



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 11:05 am GMT

PDB ID : 1Q5A
EMDB ID: : EMD-1052
Title : S-shaped trans interactions of cadherins model based on fitting C-cadherin (1L3W) to 3D map of desmosomes obtained by electron tomography
Authors : He, W.; Cowin, P.; Stokes, D.L.
Deposited on : 2003-08-06
Resolution : 30.00 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

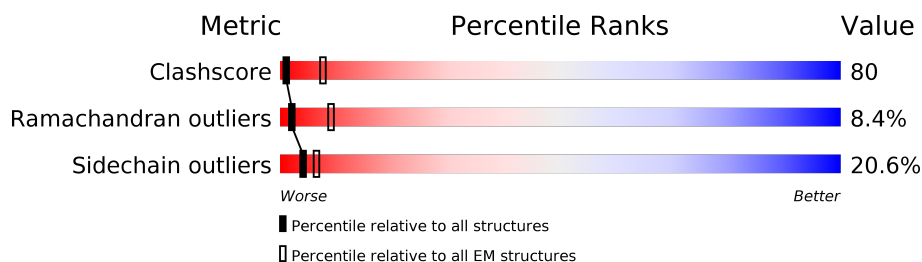
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 30.00 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	880	
1	B	880	

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
2	NAG	A	801	-	-	X	-
2	NAG	A	805	X	-	X	-
2	NAG	A	806	X	-	X	-
2	NAG	A	807	-	-	X	-
2	NAG	A	809	-	-	X	-
2	NAG	A	810	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	904	-	-	X	-
2	NAG	B	801	-	-	X	-
2	NAG	B	805	X	-	X	-
2	NAG	B	806	X	-	X	-
2	NAG	B	807	-	-	X	-
2	NAG	B	809	-	-	X	-
2	NAG	B	810	-	-	X	-
2	NAG	B	904	-	-	X	-
3	NDG	A	902	-	-	X	-
3	NDG	B	811	-	-	X	-
3	NDG	B	902	-	-	X	-

2 Entry composition [i](#)

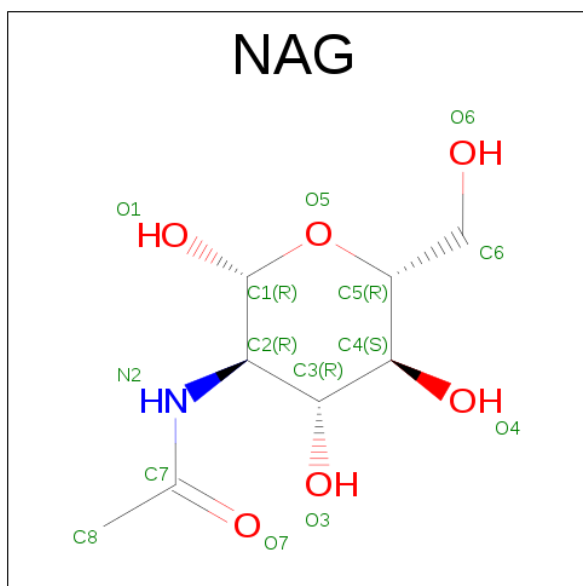
There are 4 unique types of molecules in this entry. The entry contains 8826 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 EP-cadherin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	540	Total	C	N	O	S	0	0
			4191	2635	695	850	11		
1	B	540	Total	C	N	O	S	0	0
			4191	2635	695	850	11		

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



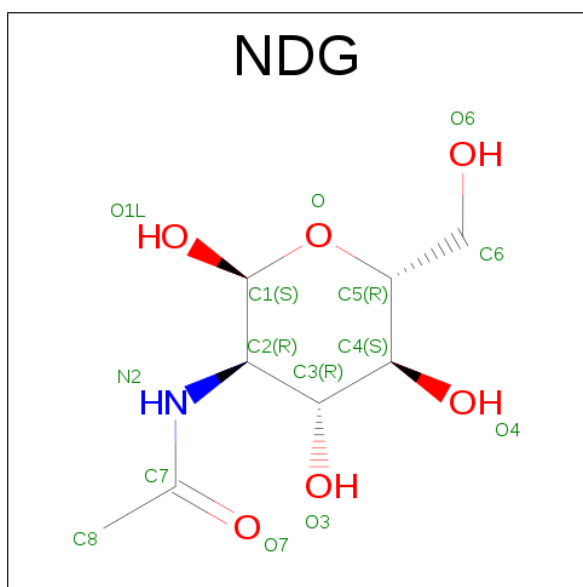
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	

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Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	B	1	Total	C	N	O	0
			154	88	11	55	
2	B	1	Total	C	N	O	0
			154	88	11	55	
2	B	1	Total	C	N	O	0
			154	88	11	55	
2	B	1	Total	C	N	O	0
			154	88	11	55	
2	B	1	Total	C	N	O	0
			154	88	11	55	
2	B	1	Total	C	N	O	0
			154	88	11	55	
2	B	1	Total	C	N	O	0
			154	88	11	55	
2	B	1	Total	C	N	O	0
			154	88	11	55	
2	B	1	Total	C	N	O	0
			154	88	11	55	

- Molecule 3 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			56	32	4	20	
3	A	1	Total	C	N	O	0
			56	32	4	20	
3	A	1	Total	C	N	O	0
			56	32	4	20	
3	A	1	Total	C	N	O	0
			56	32	4	20	
3	B	1	Total	C	N	O	0
			56	32	4	20	
3	B	1	Total	C	N	O	0
			56	32	4	20	
3	B	1	Total	C	N	O	0
			56	32	4	20	

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
4	B	12	Total	Ca	0
			12	12	
4	A	12	Total	Ca	0
			12	12	

ASN	SER	SER	ASN	SER	ASN	ASP	GLU	HIS	ASP	TYR	ASN	TYR	LEU	SER	ASP	TRP	GLY	SER	ARG	PHE	ARG	LYS	LEU	ALA	ASP	MET	TYR	GLY	GLY	ASP	ASP	ASP	GLU	GLU
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- Molecule 1: EP-cadherin

Chain B: 16% 30% 11% • 39%

MET	GLY	SER	THR	ARG	LEU	ARG	ASN	ALA	SER	ALA	VAL	TRP	LEU	CYS	GLY	LEU	LEU	GLN	VAL	VAL	PRO	SER	ILE	ASN	ALA	ASP	VAL	SER	GLY	CYS	LYS	PRO	GLY	PHE	SER	SER	ALA	GLU	TYR	ILE	PHE	SER	VAL	ASN	ARG	ARG	GLU	LEU	GLU	GLY	GLY	LYS	VAL
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ASN	PHE	SER	ASP	CYS	THR	THR	ARG	ARG	HIS	GLY	LEU	TYR	ASP	VAL	GLY	ASP	SER	ARG	PHE	ARG	ARG	VAL	LEU	PRO	ASP	GLY	THR	VAL	VAL	VAL	LYS	ARG	HIS	VAL	VAL	LYS	LEU	LYS	HIS	ASP	ASP	THR	THR	PHE	THR	ILE	SER	THR	TRP	ASP	ALA	ARG	GLY	ILE	LYS	HIS	SER	THR	ASN	ILE	ALA	VAL
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ALA	SER	LYS	ARG	HIS	ARG	SER	GLY	GLU	GLU	ALA	ALA	HIS	SER	ARG	SER	SER	LYS	LEU	LEU	PRO	VAL	LEU	THR	PHE	PRO	GLU	THR	HIS	HIS	THR	GLY	LEU	LYS	ARG	LYS	LYS	LYS	ARG	D1	W2	V3	I4	P5	P6	P6	I7	K8	E11	P16	F17	P18	K19	K20	V22	Q23	K24	K25	S26	K27	N28	K28	D29	E30
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[illegible]

R105	R106	R107	R108	T109	Q110	D111	V112	S116	V117	R118	E119		V127	M128	A129	V130	S131	A132	T133	D134		D137	M138	I139		L142		L146	S147		V150	L151	K152	Q153	D154	P155	E156	E157	P158	I159	P160	M161	L162	F163	T164	L165	R166	E167	E168	T169	G170	V171		L174	I175	G176	
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R181	E186	Y187	T188	L189	T190	V191	Q192	A193	T194	D195	L196	E197	G198	A199	G200	Z201	S202	Z203		Z208	T209	Q210	I211	T212	T213		D216	N217		Z220	Z221	Z222	Z223	Z224	Z225	Z226	T227	Z228	Z229	Z230	Z231	Z232	Z233	Z234	Z235	Z236	Z237	Z238	Z239	Q240	Q241	Z242	Z243	Z244	Z245	D246	Z247	Z248
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Y249	Y250	Y251	Y252	Y253	Y254	Y255	Y256	Y257	Y258	Y259	Y260	Y261	Y262	Y263	Y264	Y265	Y266	Y267	Y268	Y269	Y270	Y271	Y272	Y273	Y274	Y275	Y276	Y277	Y278	Y279	Y280	Y281	Y282	Y283	Y284	Y285	Y286	Y287	Y288	Y289	Y290	Y291	Y292	Y293	Y294	Y295	Y296	Y297	Y298	Y299	Y300	Y301	Y302	Y303	Y304	Y305	Y306	Y307	Y308	Y309	Y310	Y311	Y312	Y313	Y314	Y315	Y316	Y317	Y318	Y319	Y320	Y321	Y322	Y323	Y324	Y325	Y326	Y327	Y328	Y329	Y330	Y331	Y332	Y333	Y334	Y335	Y336	Y337	Y338	Y339	Y340	Y341	Y342	Y343	Y344	Y345	Y346	Y347	Y348	Y349	Y350	Y351	Y352	Y353	Y354	Y355	Y356	Y357	Y358	Y359	Y360	Y361	Y362	Y363	Y364	Y365	Y366	Y367	Y368	Y369	Y370	Y371	Y372	Y373	Y374	Y375	Y376	Y377	Y378	Y379	Y380	Y381	Y382	Y383	Y384	Y385	Y386	Y387	Y388	Y389	Y390	Y391	Y392	Y393	Y394	Y395	Y396	Y397	Y398	Y399	Y400	Y401	Y402	Y403	Y404	Y405	Y406	Y407	Y408	Y409	Y410	Y411	Y412	Y413	Y414	Y415	Y416	Y417	Y418	Y419	Y420	Y421	Y422	Y423	Y424	Y425	Y426	Y427	Y428	Y429	Y430	Y431	Y432	Y433	Y434	Y435	Y436	Y437	Y438	Y439	Y440	Y441	Y442	Y443	Y444	Y445	Y446	Y447	Y448	Y449	Y450	Y451	Y452	Y453	Y454	Y455	Y456	Y457	Y458	Y459	Y460	Y461	Y462	Y463	Y464	Y465	Y466	Y467	Y468	Y469	Y470	Y471	Y472	Y473	Y474	Y475	Y476	Y477	Y478	Y479	Y480	Y481	Y482	Y483	Y484	Y485	Y486	Y487	Y488	Y489	Y490	Y491	Y492	Y493	Y494	Y495	Y496	Y497	Y498	Y499	Y500	Y501	Y502	Y503	Y504	Y505	Y506	Y507	Y508	Y509	Y510	Y511	Y512	Y513	Y514	Y515	Y516	Y517	Y518	Y519	Y520	Y521	Y522	Y523	Y524	Y525	Y526	Y527	Y528	Y529	Y530	Y531	Y532	Y533	Y534	Y535	Y536	Y537	Y538	Y539	Y540	Y541	Y542	Y543	Y544	Y545	Y546	Y547	Y548	Y549	Y550	Y551	Y552	Y553	Y554	Y555	Y556	Y557	Y558	Y559	Y560	Y561	Y562	Y563	Y564	Y565	Y566	Y567	Y568	Y569	Y570	Y571	Y572	Y573	Y574	Y575	Y576	Y577	Y578	Y579	Y580	Y581	Y582	Y583	Y584	Y585	Y586	Y587	Y588	Y589	Y590	Y591	Y592	Y593	Y594	Y595	Y596	Y597	Y598	Y599	Y600	Y601	Y602	Y603	Y604	Y605	Y606	Y607	Y608	Y609	Y610	Y611	Y612	Y613	Y614	Y615	Y616	Y617	Y618	Y619	Y620	Y621	Y622	Y623	Y624	Y625	Y626	Y627	Y628	Y629	Y630	Y631	Y632	Y633	Y634	Y635	Y636	Y637	Y638	Y639	Y640	Y641	Y642	Y643	Y644	Y645	Y646	Y647	Y648	Y649	Y650	Y651	Y652	Y653	Y654	Y655	Y656	Y657	Y658	Y659	Y660	Y661	Y662	Y663	Y664	Y665	Y666	Y667	Y668	Y669	Y670	Y671	Y672	Y673	Y674	Y675	Y676	Y677	Y678	Y679	Y680	Y681	Y682	Y683	Y684	Y685	Y686	Y687	Y688	Y689	Y690	Y691	Y692	Y693	Y694	Y695	Y696	Y697	Y698	Y699	Y700	Y701	Y702
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S315	S316	S317	S318	S319	T320	T321	T322	T323	T324			N327	P330	F331	F332	F333	F334	F335	F336	F337	F338	F339	D340	D341	D342	D343	D344	D345	D346	D347	D348	E349	E350	I351	I352	S353	S354	S355	S356	S357	S358	S359	S360	S361	S362	S363	S364	S365	S366	S367	S368	S369	S370	S371	S372	S373	S374	S375	S376	S377	S378
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L379	L380	L381	L382	L383	L384	L385	L386	L387	L388	L389	L390	L391	L392	L393	L394	L395	L396	L397	L398	L399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424	L425	L426	L427	L428	L429	L430	L431	L432	L433	L434	L435	L436	L437	L438	L439	L440	L441	L442	L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	L481	L482	L483	L484	L485	L486	L487	L488	L489	L490	L491	L492	L493	L494	L495	L496	L497	L498	L499	L500	L501	L502	L503	L504	L505	L506	L507	L508	L509	L510	L511	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	L811	L812	L813	L814	L815	L816	L817	L818	L819	L820	L821	L822	L823	L824	L825	L826	L827	L828	L829	L830	L831	L832	L833	L834	L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849	L850	L851	L852	L853	L854	L855	L856	L857	L858	L859	L860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889
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ASN	ASP	VAL	PRO	THR	LEU	MET	PRO	ALA	ALA	HIS	ARG	ARG	ARG	SER	ASN	PRO	GLU	ASP	ILE	GLY	ASN	PHE	ILE	ASP	GLU	ASN	LEU	ASP	ALA	ALA	ASP	ASN	ASP	THR	THR	PRO	PRO	Tyr	LEU	SER	LEU	VAL	PHE	ASP	TYR	GLY	GLY	SER	GLY	SER	GLU	ALA	ALA	FER
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4 Experimental information

Property	Value	Source
Reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	no CTF correction. Imaging at underfocus 0.4 micron with CM200FEG microscope at 50,000 magnification	Depositor
Microscope	FEI/PHILIPS CM200FEG	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	120000	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	500	Depositor
Magnification	68276	Depositor
Image detector	GATAN 794	Depositor

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: CA, NAG, NDG

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 >2	RMSZ	# Z >2
1	A	0.70	8/4276 (0.2%)	1.44	81/5839 (1.4%)
1	B	0.70	8/4276 (0.2%)	1.39	79/5839 (1.4%)
All	All	0.70	16/8552 (0.2%)	1.42	160/11678 (1.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	4
1	B	0	4
All	All	1	8

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	335	ALA	CA-CB	-8.37	1.34	1.52
1	B	335	ALA	CA-CB	-8.33	1.34	1.52
1	A	539	CYS	CB-SG	8.17	1.96	1.82
1	B	539	CYS	CB-SG	8.15	1.96	1.82
1	B	223	PRO	CG-CD	7.02	1.73	1.50

The worst 5 of 160 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	490	LYS	N-CA-CB	-28.44	59.41	110.60
1	A	520	PRO	CA-C-N	-13.30	87.95	117.20
1	B	520	PRO	CA-C-N	-13.28	87.99	117.20
1	B	290	PHE	N-CA-C	12.73	145.38	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	235	ILE	N-CA-C	12.72	145.34	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	490	LYS	CA

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	17	PHE	Sidechain
1	A	18	PRO	Mainchain
1	A	222	ASP	Mainchain
1	A	520	PRO	Mainchain
1	B	17	PHE	Sidechain

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	4191	0	4085	707	0
1	B	4191	0	4090	720	0
2	A	154	0	143	85	0
2	B	154	0	143	84	0
3	A	56	0	52	16	0
3	B	56	0	52	17	0
4	A	12	0	0	0	0
4	B	12	0	0	0	0
All	All	8826	0	8565	1392	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 80.

The worst 5 of 1392 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:B:464:ILE:HD12	1:B:465:PRO:CD	1.30	1.58
1:A:464:ILE:HD12	1:A:465:PRO:CD	1.30	1.55
1:A:87:PRO:CG	1:B:89:GLU:HB3	1.16	1.54
1:B:464:ILE:CD1	1:B:465:PRO:HD2	1.50	1.41
1:A:464:ILE:CD1	1:A:465:PRO:HD2	1.50	1.37

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 PDB entries followed by that with respect to all EM entries.

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	538/880 (61%)	401 (74%)	92 (17%)	45 (8%)	1	15
1	B	538/880 (61%)	401 (74%)	92 (17%)	45 (8%)	1	15
All	All	1076/1760 (61%)	802 (74%)	184 (17%)	90 (8%)	2	15

5 of 90 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	PRO
1	A	155	PRO
1	A	235	ILE
1	A	347	ARG
1	A	363	GLN

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 PDB entries followed by that with respect to all EM entries.

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	480/779 (62%)	381 (79%)	99 (21%)	1	8
1	B	480/779 (62%)	381 (79%)	99 (21%)	1	8
All	All	960/1558 (62%)	762 (79%)	198 (21%)	4	8

5 of 198 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	509	ILE
1	B	117	VAL
1	B	464	ILE
1	A	518	ASN
1	B	18	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	517	GLN
1	B	45	ASN
1	B	455	GLN
1	B	12	ASN
1	B	79	HIS

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 54 ligands modelled in this entry, 24 are monoatomic - leaving 30 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	$\# Z > 2$
2	NAG	A	801	1	14,14,15	0.67	0	15,19,21	0.99	1 (6%)
2	NAG	A	802	1	14,14,15	0.73	0	15,19,21	0.92	0
2	NAG	A	803	1	14,14,15	0.94	1 (7%)	15,19,21	1.20	2 (13%)
3	NDG	A	804	1	14,14,15	0.63	0	15,19,21	0.82	0
2	NAG	A	805	1	14,14,15	0.69	0	15,19,21	1.07	1 (6%)
2	NAG	A	806	1	14,14,15	0.55	0	15,19,21	1.44	3 (20%)
2	NAG	A	807	1	14,14,15	0.65	0	15,19,21	1.25	2 (13%)
2	NAG	A	808	1	14,14,15	0.66	0	15,19,21	0.68	0
2	NAG	A	809	1	14,14,15	0.76	1 (7%)	15,19,21	0.86	0
2	NAG	A	810	1	14,14,15	0.65	0	15,19,21	1.40	4 (26%)
3	NDG	A	811	1	14,14,15	0.86	0	15,19,21	1.95	1 (6%)
2	NAG	A	812	1	14,14,15	0.84	1 (7%)	15,19,21	0.75	1 (6%)
3	NDG	A	902	1	14,14,15	1.10	1 (7%)	15,19,21	1.14	1 (6%)
3	NDG	A	903	1	14,14,15	0.52	0	15,19,21	0.80	0
2	NAG	A	904	1	14,14,15	0.77	1 (7%)	15,19,21	0.64	0
2	NAG	B	801	1	14,14,15	0.66	0	15,19,21	1.00	1 (6%)
2	NAG	B	802	1	14,14,15	0.74	0	15,19,21	0.91	0
2	NAG	B	803	1	14,14,15	0.94	1 (7%)	15,19,21	1.21	2 (13%)
3	NDG	B	804	1	14,14,15	0.62	0	15,19,21	0.82	0
2	NAG	B	805	1	14,14,15	0.70	0	15,19,21	1.07	1 (6%)
2	NAG	B	806	1	14,14,15	0.55	0	15,19,21	1.45	3 (20%)
2	NAG	B	807	1	14,14,15	0.64	0	15,19,21	1.25	2 (13%)
2	NAG	B	808	1	14,14,15	0.68	0	15,19,21	0.67	0
2	NAG	B	809	1	14,14,15	0.77	1 (7%)	15,19,21	0.86	0
2	NAG	B	810	1	14,14,15	0.64	0	15,19,21	1.40	4 (26%)
3	NDG	B	811	1	14,14,15	0.84	0	15,19,21	1.96	1 (6%)
2	NAG	B	812	1	14,14,15	0.85	1 (7%)	15,19,21	0.75	0
3	NDG	B	902	1	14,14,15	1.09	1 (7%)	15,19,21	1.14	1 (6%)
3	NDG	B	903	1	14,14,15	0.52	0	15,19,21	0.80	0
2	NAG	B	904	1	14,14,15	0.77	1 (7%)	15,19,21	0.65	0

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
2	NAG	A	801	1	-	0/6/23/26	0/1/1/1
2	NAG	A	802	1	-	0/6/23/26	0/1/1/1
2	NAG	A	803	1	-	0/6/23/26	0/1/1/1
3	NDG	A	804	1	-	0/6/23/26	0/1/1/1
2	NAG	A	805	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	806	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	807	1	-	0/6/23/26	0/1/1/1
2	NAG	A	808	1	-	0/6/23/26	0/1/1/1
2	NAG	A	809	1	-	0/6/23/26	0/1/1/1
2	NAG	A	810	1	-	0/6/23/26	0/1/1/1
3	NDG	A	811	1	-	0/6/23/26	0/1/1/1
2	NAG	A	812	1	-	0/6/23/26	0/1/1/1
3	NDG	A	902	1	-	0/6/23/26	0/1/1/1
3	NDG	A	903	1	-	0/6/23/26	0/1/1/1
2	NAG	A	904	1	-	0/6/23/26	0/1/1/1
2	NAG	B	801	1	-	0/6/23/26	0/1/1/1
2	NAG	B	802	1	-	0/6/23/26	0/1/1/1
2	NAG	B	803	1	-	0/6/23/26	0/1/1/1
3	NDG	B	804	1	-	0/6/23/26	0/1/1/1
2	NAG	B	805	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	B	806	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	B	807	1	-	0/6/23/26	0/1/1/1
2	NAG	B	808	1	-	0/6/23/26	0/1/1/1
2	NAG	B	809	1	-	0/6/23/26	0/1/1/1
2	NAG	B	810	1	-	0/6/23/26	0/1/1/1
3	NDG	B	811	1	-	0/6/23/26	0/1/1/1
2	NAG	B	812	1	-	0/6/23/26	0/1/1/1
3	NDG	B	902	1	-	0/6/23/26	0/1/1/1
3	NDG	B	903	1	-	0/6/23/26	0/1/1/1
2	NAG	B	904	1	-	0/6/23/26	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	904	NAG	C1-C2	-2.44	1.49	1.52
2	A	904	NAG	C1-C2	-2.42	1.49	1.52
2	B	812	NAG	C1-C2	-2.37	1.49	1.52
2	A	812	NAG	C1-C2	-2.36	1.49	1.52
2	B	809	NAG	C1-C2	-2.05	1.49	1.52

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	811	NDG	C2-N2-C7	-6.87	112.92	122.94
3	A	811	NDG	C2-N2-C7	-6.85	112.95	122.94
2	A	806	NAG	C2-N2-C7	-3.36	118.04	122.94
2	B	806	NAG	C2-N2-C7	-3.35	118.05	122.94
2	B	805	NAG	C2-N2-C7	-2.97	118.61	122.94

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	806	NAG	C1
2	A	806	NAG	C1
2	B	805	NAG	C1
2	A	805	NAG	C1

There are no torsion outliers.

There are no ring outliers.

26 monomers are involved in 202 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	NAG	21	0
2	A	803	NAG	4	0
3	A	804	NDG	2	0
2	A	805	NAG	7	0
2	A	806	NAG	12	0
2	A	807	NAG	17	0
2	A	808	NAG	2	0
2	A	809	NAG	8	0
2	A	810	NAG	13	0
3	A	811	NDG	6	0
2	A	812	NAG	3	0
3	A	902	NDG	8	0
2	A	904	NAG	8	0
2	B	801	NAG	21	0
2	B	803	NAG	4	0
3	B	804	NDG	2	0
2	B	805	NAG	7	0
2	B	806	NAG	12	0
2	B	807	NAG	16	0
2	B	808	NAG	2	0
2	B	809	NAG	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	810	NAG	13	0
3	B	811	NDG	7	0
2	B	812	NAG	3	0
3	B	902	NDG	8	0
2	B	904	NAG	8	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.