



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:04 PM GMT

PDB ID : 1WDM
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

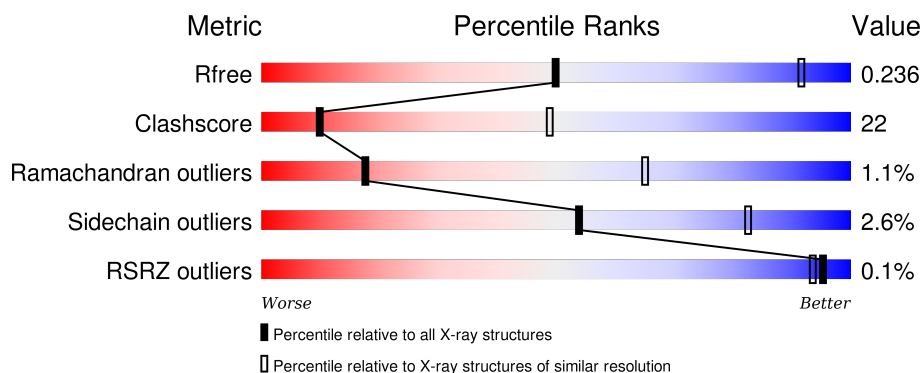
1 Overall quality at a glance

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}	91344	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	 61% 37% ..
1	B	715	 59% 39% ..
2	C	390	 56% 42% .
2	D	390	 55% 43% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ACO	A	1002	-	-	-	X
4	ACO	C	3001	-	-	-	X
4	ACO	D	4001	-	-	-	X
5	NAD	A	1001	-	-	-	X
5	NAD	B	2001	-	-	-	X

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 (three-letter code: ZN) (formula: Zn).

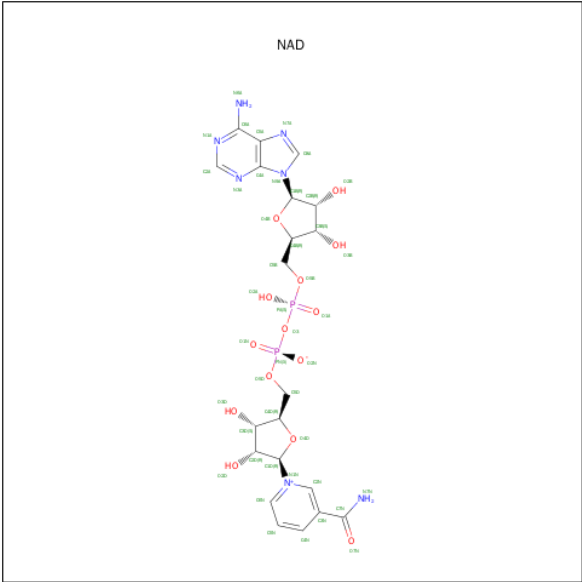
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is ACETYL COENZYME *A (three-letter code: 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 (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).

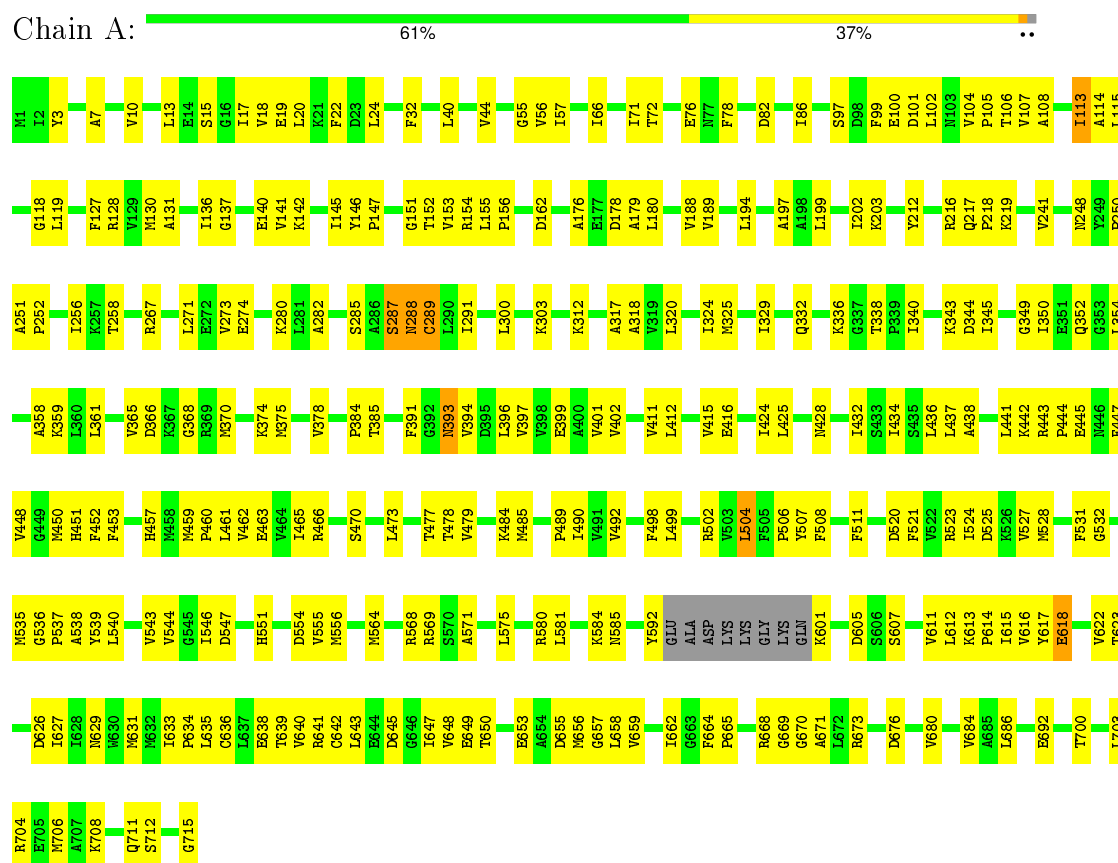


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
5	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

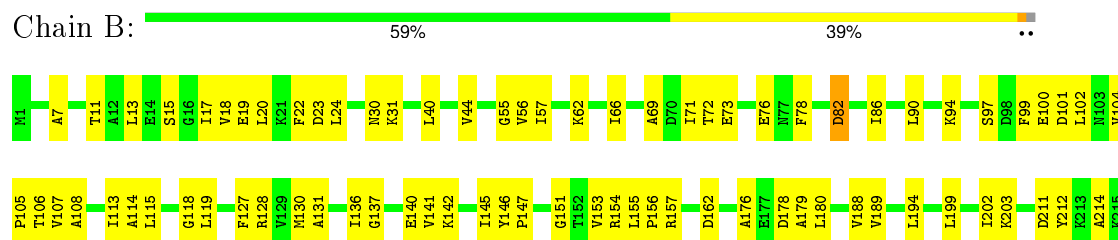
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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



G351	G352	G353	G354	G355	G356	G357	G358	G359	G360	G361	G362	G363	G364	G365	G366	G367	G368	G369	G370	G371	G372	G373	G374	G375	G376	G377	G378	G379	G380	G381	G382	G383	G384	G385	G386	G387	G388	G389	G390	G391	G392	G393	G394	G395	G396	G397	G398	G399	G400	G401	G402	G403	G404	G405	G406	G407	G408	G409	G410	G411	G412	G413	G414	G415	G416	G417	G418	G419	G420	G421	G422	G423	G424	G425	G426	G427	G428	G429	G430	G431	G432	G433	G434	G435	G436	G437	G438	G439	G440	G441	G442	G443	G444	G445	G446	G447	G448	G449	G450	G451	G452	G453	G454	G455	G456	G457	G458	G459	G460	G461	G462	G463	G464	G465	G466	G467	G468	G469	G470	G471	G472	G473	G474	G475	G476	G477	G478	G479	G480	G481	G482	G483	G484	G485	G486	G487	G488	G489	G490	G491	G492	G493	G494	G495	G496	G497	G498	G499	G500	G501	G502	G503	G504	G505	G506	G507	G508	G509	G510	G511	G512	G513	G514	G515	G516	G517	G518	G519	G520	G521	G522	G523	G524	G525	G526	G527	G528	G529	G530	G531	G532	G533	G534	G535	G536	G537	G538	G539	G540	G541	G542	G543	G544	G545	G546	G547	G548	G549	G550	G551	G552	G553	G554	G555	G556	G557	G558	G559	G560	G561	G562	G563	G564	G565	G566	G567	G568	G569	G570	G571	G572	G573	G574	G575	G576	G577	G578	G579	G580	G581	G582	G583	G584	G585	G586	G587	G588	G589	G590	G591	G592	G593	G594	G595	G596	G597	G598	G599	G600	G601	G602	G603	G604	G605	G606	G607	G608	G609	G610	G611	G612	G613	G614	G615	G616	G617	G618	G619	G620	G621	G622	G623	G624	G625	G626	G627	G628	G629	G630	G631	G632	G633	G634	G635	G636	G637	G638	G639	G640	G641	G642	G643	G644	G645	G646	G647	G648	G649	G650	G651	G652	G653	G654	G655	G656	G657	G658	G659	G660	G661	G662	G663	G664	G665	G666	G667	G668	G669	G670	G671	G672	G673	G674	G675	G676	G677	G678	G679	G680	G681	G682	G683	G684	G685	G686	G687	G688	G689	G690	G691	G692	G693	G694	G695	G696	G697	G698	G699	G700	G701	G702	G703	G704	G705	G706	G707	G708	G709	G710	G711	G712	G713	G714	G715	G716	G717	G718	G719	G720	G721	G722	G723	G724	G725	G726	G727	G728	G729	G730	G731	G732	G733	G734	G735	G736	G737	G738	G739	G740	G741	G742	G743	G744	G745	G746	G747	G748	G749	G750	G751	G752	G753	G754	G755	G756	G757	G758	G759	G760	G761	G762	G763	G764	G765	G766	G767	G768	G769	G770	G771	G772	G773	G774	G775	G776	G777	G778	G779	G780	G781	G782	G783	G784	G785	G786	G787	G788	G789	G790	G791	G792	G793	G794	G795	G796	G797	G798	G799	G800	G801	G802	G803	G804	G805	G806	G807	G808	G809	G810	G811	G812	G813	G814	G815	G816	G817	G818	G819	G820	G821	G822	G823	G824	G825	G826	G827	G828	G829	G830	G831	G832	G833	G834	G835	G836	G837	G838	G839	G840	G841	G842	G843	G844	G845	G846	G847	G848	G849	G850	G851	G852	G853	G854	G855	G856	G857	G858	G859	G860	G861	G862	G863	G864	G865	G866	G867	G868	G869	G870	G871	G872	G873	G874	G875	G876	G877	G878	G879	G880	G881	G882	G883	G884	G885	G886	G887	G888	G889	G890	G891	G892	G893	G894	G895	G896	G897	G898	G899	G900	G901	G902	G903	G904	G905	G906	G907	G908	G909	G910	G911	G912	G913	G914	G915	G916	G917	G918	G919	G920	G921	G922	G923	G924	G925	G926	G927	G928	G929	G930	G931	G932	G933	G934	G935	G936	G937	G938	G939	G940	G941	G942	G943	G944	G945	G946	G947	G948	G949	G950	G951	G952	G953	G954	G955	G956	G957	G958	G959	G960	G961	G962	G963	G964	G965	G966	G967	G968	G969	G970	G971	G972	G973	G974	G975	G976	G977	G978	G979	G980	G981	G982	G983	G984	G985	G986	G987	G988	G989	G990	G991	G992	G993	G994	G995	G996	G997	G998	G999
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

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 19.99 – 3.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-3.80) 98.4 (19.99-3.80)	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	1709 reflections (6.86%)	DCC
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 , 21.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 24902 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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, ACO, NAD

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	0.29	0/5343	0.51	0/7237
1	B	0.28	0/5388	0.51	0/7291
2	C	0.29	0/2919	0.52	0/3944
2	D	0.30	0/2917	0.52	0/3941
All	All	0.29	0/16567	0.51	0/22413

There are no bond length outliers.

There are no bond angle outliers.

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	217	0
1	B	5302	0	5314	232	0
2	C	2871	0	2848	146	0
2	D	2869	0	2849	152	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	44	0	26	1	0
All	All	16541	0	16408	727	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 22.

The worst 5 of 727 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:289:VAL:HG13	2:D:290:PRO:HD3	1.55	0.87
2:D:98:SER:HB3	2:D:353:GLY:HA3	1.59	0.85
1:B:130:MET:HE1	1:B:176:ALA:HA	1.57	0.84

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%)	26	72
1	B	706/715 (99%)	628 (89%)	73 (10%)	5 (1%)	26	72
2	C	388/390 (100%)	343 (88%)	37 (10%)	8 (2%)	9	53
2	D	388/390 (100%)	346 (89%)	35 (9%)	7 (2%)	11	55
All	All	2185/2210 (99%)	1949 (89%)	211 (10%)	25 (1%)	17	65

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	324	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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%)	61	86
1	B	539/562 (96%)	527 (98%)	12 (2%)	60	85
2	C	302/307 (98%)	292 (97%)	10 (3%)	45	79
2	D	301/307 (98%)	291 (97%)	10 (3%)	45	79
All	All	1674/1738 (96%)	1631 (97%)	43 (3%)	54	82

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	554	ASP
2	C	158	LEU
2	D	318	GLN
1	B	673	ARG
1	B	676	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	409	GLN
2	C	46	ASN
2	D	293	GLN
1	B	428	ASN
1	B	629	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	A	1001	-	38,48,48	1.34	3 (7%)	47,73,73	1.74	8 (17%)
4	ACO	A	1002	-	43,53,53	0.79	1 (2%)	55,79,79	1.00	4 (7%)
5	NAD	B	2001	-	38,48,48	1.31	3 (7%)	47,73,73	1.76	9 (19%)
4	ACO	C	3001	-	43,53,53	0.82	0	55,79,79	1.05	4 (7%)
4	ACO	D	4001	-	43,53,53	0.75	0	55,79,79	0.93	3 (5%)

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	A	1001	-	-	0/22/62/62	0/5/5/5
4	ACO	A	1002	-	-	2/47/67/67	0/3/3/3
5	NAD	B	2001	-	-	0/22/62/62	0/5/5/5
4	ACO	C	3001	-	-	2/47/67/67	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ACO	D	4001	-	-	2/47/67/67	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1002	ACO	C2A-N3A	2.13	1.36	1.32
5	A	1001	NAD	C6N-N1N	2.90	1.43	1.35
5	B	2001	NAD	C6N-N1N	2.98	1.43	1.35
5	A	1001	NAD	C4N-C3N	3.20	1.44	1.39
5	B	2001	NAD	C4N-C3N	3.25	1.44	1.39

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1001	NAD	C5N-C4N-C3N	-5.37	113.58	120.33
5	B	2001	NAD	C5N-C4N-C3N	-5.20	113.80	120.33
4	A	1002	ACO	P2A-O3A-P1A	-4.42	120.33	132.73
4	C	3001	ACO	P2A-O3A-P1A	-4.41	120.35	132.73
5	A	1001	NAD	PN-O3-PA	-4.03	121.40	132.73

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1002	ACO	CH3-C-S1P-C2P
4	A	1002	ACO	O-C-S1P-C2P
4	D	4001	ACO	CH3-C-S1P-C2P
4	C	3001	ACO	CH3-C-S1P-C2P
4	D	4001	ACO	O-C-S1P-C2P

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1001	NAD	1	0
4	A	1002	ACO	2	0
5	B	2001	NAD	1	0

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%)	-0.65	0 100 100	1, 21, 67, 97	0
1	B	710/715 (99%)	-0.62	2 (0%) 94 89	1, 22, 65, 99	0
2	C	390/390 (100%)	-0.71	0 100 100	1, 8, 45, 83	0
2	D	390/390 (100%)	-0.69	1 (0%) 94 89	1, 11, 45, 97	0
All	All	2197/2210 (99%)	-0.66	3 (0%) 95 93	1, 17, 61, 99	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	600	GLN	2.2
1	B	567	ASP	2.1
2	D	2	SER	2.0

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
4	ACO	A	1002	51/51	0.57	0.57	8.19	160,160,160,160	0
4	ACO	C	3001	51/51	0.76	0.44	5.74	159,159,159,159	0
4	ACO	D	4001	51/51	0.84	0.39	4.10	133,133,133,133	0
5	NAD	B	2001	44/44	0.81	0.35	2.93	123,123,123,123	0
5	NAD	A	1001	44/44	0.87	0.32	2.28	98,98,98,98	0
3	ZN	A	716	1/1	0.99	0.04	-4.35	5,5,5,5	0

6.5 Other polymers [i](#)

There are no such residues in this entry.