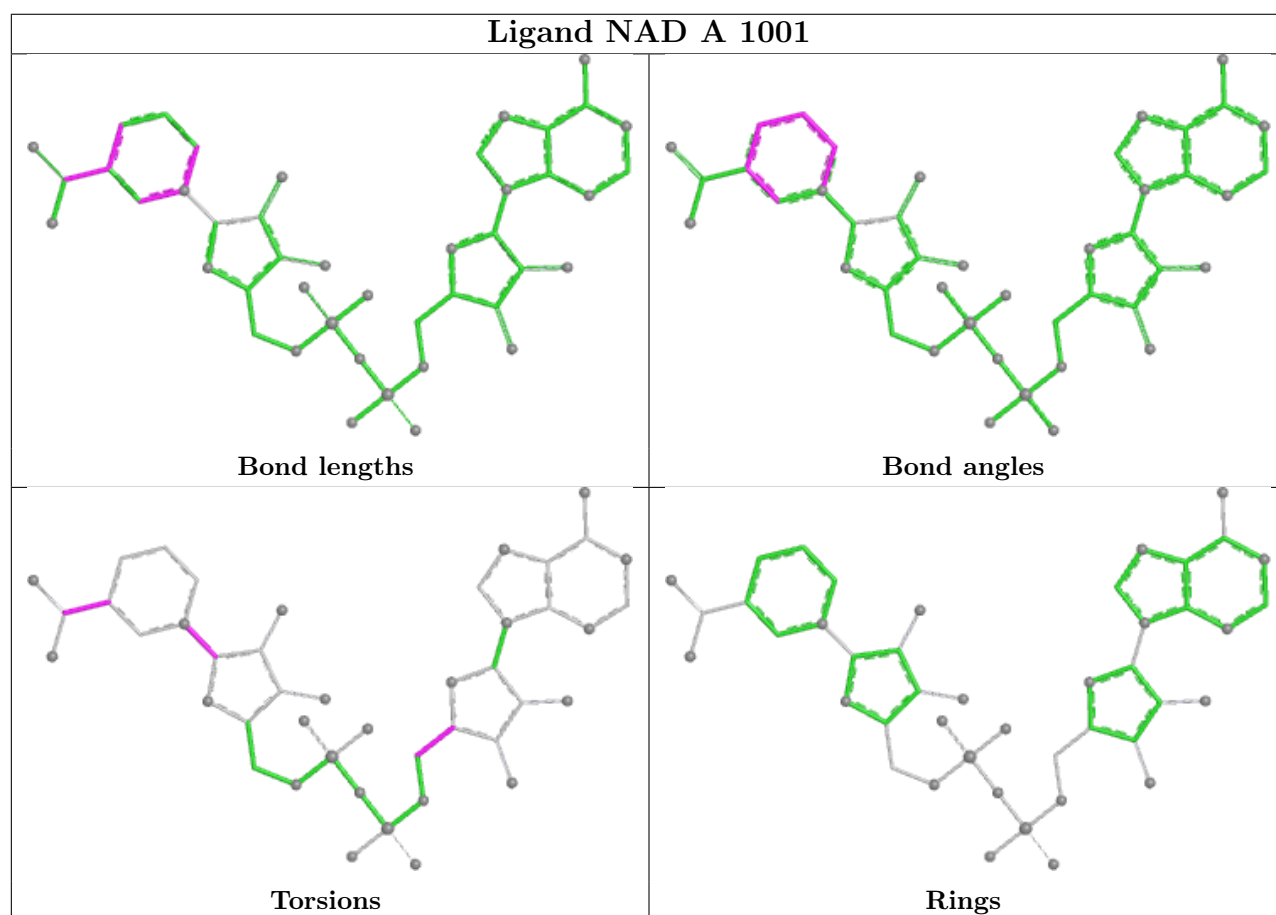
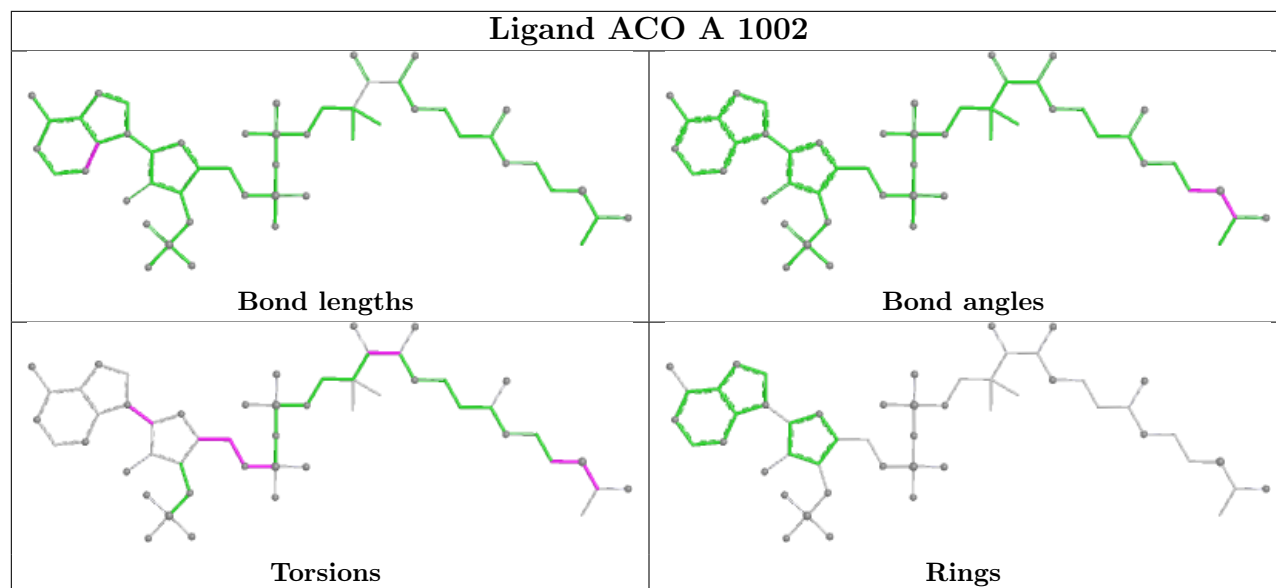
There are no ring outliers.

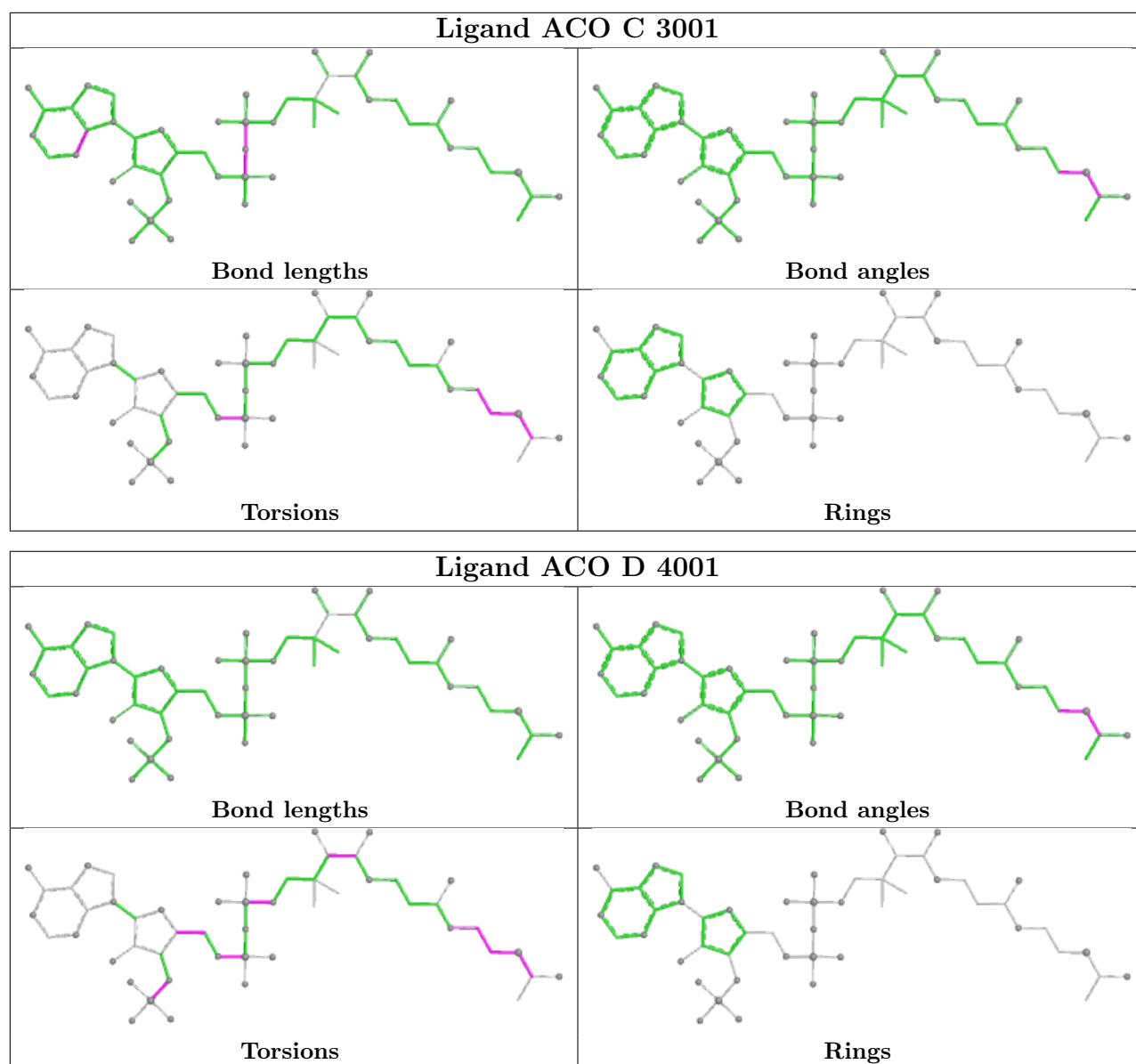
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	2001	NAD	1	0
4	A	1002	ACO	2	0
5	A	1001	NAD	1	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	707/715 (98%)	-0.34	0 100 100	1, 21, 67, 97	0
1	B	710/715 (99%)	-0.36	0 100 100	1, 22, 65, 99	0
2	C	390/390 (100%)	-0.44	0 100 100	1, 8, 45, 83	0
2	D	390/390 (100%)	-0.44	0 100 100	1, 11, 45, 97	0
All	All	2197/2210 (99%)	-0.38	0 100 100	1, 17, 61, 99	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
4	ACO	A	1002	51/51	0.67	0.26	160,160,160,160	0
4	ACO	C	3001	51/51	0.77	0.18	159,159,159,159	0
5	NAD	B	2001	44/44	0.84	0.15	123,123,123,123	0
4	ACO	D	4001	51/51	0.85	0.15	133,133,133,133	0

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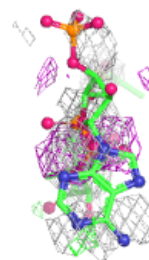
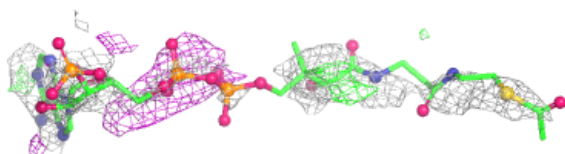
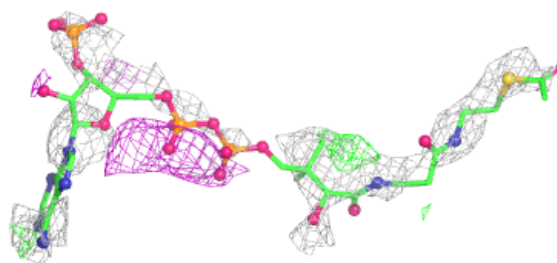
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAD	A	1001	44/44	0.88	0.13	98,98,98,98	0
3	ZN	A	716	1/1	1.00	0.03	5,5,5,5	0

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.

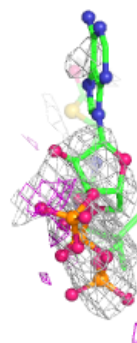
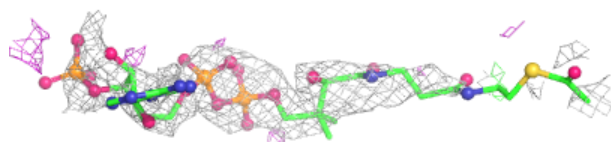
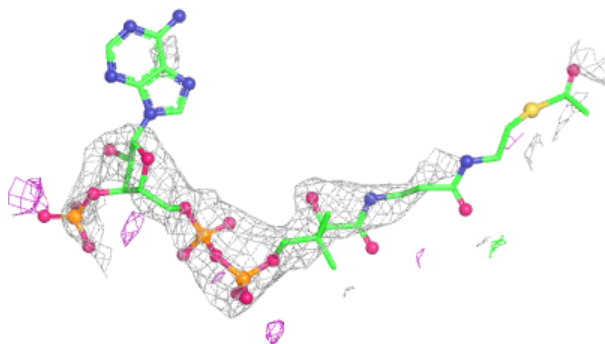
Electron density around ACO A 1002:

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

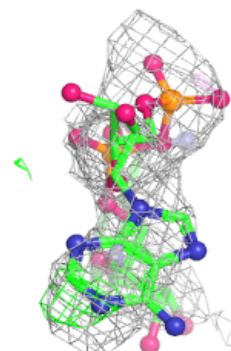
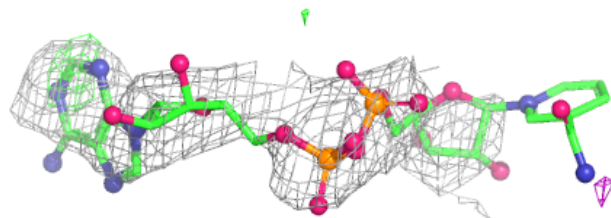
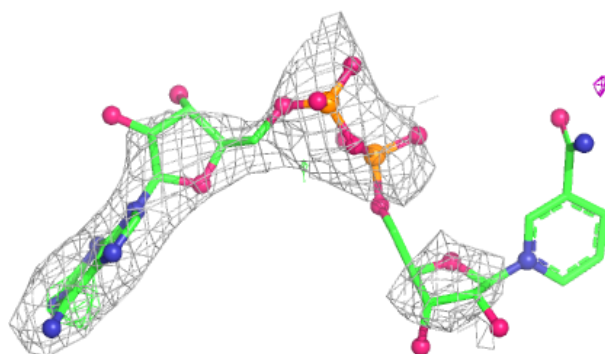


Electron density around ACO C 3001:

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

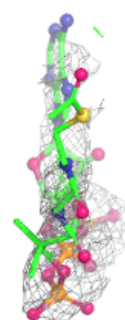
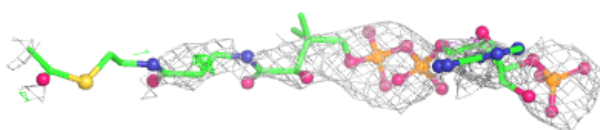
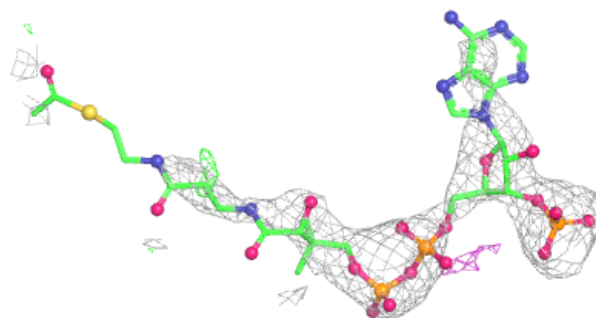
**Electron density around NAD B 2001:**

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

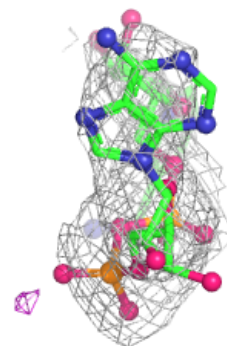
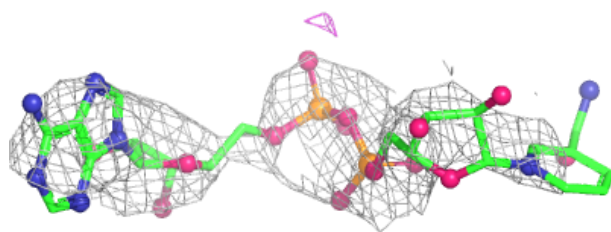
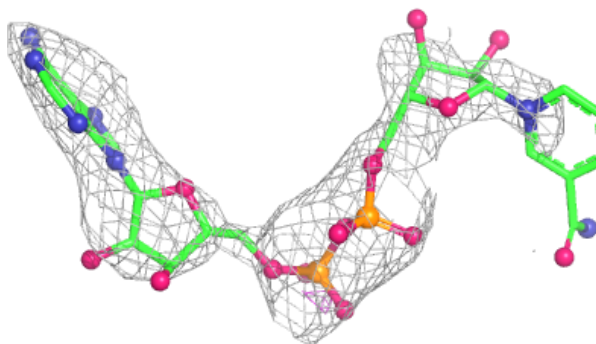


Electron density around ACO D 4001:

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

**Electron density around NAD A 1001:**

$2mF_o-DF_c$ (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.