



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:22 PM GMT

PDB ID : 1OHF
Title : THE REFINED STRUCTURE OF NUDAURELIA CAPENSIS OMEGA VIRUS
Authors : Helgstrand, C.; Munshi, S.; Johnson, J.E.; Liljas, L.
Deposited on : 2003-05-26
Resolution : 2.80 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 : **FAILED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

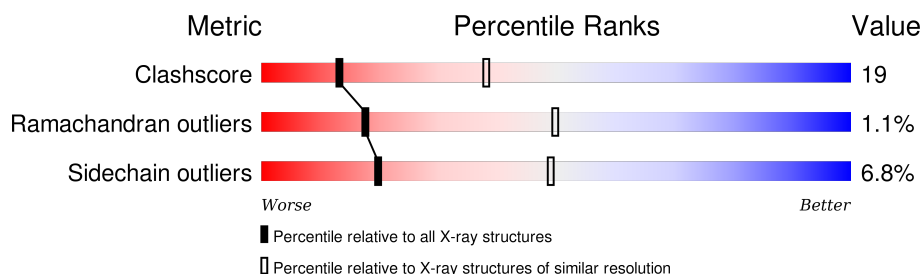
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	644	
1	B	644	
1	C	644	
1	D	644	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17851 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 NUDAURELIA CAPENSIS OMEGA VIRUS CAPSID PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	539	Total	C	N	O	S	0	0	0
			4134	2632	683	806	13			
1	B	547	Total	C	N	O	S	0	0	0
			4187	2659	694	821	13			
1	C	590	Total	C	N	O	S	0	0	0
			4519	2861	770	874	14			
1	D	587	Total	C	N	O	S	0	0	0
			4491	2846	761	870	14			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	235	VAL	CYS	SEE REMARK 999	UNP Q90063
A	283	VAL	GLU	SEE REMARK 999	UNP Q90063
B	235	VAL	CYS	SEE REMARK 999	UNP Q90063
B	283	VAL	GLU	SEE REMARK 999	UNP Q90063
C	235	VAL	CYS	SEE REMARK 999	UNP Q90063
C	283	VAL	GLU	SEE REMARK 999	UNP Q90063
D	235	VAL	CYS	SEE REMARK 999	UNP Q90063
D	283	VAL	GLU	SEE REMARK 999	UNP Q90063

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is water.

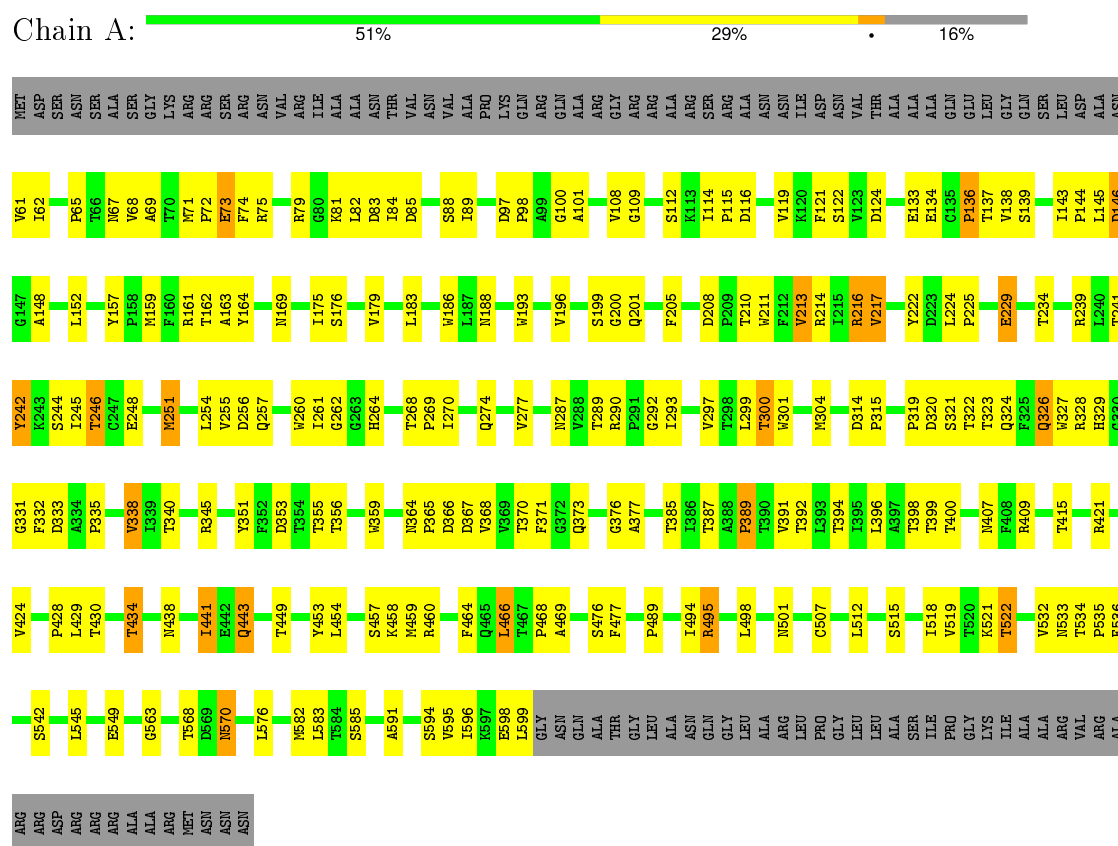
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	97	Total 97	O 97	0	0
3	B	127	Total 127	O 127	0	0
3	C	148	Total 148	O 148	0	0
3	D	144	Total 144	O 144	0	0

3 Residue-property plots

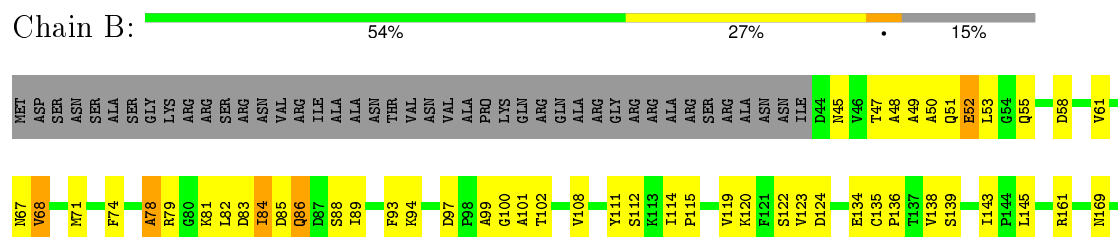
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

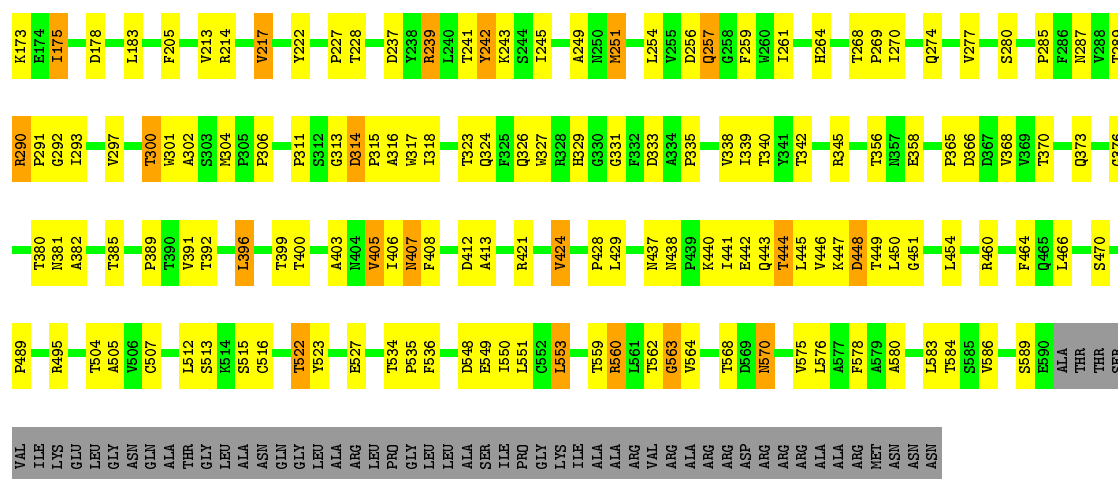
Note EDS failed to run properly.

• Molecule 1: NUDAURELIA CAPENSIS OMEGA VIRUS CAPSID PROTEIN



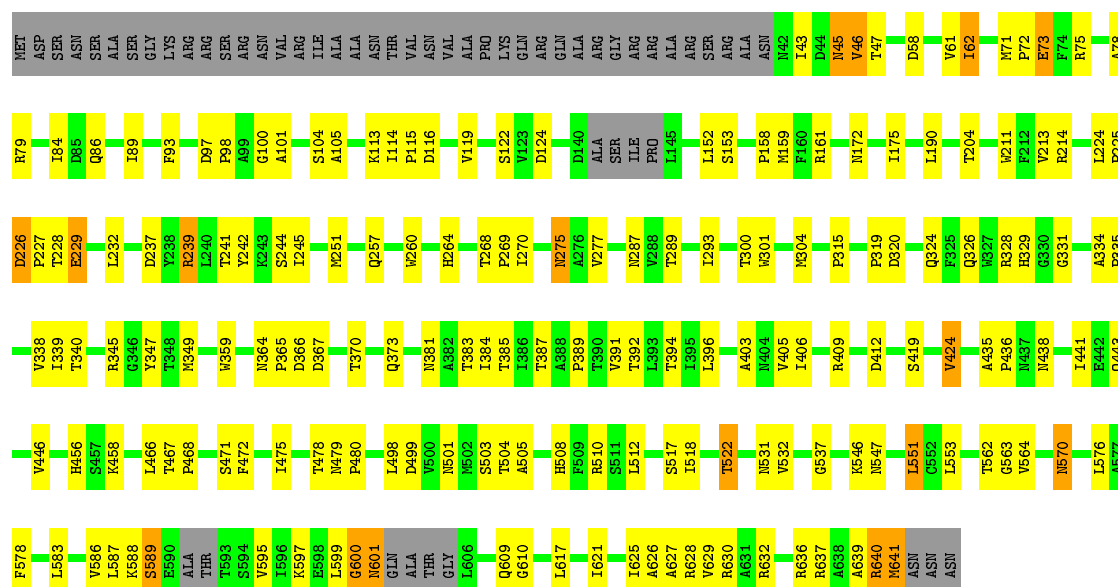
• Molecule 1: NUDAURELIA CAPENSIS OMEGA VIRUS CAPSID PROTEIN





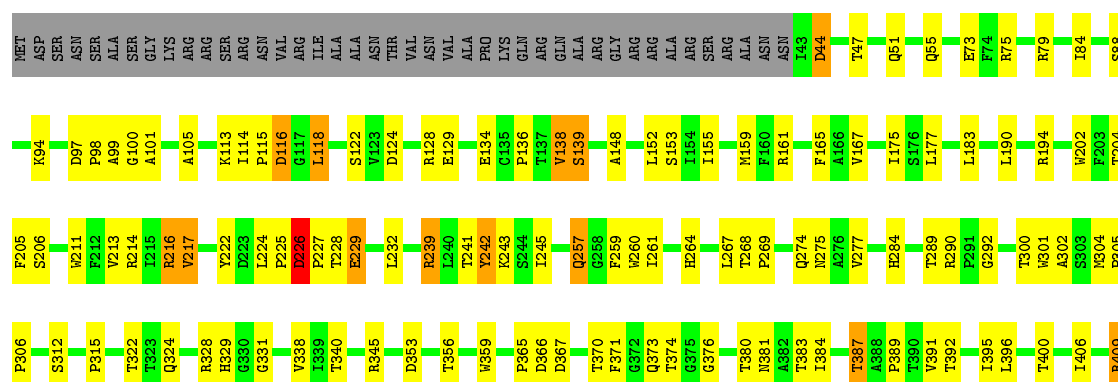
• Molecule 1: NUDAURELIA CAPENSIS OMEGA VIRUS CAPSID PROTEIN

Chain C: 64% 25% 8%



• Molecule 1: NUDAURELIA CAPENSIS OMEGA VIRUS CAPSID PROTEIN

Chain D: 62% 24% 9%



ASN	TS22	E414	TS23	E415	TS24	E416	TS25	E417	TS26	E418	TS27	E419	TS28	E420	TS29	E421	TS30	E422	TS31	E423	TS32	E424	TS33	E425	TS34	E426	TS35	E427	TS36	E428	TS37	E429	TS38	E430	TS39	E431	TS40	E432	TS41	E433	TS42	E434	TS43	E435	TS44	E436	TS45	E437	TS46	E438	TS47	E439	TS48	E440	TS49	E441	TS50	E442	TS51	E443	TS52	E444	TS53	E445	TS54	E446	TS55	E447	TS56	E448	TS57	E449	TS58	E450	TS59	E451	TS60	E452	TS61	E453	TS62	E454	TS63	E455	TS64	E456	TS65	E457	TS66	E458	TS67	E459	TS68	E460	TS69	E461	TS70	E462	TS71	E463	TS72	E464	TS73	E465	TS74	E466	TS75	E467	TS76	E468	TS77	E469	TS78	E470	TS79	E471	TS80	E472	TS81	E473	TS82	E474	TS83	E475	TS84	E476	TS85	E477	TS86	E478	TS87	E479	TS88	E480	TS89	E481	TS90	E482	TS91	E483	TS92	E484	TS93	E485	TS94	E486	TS95	E487	TS96	E488	TS97	E489	TS98	E490	TS99	E491	TS100	E492	TS101	E493	TS102	E494	TS103	E495	TS104	E496	TS105	E497	TS106	E498	TS107	E499	TS108	E500	TS109	E501	TS110	E502	TS111	E503	TS112	E504	TS113	E505	TS114	E506	TS115	E507	TS116	E508	TS117	E509	TS118	E510	TS119	E511	TS120	E512	TS121	E513	TS122	E514	TS123	E515	TS124	E516	TS125	E517	TS126	E518	TS127	E519	TS128	E520	TS129	E521	TS130	E522	TS131	E523	TS132	E524	TS133	E525	TS134	E526	TS135	E527	TS136	E528	TS137	E529	TS138	E530	TS139	E531	TS140	E532	TS141	E533	TS142	E534	TS143	E535	TS144	E536	TS145	E537	TS146	E538	TS147	E539	TS148	E540	TS149	E541	TS150	E542	TS151	E543	TS152	E544	TS153	E545	TS154	E546	TS155	E547	TS156	E548	TS157	E549	TS158	E550	TS159	E551	TS160	E552	TS161	E553	TS162	E554	TS163	E555	TS164	E556	TS165	E557	TS166	E558	TS167	E559	TS168	E560	TS169	E561	TS170	E562	TS171	E563	TS172	E564	TS173	E565	TS174	E566	TS175	E567	TS176	E568	TS177	E569	TS178	E570	TS179	E571	TS180	E572	TS181	E573	TS182	E574	TS183	E575	TS184	E576	TS185	E577	TS186	E578	TS187	E579	TS188	E580	TS189	E581	TS190	E582	TS191	E583	TS192	E584	TS193	E585	TS194	E586	TS195	E587	TS196	E588	TS197	E589	TS198	E590	TS199	E591	TS200	E592	TS201	E593	TS202	E594	TS203	E595	TS204	E596	TS205	E597	TS206	E598	TS207	E599	TS208	E600	TS209	E601	TS210	E602	TS211	E603	TS212	E604	TS213	E605	TS214	E606	TS215	E607	TS216	E608	TS217	E609	TS218	E610	TS219	E611	TS220	E612	TS221	E613	TS222	E614	TS223	E615	TS224	E616	TS225	E617	TS226	E618	TS227	E619	TS228	E620	TS229	E621	TS230	E622	TS231	E623	TS232	E624	TS233	E625	TS234	E626	TS235	E627	TS236	E628	TS237	E629	TS238	E630	TS239	E631	TS240	E632	TS241	E633	TS242	E634	TS243	E635	TS244	E636	TS245	E637	TS246	E638	TS247	E639	TS248	E640	TS249	E641	TS250	E642	TS251	E643	TS252	E644	TS253	E645	TS254	E646	TS255	E647	TS256	E648	TS257	E649	TS258	E650	TS259	E651	TS260	E652	TS261	E653	TS262	E654	TS263	E655	TS264	E656	TS265	E657	TS266	E658	TS267	E659	TS268	E660	TS269	E661	TS270	E662	TS271	E663	TS272	E664	TS273	E665	TS274	E666	TS275	E667	TS276	E668	TS277	E669	TS278	E670	TS279	E671	TS280	E672	TS281	E673	TS282	E674	TS283	E675	TS284	E676	TS285	E677	TS286	E678	TS287	E679	TS288	E680	TS289	E681	TS290	E682	TS291	E683	TS292	E684	TS293	E685	TS294	E686	TS295	E687	TS296	E688	TS297	E689	TS298	E690	TS299	E691	TS300	E692	TS301	E693	TS302	E694	TS303	E695	TS304	E696	TS305	E697	TS306	E698	TS307	E699	TS308	E700	TS309	E701	TS310	E702	TS311	E703	TS312	E704	TS313	E705	TS314	E706	TS315	E707	TS316	E708	TS317	E709	TS318	E710	TS319	E711	TS320	E712	TS321	E713	TS322	E714	TS323	E715	TS324	E716	TS325	E717	TS326	E718	TS327	E719	TS328	E720	TS329	E721	TS330	E722	TS331	E723	TS332	E724	TS333	E725	TS334	E726	TS335	E727	TS336	E728	TS337	E729	TS338	E730	TS339	E731	TS340	E732	TS341	E733	TS342	E734	TS343	E735	TS344	E736	TS345	E737	TS346	E738	TS347	E739	TS348	E740	TS349	E741	TS350	E742	TS351	E743	TS352	E744	TS353	E745	TS354	E746	TS355	E747	TS356	E748	TS357	E749	TS358	E750	TS359	E751	TS360	E752	TS361	E753	TS362	E754	TS363	E755	TS364	E756	TS365	E757	TS366	E758	TS367	E759	TS368	E760	TS369	E761	TS370	E762	TS371	E763	TS372	E764	TS373	E765	TS374	E766	TS375	E767	TS376	E768	TS377	E769	TS378	E770	TS379	E771	TS380	E772	TS381	E773	TS382	E774	TS383	E775	TS384	E776	TS385	E777	TS386	E778	TS387	E779	TS388	E780	TS389	E781	TS390	E782	TS391	E783	TS392	E784	TS393	E785	TS394	E786	TS395	E787	TS396	E788	TS397	E789	TS398	E790	TS399	E791	TS400	E792	TS401	E793	TS402	E794	TS403	E795	TS404	E796	TS405	E797	TS406	E798	TS407	E799	TS408	E800	TS409	E801	TS410	E802	TS411	E803	TS412	E804	TS413	E805	TS414	E806	TS415	E807	TS416	E808	TS417	E809	TS418	E810	TS419	E811	TS420	E812	TS421	E813	TS422	E814	TS423	E815	TS424	E816	TS425	E817	TS426	E818	TS427	E819	TS428	E820	TS429	E821	TS430	E822	TS431	E823	TS432	E824	TS433	E825	TS434	E826	TS435	E827	TS436	E828	TS437	E829	TS438	E830	TS439	E831	TS440	E832	TS441	E833	TS442	E834	TS443	E835	TS444	E836	TS445	E837	TS446	E838	TS447	E839	TS448	E840	TS449	E841	TS450	E842	TS451	E843	TS452	E844	TS453	E845	TS454	E846	TS455	E847	TS456	E848	TS457	E849	TS458	E850	TS459	E851	TS460	E852	TS461	E853	TS462	E854	TS463	E855	TS464	E856	TS465	E857	TS466	E858	TS467	E859	TS468	E860	TS469	E861	TS470	E862	TS471	E863	TS472	E864	TS473	E865	TS474	E866	TS475	E867	TS476	E868	TS477	E869	TS478	E870	TS479	E871	TS480	E872	TS481	E873	TS482	E874	TS483	E875	TS484	E876	TS485	E877	TS486	E878	TS487	E879	TS488	E880	TS489	E881	TS490	E882	TS491	E883	TS492	E884	TS493	E885	TS494	E886	TS495	E887	TS496	E888	TS497	E889	TS498	E890	TS499	E891	TS500	E892	TS501	E893	TS502	E894	TS503	E895	TS504	E896	TS505	E897	TS506	E898	TS507	E899	TS508	E900	TS509	E901	TS510	E902	TS511	E903	TS512	E904	TS513	E905	TS514	E906	TS515	E907	TS516	E908	TS517	E909	TS518	E910	TS519	E911	TS520	E912	TS521	E913	TS522	E914	TS523	E915	TS524	E916	TS525	E917	TS526	E918	TS527	E919	TS528	E920	TS529	E921	TS530	E922	TS531	E923	TS532	E924	TS533	E925	TS534	E926	TS535	E927	TS536	E928	TS537	E929	TS538	E930	TS539	E931	TS540	E932	TS541	E933	TS542	E934	TS543	E935	TS544	E936	TS545	E937	TS546	E938	TS547	E939	TS548	E940	TS549	E941	TS550	E942	TS551	E943	TS552	E944	TS553	E945	TS554	E946	TS555	E947	TS556	E948	TS557	E949	TS558	E950	TS559	E951	TS560	E952	TS561	E953	TS562	E954	TS563	E955	TS564	E956	TS565	E957	TS566	E958	TS567	E959	TS568	E960	TS569	E961	TS570	E962	TS571	E963	TS572	E964	TS573	E965	TS574	E966	TS575	E967	TS576	E968	TS577	E969	TS578	E970	TS579	E971	TS580	E972	TS581	E973	TS582	E974	TS583	E975	TS584	E976	TS585	E977	TS586	E978	TS587	E979	TS588	E980	TS589	E981	TS590	E982	TS591	E983	TS592	E984	TS593	E985	TS594	E986	TS595	E987	TS596	E988	TS597	E989	TS598	E990	TS599	E991	TS600	E992	TS601	E993	TS602	E994	TS603	E995	TS604	E996	TS605	E997	TS606	E998	TS607	E999	TS608	E1000	TS609	E1001	TS610	E1002	TS611	E1003	TS612	E1004	TS613	E1005	TS614	E1006	TS615	E1007	TS616	E1008	TS617	E1009	TS618	E1010	TS619	E1011	TS620	E1012	TS621	E1013	TS622	E1014	TS623	E1015	TS624	E1016	TS625	E1017	TS626	E1018	TS627	E1019	TS628	E1020	TS629	E1021	TS630	E1022	TS631	E1023	TS632	E1024	TS633	E1025	TS634	E1026	TS635	E1027	TS636	E1028	TS637	E1029	TS638	E1030	TS639	E1031	TS640	E1032	TS641	E1033	TS642	E1034	TS643	E1035	TS644	E1036	TS645	E1037	TS646	E1038	TS647	E1039	TS648	E1040	TS649	E1041	TS650	E1042	TS651	E1043	TS652	E1044	TS653	E1045	TS654	E1046	TS655	E1047	TS656	E1048	TS657	E1049	TS658	E1050	TS659	E1051	TS660	E1052	TS661	E1053	TS662	E1054	TS663	E1055	TS664	E1056	TS665	E1057	TS666	E1058	TS667	E1059	TS668	E1060	TS669	E1061	TS670	E1062	TS671	E1063	TS672	E1064	TS673	E1065	TS674	E1066	TS675	E1067	TS676	E1068	TS677	E1069	TS678	E1070	TS679	E1071	TS680	E1072	TS681	E1073	TS682	E1074	TS683	E1075	TS684	E1076	TS685	E1077	TS686	E1078	TS687	E1079	TS688	E1080	TS689	E1081	TS690	E1082	TS691	E1083	TS692	E1084	TS693	E1085	TS694	E1086	TS695	E1087	TS696	E1088	TS697	E1089	TS698	E1090	TS699	E1091	TS700	E1092	TS701	E1093	TS702	E1094	TS703	E1095	TS704	E1096	TS705	E1097	TS706	E1098	TS707	E1099	TS710	E1100	TS711	E1101	TS712	E1102	TS713	E1103	TS714	E1104	TS715	E1105	TS716	E1106	TS717	E1107	TS718	E1108	TS719	E1109	TS720	E1110	TS721	E1111	TS722	E1112	TS723	E1113	TS724	E1114	TS725	E1115	TS726	E1116	TS727	E1117	TS728	E1118	TS729	E1119	TS730	E1120	TS731	E1121	TS732	E1122	TS733	E1123	TS734	E1124	TS735	E1125	TS736	E1126	TS737	E1127	TS738	E1128	TS739	E1129	TS740	E1130	TS741	E1131	TS742	E1132	TS743	E1133
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4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	413.55Å 410.22Å 419.67Å 59.13° 58.90° 64.04°	Depositor
Resolution (Å)	20.00 – 2.80	Depositor
% Data completeness (in resolution range)	50.9 (20.00-2.80)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.07 (at 2.79Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.219 , 0.221	Depositor
Wilson B-factor (Å ²)	36.1	Xtriage
Anisotropy	0.126	Xtriage
Estimated twinning fraction	0.045 for h-l,h,h-k 0.045 for k,k-l,-h+k 0.046 for -k,-h,-l 0.046 for -h+l,-k+l,l 0.046 for k-l,h-l,-l 0.046 for -h,-h+l,-h+k 0.046 for -k+l,-k,h-k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 2465275 reflections	Xtriage
Total number of atoms	17851	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.43	0/4244	0.67	0/5816
1	B	0.44	0/4297	0.67	0/5889
1	C	0.42	0/4627	0.65	0/6324
1	D	0.43	0/4602	0.68	0/6296
All	All	0.43	0/17770	0.67	0/24325

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	4134	0	3987	189	0
1	B	4187	0	4021	175	0
1	C	4519	0	4389	169	0
1	D	4491	0	4363	154	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	97	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	127	0	0	5	0
3	C	148	0	0	2	0
3	D	144	0	0	4	0
All	All	17851	0	16760	643	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 19.

The worst 5 of 643 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:428:PRO:HB2	1:A:434:THR:HG22	1.34	1.08
1:A:175:ILE:HD11	1:A:429:LEU:HB3	1.37	1.06
1:B:342:THR:HG22	1:B:368:VAL:HG22	1.35	1.04
1:B:269:PRO:HB3	1:B:424:VAL:HG13	1.39	0.99
1:A:329:HIS:CE1	1:A:373:GLN:HE22	1.79	0.98

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	535/644 (83%)	495 (92%)	37 (7%)	3 (1%)	30	65
1	B	543/644 (84%)	500 (92%)	36 (7%)	7 (1%)	15	44
1	C	580/644 (90%)	552 (95%)	22 (4%)	6 (1%)	19	52
1	D	581/644 (90%)	540 (93%)	33 (6%)	8 (1%)	14	42
All	All	2239/2576 (87%)	2087 (93%)	128 (6%)	24 (1%)	17	50

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	589	SER
1	D	139	SER
1	D	615	PRO
1	D	640	ARG
1	A	200	GLY

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	450/527 (85%)	415 (92%)	35 (8%)	16	41
1	B	454/527 (86%)	421 (93%)	33 (7%)	17	44
1	C	486/527 (92%)	459 (94%)	27 (6%)	26	59
1	D	484/527 (92%)	451 (93%)	33 (7%)	20	49
All	All	1874/2108 (89%)	1746 (93%)	128 (7%)	20	49

5 of 128 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	424	VAL
1	C	86	GLN
1	D	495	ARG
1	B	504	THR
1	B	568	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	479	ASN
1	C	329	HIS
1	D	533	ASN
1	C	86	GLN
1	C	275	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.