



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 11:06 am GMT

PDB ID : 1Q55  
EMDB ID: : EMD-1052  
Title : W-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](mailto: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.

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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

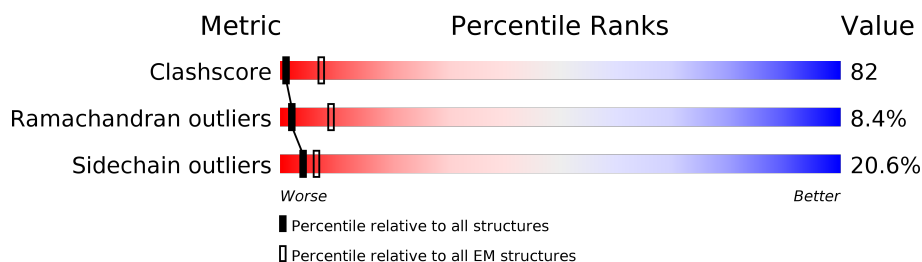
# 1 Overall quality at a glance

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  $\geq 3$ , 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	
1	C	880	
1	D	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	-

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

## 2 Entry composition [i](#)

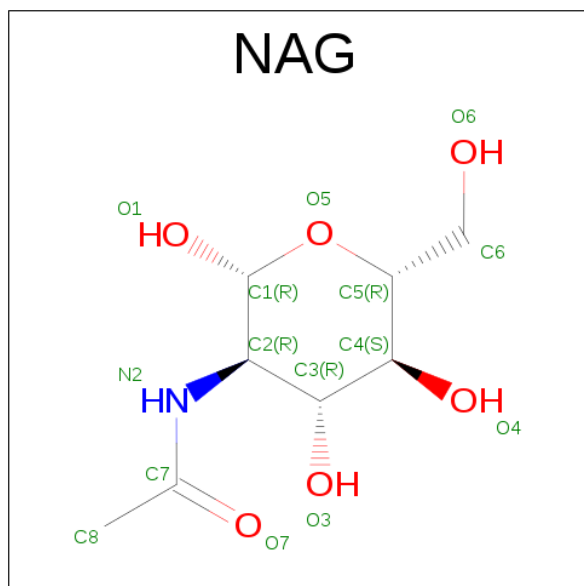
There are 4 unique types of molecules in this entry. The entry contains 17652 atoms, of which 0 are hydrogens and 0 are deuteriums.

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		
1	C	540	Total	C	N	O	S	0	0
			4191	2635	695	850	11		
1	D	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	

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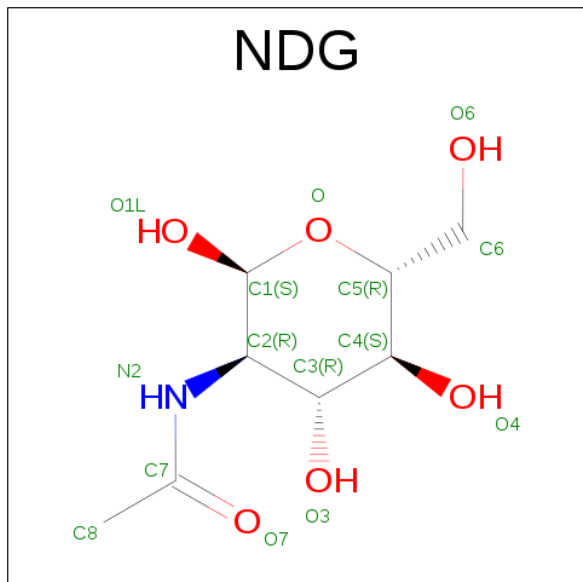
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	B	1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

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Mol	Chain	Residues	Atoms				AltConf
2	C	1	Total	C	N	O	0
			154	88	11	55	
2	C	1	Total	C	N	O	0
			154	88	11	55	
2	C	1	Total	C	N	O	0
			154	88	11	55	
2	C	1	Total	C	N	O	0
			154	88	11	55	
2	C	1	Total	C	N	O	0
			154	88	11	55	
2	C	1	Total	C	N	O	0
			154	88	11	55	
2	C	1	Total	C	N	O	0
			154	88	11	55	
2	C	1	Total	C	N	O	0
			154	88	11	55	
2	D	1	Total	C	N	O	0
			154	88	11	55	
2	D	1	Total	C	N	O	0
			154	88	11	55	
2	D	1	Total	C	N	O	0
			154	88	11	55	
2	D	1	Total	C	N	O	0
			154	88	11	55	
2	D	1	Total	C	N	O	0
			154	88	11	55	
2	D	1	Total	C	N	O	0
			154	88	11	55	
2	D	1	Total	C	N	O	0
			154	88	11	55	
2	D	1	Total	C	N	O	0
			154	88	11	55	
2	D	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:  $C_8H_{15}NO_6$ ).



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	
3	B	1	Total	C	N	O	0
			56	32	4	20	
3	C	1	Total	C	N	O	0
			56	32	4	20	
3	C	1	Total	C	N	O	0
			56	32	4	20	
3	C	1	Total	C	N	O	0
			56	32	4	20	

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Mol	Chain	Residues	Atoms				AltConf
3	D	1	Total	C	N	O	0
			56	32	4	20	
3	D	1	Total	C	N	O	0
			56	32	4	20	
3	D	1	Total	C	N	O	0
			56	32	4	20	
3	D	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	
4	D	12	Total	Ca	0
			12	12	
4	C	12	Total	Ca	0
			12	12	





LEU SER SER LEU ASN SER SER ASN 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

- Molecule 1: EP-cadherin

Chain B:  16% 30% 11% 1% 42%

MET	GLY	SER	THR	ARG	LEU	ARG	ASN	ALA	SER	VAL	TRP	CYS	GLY	LEU	LEU	CYS	LEU	GLN	VAL	VAL	PRO	SER	ILE	ASN	ASP	VAL	SER	GLY	CYS	LYS	PRO	GLY	PHE	SER	SER	ALA	GLU	TYP	ILE	PHE	SER	VAL	ASN	ARG	ARG	GLU	LEU	GLU	ARG	GLY	LYS
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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 GLY VAL VAL VAL LYS ARG ARG HIS VAL VAL LYS LEU LEU HIS LYS ASP ASP THR THR PHE THR THR SER SER THR TRP ASP ALA ARG ARG GLY LEU LYS HIS SER THR THR ASN ALA

[illegible]

K33	Y36	S37	I38	T39	G40	Q41	G42	N45	P46	P47	Q48	G49	V50	F51	F52	I53	E54	E55	E56	T57	G58	W59	M60	L61	V62	T63	L66	D67	R68	E69	A90	E93	S96	P97	V98	E99	E90	P91	M92	E93	E93	I94	T95	I96	T100	Q101	R105	P106
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F108	T109	T110	T111	T112	S116	S117	R118	E119	T127	M128	A129	V130	S131	A132	T133	L134	D137	M138	L139	L142	L146	S147	I150	L151	K152	Q153	D154	P155	E156	S157	P158	I159	P160	N161	L162	F163	T164	L165	N166	L167	T169	G170	V171	L174	L175	G176	L179	D180	R181
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[illegible]

P250	P251	P252	P253	P254	P255	P256	P257	P258	P259	P260	P261	P262	P263	P264	P265	P266	P267	P268	P269	P270	P271	P272	P273	P274	P275	P276	P277	P278	P279	P280	P281	P282	P283	P284	P285	P286	P287	P288	P289	P290	P291	P292	P293	P294	P295	P296	P297	P298	P299	P300	P301	P302	P303	P304	P305	P306	P307	P308	P309	P310	P311	P312	P313	P314	P315	P316	P317	P318	P319	P320	P321	P322	P323	P324	P325	P326	P327	P328	P329	P330	P331	P332	P333	P334	P335	P336	P337	P338	P339	P340	P341	P342	P343	P344	P345	P346	P347	P348	P349	P350	P351	P352	P353	P354	P355	P356	P357	P358	P359	P360	P361	P362	P363	P364	P365	P366	P367	P368	P369	P370	P371	P372	P373	P374	P375	P376	P377	P378	P379	P380	P381	P382	P383	P384	P385	P386	P387	P388	P389	P390	P391	P392	P393	P394	P395	P396	P397	P398	P399	P400	P401	P402	P403	P404	P405	P406	P407	P408	P409	P410	P411	P412	P413	P414	P415	P416	P417	P418	P419	P420	P421	P422	P423	P424	P425	P426	P427	P428	P429	P430	P431	P432	P433	P434	P435	P436	P437	P438	P439	P440	P441	P442	P443	P444	P445	P446	P447	P448	P449	P450	P451	P452	P453	P454	P455	P456	P457	P458	P459	P460	P461	P462	P463	P464	P465	P466	P467	P468	P469	P470	P471	P472	P473	P474	P475	P476	P477	P478	P479	P480	P481	P482	P483	P484	P485	P486	P487	P488	P489	P490	P491	P492	P493	P494	P495	P496	P497	P498	P499	P500	P501	P502	P503	P504	P505	P506	P507	P508	P509	P510	P511	P512	P513	P514	P515	P516	P517	P518	P519	P520	P521	P522	P523	P524	P525	P526	P527	P528	P529	P530	P531	P532	P533	P534	P535	P536	P537	P538	P539	P540	P541	P542	P543	P544	P545	P546	P547	P548	P549	P550	P551	P552	P553	P554	P555	P556	P557	P558	P559	P560	P561	P562	P563	P564	P565	P566	P567	P568	P569	P570	P571	P572	P573	P574	P575	P576	P577	P578	P579	P580	P581	P582	P583	P584	P585	P586	P587	P588	P589	P590	P591	P592	P593	P594	P595	P596	P597	P598	P599	P600	P601	P602	P603	P604	P605	P606	P607	P608	P609	P610	P611	P612	P613	P614	P615	P616	P617	P618	P619	P620	P621	P622	P623	P624	P625	P626	P627	P628	P629	P630	P631	P632	P633	P634	P635	P636	P637	P638	P639	P640	P641	P642	P643	P644	P645	P646	P647	P648	P649	P650	P651	P652	P653	P654	P655	P656	P657	P658	P659	P660	P661	P662	P663	P664	P665	P666	P667	P668	P669	P670	P671	P672	P673	P674	P675	P676	P677	P678	P679	P680	P681	P682	P683	P684	P685	P686	P687	P688	P689	P690	P691	P692	P693	P694	P695	P696	P697	P698	P699	P700	P701	P702	P703	P704	P705	P706	P707	P708	P709	P710	P711	P712	P713	P714	P715	P716	P717	P718	P719	P720	P721	P722	P723	P724	P725	P726	P727	P728	P729	P730	P731	P732	P733	P734	P735	P736	P737	P738	P739	P740	P741	P742	P743	P744	P745	P746	P747	P748	P749	P750	P751	P752	P753	P754	P755	P756	P757	P758	P759	P760
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T316	T317	T318	T319	T320	T321	T322	T323	T324	T325	T326	T327	T328	T329	T330	T331	T332	T333	T334	T335	T336	T337	T338	T339	T340	T341	T342	T343	T344	T345	T346	T347	T348	T349	T350	T351	T352	T353	T354	T355	T356	T357	T358	T359	T360	T361	T362	T363	T364	T365	T366	T367	T368	T369	T370	T371	T372	T373	T374	T375	T376	T377	T378	T379	T380	T381	T382	T383	T384	T385	T386	T387	T388	T389	T390	T391	T392	T393	T394	T395	T396	T397	T398	T399	T400	T401	T402	T403	T404	T405	T406	T407	T408	T409	T410	T411	T412	T413	T414	T415	T416	T417	T418	T419	T420	T421	T422	T423	T424	T425	T426	T427	T428	T429	T430	T431	T432	T433	T434	T435	T436	T437	T438	T439	T440	T441	T442	T443	T444	T445	T446	T447	T448	T449	T450	T451	T452	T453	T454	T455	T456	T457	T458	T459	T460	T461	T462	T463	T464	T465	T466	T467	T468	T469	T470	T471	T472	T473	T474	T475	T476	T477	T478	T479	T480	T481	T482	T483	T484	T485	T486	T487	T488	T489	T490	T491	T492	T493	T494	T495	T496	T497	T498	T499	T500	T501	T502	T503	T504	T505	T506	T507	T508	T509	T510	T511	T512	T513	T514	T515	T516	T517	T518	T519	T520	T521	T522	T523	T524	T525	T526	T527	T528	T529	T530	T531	T532	T533	T534	T535	T536	T537	T538	T539	T540	T541	T542	T543	T544	T545	T546	T547	T548	T549	T550	T551	T552	T553	T554	T555	T556	T557	T558	T559	T560	T561	T562	T563	T564	T565	T566	T567	T568	T569	T570	T571	T572	T573	T574	T575	T576	T577	T578	T579	T580	T581	T582	T583	T584	T585	T586	T587	T588	T589	T590	T591	T592	T593	T594	T595	T596	T597	T598	T599	T600	T601	T602	T603	T604	T605	T606	T607	T608	T609	T610	T611	T612	T613	T614	T615	T616	T617	T618	T619	T620	T621	T622	T623	T624	T625	T626	T627	T628	T629	T630	T631	T632	T633	T634	T635	T636	T637	T638	T639	T640	T641	T642	T643	T644	T645	T646	T647	T648	T649	T650	T651	T652	T653	T654	T655	T656	T657	T658	T659	T660	T661	T662	T663	T664	T665	T666	T667	T668	T669	T670	T671	T672	T673	T674	T675	T676	T677	T678	T679	T680	T681	T682	T683	T684	T685	T686	T687	T688	T689	T690	T691	T692	T693	T694	T695	T696	T697	T698	T699	T700	T701	T702	T703	T704	T705	T706	T707	T708	T709	T710	T711	T712	T713	T714	T715	T716	T717	T718	T719	T720	T721	T722	T723	T724	T725	T726	T727	T728	T729	T730	T731	T732	T733	T734	T735	T736	T737	T738	T739	T740	T741	T742	T743	T744	T745	T746	T747	T748	T749	T750	T751	T752	T753	T754	T755	T756	T757	T758	T759	T760	T761	T762	T763	T764	T765	T766	T767	T768	T769	T770	T771	T772	T773	T774	T775	T776	T777	T778	T779	T780	T781	T782	T783	T784	T785	T786	T787	T788	T789	T790	T791	T792	T793	T794	T795	T796	T797	T798	T799	T800	T801	T802	T803	T804	T805	T806	T807	T808	T809	T810	T811	T812	T813	T814	T815	T816	T817	T818	T819	T820	T821	T822	T823	T824	T825	T826
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T380	T381	T382	T383	T384	T385	T386	T387	T388	T389	T390	T391	T392	T393	T394	T395	T396	T397	T398	T399	T400	T401	T402	T403	T404	T405	T406	T407	T408	T409	T410	T411	T412	T413	T414	T415	T416	T417	T418	T419	T420	T421	T422	T423	T424	T425	T426	T427	T428	T429	T430	T431	T432	T433	T434	T435	T436	T437	T438	T439	T440	T441	T442	T443	T444	T445	T446	T447	T448	T449	T450	T451	T452	T453	T454	T455	T456	T457	T458	T459	T460	T461	T462	T463	T464	T465	T466	T467	T468	T469	T470	T471	T472	T473	T474	T475	T476	T477	T478	T479	T480	T481	T482	T483	T484	T485	T486	T487	T488	T489	T490	T491	T492	T493	T494	T495	T496	T497	T498	T499	T500
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S8411	P442	P443	T446	T447	C446	D449	Q450	N451	P452	L457	T458	L459	S460	D461	T464	P465	P466	T467	T468	T469	P470	L471	L472	V473	S474	L475	S476	H477	G478	S479	D480	L481	T482	L483	L484	L485	L486	L487	D488	S489	L490	Q491	T492	S493	N494	L495	L496	S497	P498	T499	W500	W501	L502	S503	S504
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B506	B507	B508	B509	B510	B511	B512	B513	B514	B515	B516	B517	B518	B519	B520	B521	B522	B523	B524	B525	B526	B527	B528	B529	B530	B531	B532	B533	B534	B537	B538	B539	B540	B541	B542	B543	B544	B545	B546	B547	B548	B549	B550	B551	B552	B553	B554	B555	B556	B557	B558	B559	B560	B561	B562	B563	B564	B565	B566	B567	B568	B569	B570	B571	B572	B573	B574	B575	B576	B577	B578	B579	B580	B581	B582	B583	B584	B585	B586	B587	B588	B589	B590	B591	B592	B593	B594	B595	B596	B597	B598	B599	B600	B601	B602	B603	B604	B605	B606	B607	B608	B609	B610	B611	B612	B613	B614	B615	B616	B617	B618	B619	B620	B621	B622	B623	B624	B625	B626	B627	B628	B629	B630	B631	B632	B633	B634	B635	B636	B637	B638	B639	B640	B641	B642	B643	B644	B645	B646	B647	B648	B649	B650	B651	B652	B653	B654	B655	B656	B657	B658	B659	B660	B661	B662	B663	B664	B665	B666	B667	B668	B669	B670	B671	B672	B673	B674	B675	B676	B677	B678	B679	B680	B681	B682	B683	B684	B685	B686	B687	B688	B689	B690	B691	B692	B693	B694	B695	B696	B697	B698	B699	B700	B701	B702	B703	B704	B705	B706	B707	B708	B709	B710	B711	B712	B713	B714	B715	B716	B717	B718	B719	B720	B721	B722	B723	B724	B725	B726	B727	B728	B729	B730	B731	B732	B733	B734	B735	B736	B737	B738	B739	B740	B741	B742	B743	B744	B745	B746	B747	B748	B749	B750	B751	B752	B753	B754	B755	B756	B757	B758	B759	B760	B761	B762	B763	B764	B765	B766	B767	B768	B769	B770	B771	B772	B773	B774	B775	B776	B777	B778	B779	B780	B781	B782	B783	B784	B785	B786	B787	B788	B789	B790	B791	B792	B793	B794	B795	B796	B797	B798	B799	B800	B801	B802	B803	B804	B805	B806	B807	B808	B809	B810	B811	B812	B813	B814	B815	B816	B817	B818	B819	B820	B821	B822	B823	B824	B825	B826	B827	B828	B829	B830	B831	B832	B833	B834	B835	B836	B837	B838	B839	B840	B841	B842	B843	B844	B845	B846	B847	B848	B849	B850	B851	B852	B853	B854	B855	B856	B857	B858	B859	B860	B861	B862	B863	B864	B865	B866	B867	B868	B869	B870	B871	B872	B873	B874	B875	B876	B877	B878	B879	B880	B881	B882	B883	B884	B885	B886	B887	B888	B889	B890	B891	B892	B893	B894	B895	B896	B897	B898	B899	B900	B901	B902	B903	B904	B905	B906	B907	B908	B909	B910	B911	B912	B913	B914	B915	B916	B917	B918	B919	B920	B921	B922	B923	B924	B925	B926	B927	B928	B929	B930	B931	B932	B933	B934	B935	B936	B937	B938	B939	B940	B941	B942	B943	B944	B945	B946	B947	B948	B949	B950	B951	B952	B953	B954	B955	B956	B957	B958	B959	B960	B961	B962	B963	B964	B965	B966	B967	B968	B969	B970	B971	B972	B973	B974	B975	B976	B977	B978	B979	B980	B981	B982	B983	B984	B985	B986	B987	B988	B989	B990	B991	B992	B993	B994	B995	B996	B997	B998	B999	B1000	B1001	B1002	B1003	B1004	B1005	B1006	B1007	B1008	B1009	B1010	B1011	B1012	B1013	B1014	B1015	B1016</
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LEU	LEU	LEU	LEU	PHE	PHE	LEU	LYS	ARG	ARG	LYS	LYS	LYS	VAL	VAL	LYS	GLU	GLU	PRO	PRO	LEU	LEU	LEU	LEU	PRO	ASP	ASP	THR	THR	ARG	ASP	ASN	ILE	PHE	PHE	TYR	GLY	GLY	GLU	GLU	GLY	GLY	GLY	GLU	GLU	ASP	ASP	GLN	ASP	ASP	THR	LEU	SER	GLN	HIS	ARG	GLY	LEU	ASP	ASP	SER	ARG	ARG	MET	ARG
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ASP	VAL	VAL	PRO	THR	LEU	MET	PRO	PRO	ALA	HIS	TYR	ARG	ARG	PRO	PRO	PRO	SER	ASN	ASN	ASP	GLU	ILE	GLY	ASN	PHE	ILE	ASP	GLU	ASN	LEU	ASP	ALA	ALA	ASP	ASN	ASP	PRO	THR	ALA	PRO	PRO	TYR	ASP	SER	LEU	LEU	VAL	PHE	ASP	TYR	GLY	SER	GLY	GLU	ALA	ALA	SER
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SER SER SER LEU ASN ASN SER SER ASN ASN ASP GLU HIS ASP TYR ASN ASN TYR LEU SER ASP TRP GLY SER SER ARG PHE ARG ARG LYS LEU ALA ASP MET TYR GLY GLY ASP ASP ASP ASP GLU GLU

- Molecule 1: EP-cadherin

Chain C:  16% 30% 11% • 39%

[illegible]

- Molecule 1: EP-cadherin

Chain D:  17% 30% 11% • 39%

[illegible]

LEU	ASN	VAL	LEU	S508	R443	N382	V319	P253	L189	P106	F31	ALA
ASP	SER	PRO	LEU	I509	T446	K383	T320	A254	T190	K107	N32	SER
ASP	SER	THR	PHE	Y510	T447	D384	T321	Q256	V191	F108	K33	ARG
ASN	ASN	MET	LEU	Y511	M447	N385	T322	Q256	Q192	T109		ARG
SER	ASN	PRO	LYS	L512	C448	G386	V323	A257	A193	A257	Y36	HIS
ASN	ASN	ALA	ARG	L513	D449	I387	E324	V258	T194	D111	I38	ARG
ASP	ASN	PRO	LYS	S514	Q450	V388		Y259	D195	V112	I38	SER
ASP	GLU	PRO	LYS	D515	N451		N327	K260	L196		T39	GLY
HIS	GLU	HIS	VAL	A516	P452		E328	K261	E197	S116	G40	GLU
TYR	HIS	TYR	VAL	Q517	P457	G392	A329	R262	G198	V117	Q41	GLU
ARG	ASP	ARG	LYS	N518	L457	N393	P330	V263	A199	R118	Q42	ALA
PRO	GLU	PRO	GLU	N619	T458	L394	F331	N264	G200	E119		HIS
ASN	ASN	ARG	PRO	N620	T459	D395	F332	E265	L201		N45	SER
TYR	TYR	PRO	LEU	Q521	S460	R396	V333	G266	S202	V127	P46	SER
SER	LEU	SER	LEU	L522	D461	E397	P334	G267	V203	M128	P47	ARG
ASN	ASN	ASN	LEU	T523		S398	A335	F268		A129	Q48	SER
ASP	PRO	ASP	PRO	V524	T464	E399	V336	F269	T208	V130	G49	LYS
TRP	TRP	ASP	GLU	V525	P465	Y400	S337	N270	T209	S131	V50	LEU
GLY	GLY	GLU	ASP	N526	P466	V401	R338	I271	Q210	A132	F51	PRO
SER	SER	ILE	ASP		M467	N403	V339	T272	T211	T133	R52	VAL
ARG	ARG	GLY	THR	V529	T468	K402	D340	T273	T212	D134	I53	LEU
PHE	ASN	ASN	ARG	C530	Y469	N404	V341	D274	D213		E54	THR
ARG	PHE	PHE	ASP	S531	P470	T405	S342	P275	A214	D137	W55	PHE
LYS	ILE	ILE	ASN	C532	Y471	Y406	E343	S276	N215	N138	E56	PRO
LEU	ASP	ASP	ILE	E533	K472	T407	D344	S277	D216	I139	T57	GLY
ALA	GLU	GLU	PHE	G534	V473	V408	L345	N278	N217		G53	THR
ASP	ASN	ASN	TYR		S474	I409	S346	Q279		L142	W59	HIS
MET	MET	LEU	TYR	I537	L475	M410	R347	G280	T220		M60	THR
TYR	TYR	ASP	GLY	K538	S476	L411	G348	I281	F221	L146	L61	GLY
GLY	GLY	ALA	GLU	C539	H477	V412	E349	L282	D222		V62	LEU
GLY	GLY	ALA	GLY	Q540	S478	T413	K360	T283	P223	I150	T63	LYS
ASP	ASP	ASP	GLY	GLU	S479	D414	I351	T284	K224	L151	L66	ARG
ASP	ASN	ASN	LYS	LYS	P490	I352	I352	A285	T225	L25	D67	LYS
ASP	ASP	ASP	GLY	LEU	L481	S353	S353	K286	Y226	Q153	R68	LYS
GLU	GLU	PRO	GLU	VAL	T482	G416	L354	G287	D154	D154	E69	ARG
GLU	THR	THR	GLU	GLY	W483	V417		L288	A228	P155		D1
ALA	ALA	ALA	ASP	GLY	K484	S418	D358	D289	L229	E156	W2	W2
PRO	PRO	PRO	GLN	PHE	A485	G420	P359	F290	V230	E157	V3	V3
PRO	ASP	PRO	ASP	ASP	E486	T421	D360	E291	P231	P158	I4	I4
TYR	TYR	TYR	TYR	LEU	L487	G422	K361	L292	E232	T159	P5	P5
ASP	ASP	ASP	ASP	PRO	D488	T423	Q362	R293	N233	P160	P6	P6
SER	SER	SER	LEU	ILE	S489	G424	Q363		K234	N161	I7	I7
LEU	LEU	LEU	SER	ILE	K490	T425	I364	Y296	E235	L162	K8	K8
LEU	LEU	LEU	GLN	ILE	C491	L426	Q365	V297	G236	F163		E11
VAL	VAL	VAL	LEU	VAL	T492	I427	K366	L298	F237	T164	S86	S86
PHE	PHE	PHE	HIS	ILE	S493	L428	L367	Q299	E238	I165	P87	P87
ASP	ASP	ASP	ARG	LEU	M494	H429	S368	I300	V239		V88	V88
TYR	TYR	TYR	GLY	GLY	L495	V430	Y369	T301	Q240	T169	E89	E89
GLY	GLY	GLY	LEU	SER	L496	L431	F370		R241	G170	E90	E90
GLY	GLY	GLY	ASP	VAL	S497	D432	I371	P307	L242	V171	P91	P91
SER	SER	SER	ASP	LEU	P498	V433	G372	F308	S243		N92	N92
GLY	GLY	GLY	ARG	ALA	T499	N434	N373	S309	V244	L174	E93	E93
PRO	PRO	PRO	PRO	LEU	Q500	D435	D374	V310	T245	I175	I94	I94
GLU	GLU	GLU	ASP	LEU	Q501	N436	P375	P311	D246	G176	T95	T95
ALA	ALA	ALA	ILE	ILE	L502	G437	A376	L312	L247		I96	I96
ALA	ALA	ALA	ILE	ILE	K503	P438	R377		D248	R181	S26	S26
SER	SER	SER	MET	LEU	K504	V439	W378		N249		D100	D100
LEU	LEU	LEU	ARG	PHE	G505	P440	W379	S315	E250	E186	Q101	Q101
SER	SER	SER	ASN	LEU	D506	S441	T380	A317	G251	Y187	D29	D29
SER	SER	SER	VAL	LEU	Y507	P442	V381	T318	T252	T188	R105	R105

## 4 Experimental information

Property	Value	Source
Reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of tilted 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/UT	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 ⓘ

### 5.1 Standard geometry ⓘ

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%)	1.39	78/5839 (1.3%)
1	B	0.70	8/4276 (0.2%)	1.39	78/5839 (1.3%)
1	C	0.70	8/4276 (0.2%)	1.39	78/5839 (1.3%)
1	D	0.70	8/4276 (0.2%)	1.39	78/5839 (1.3%)
All	All	0.70	32/17104 (0.2%)	1.39	312/23356 (1.3%)

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	0	4
1	B	0	4
1	C	0	4
1	D	0	4
All	All	0	16

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	335	ALA	CA-CB	-8.36	1.34	1.52
1	C	335	ALA	CA-CB	-8.34	1.34	1.52
1	A	335	ALA	CA-CB	-8.33	1.34	1.52
1	D	335	ALA	CA-CB	-8.33	1.34	1.52
1	D	539	CYS	CB-SG	8.16	1.96	1.82

The worst 5 of 312 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	520	PRO	CA-C-N	-13.29	87.96	117.20
1	A	520	PRO	CA-C-N	-13.29	87.96	117.20
1	D	520	PRO	CA-C-N	-13.27	88.01	117.20
1	C	520	PRO	CA-C-N	-13.27	88.02	117.20
1	C	235	ILE	N-CA-C	12.74	145.40	111.00

There are no chirality outliers.

5 of 16 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	4086	757	0
1	B	4191	0	4089	752	0
1	C	4191	0	4087	717	0
1	D	4191	0	4086	711	0
2	A	154	0	143	84	0
2	B	154	0	143	83	0
2	C	154	0	143	84	0
2	D	154	0	143	84	0
3	A	56	0	52	16	0
3	B	56	0	52	16	0
3	C	56	0	52	16	0
3	D	56	0	52	15	0
4	A	12	0	0	0	0
4	B	12	0	0	0	0
4	C	12	0	0	0	0
4	D	12	0	0	0	0
All	All	17652	0	17128	2836	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 82.

The worst 5 of 2836 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	1.61
1:D:464:ILE:HD12	1:D:465:PRO:CD	1.30	1.59
1:A:464:ILE:HD12	1:A:465:PRO:CD	1.30	1.56
1:C:464:ILE:HD12	1:C:465:PRO:CD	1.30	1.56
1:C:24:ILE:HG21	1:D:2:TRP:CA	1.42	1.48

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
1	C	538/880 (61%)	401 (74%)	92 (17%)	45 (8%)	1	15
1	D	538/880 (61%)	401 (74%)	92 (17%)	45 (8%)	1	15
All	All	2152/3520 (61%)	1604 (74%)	368 (17%)	180 (8%)	2	15

5 of 180 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 ⓘ

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
1	C	480/779 (62%)	381 (79%)	99 (21%)	1	8
1	D	480/779 (62%)	381 (79%)	99 (21%)	1	8
All	All	1920/3116 (62%)	1524 (79%)	396 (21%)	4	8

5 of 396 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	447	MET
1	C	217	ASN
1	D	398	SER
1	B	466	PRO
1	C	27	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 91 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	455	GLN
1	C	110	GLN
1	D	391	ASN
1	B	467	ASN
1	C	27	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 108 ligands modelled in this entry, 48 are monoatomic - leaving 60 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	0.66	0	15,19,21	1.00	1 (6%)
2	NAG	A	802	1	14,14,15	0.75	1 (7%)	15,19,21	0.91	0
2	NAG	A	803	1	14,14,15	0.94	1 (7%)	15,19,21	1.21	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	0.71	0	15,19,21	1.06	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	1.24	2 (13%)
2	NAG	A	808	1	14,14,15	0.67	0	15,19,21	0.67	0
2	NAG	A	809	1	14,14,15	0.77	1 (7%)	15,19,21	0.85	0
2	NAG	A	810	1	14,14,15	0.66	0	15,19,21	1.40	4 (26%)
3	NDG	A	811	1	14,14,15	0.84	0	15,19,21	1.95	1 (6%)
2	NAG	A	812	1	14,14,15	0.85	1 (7%)	15,19,21	0.74	0
3	NDG	A	902	1	14,14,15	1.11	1 (7%)	15,19,21	1.13	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	0.65	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	1 (7%)	15,19,21	0.91	0
2	NAG	B	803	1	14,14,15	0.95	1 (7%)	15,19,21	1.21	2 (13%)
3	NDG	B	804	1	14,14,15	0.63	0	15,19,21	0.81	0
2	NAG	B	805	1	14,14,15	0.70	0	15,19,21	1.06	1 (6%)
2	NAG	B	806	1	14,14,15	0.55	0	15,19,21	1.44	3 (20%)
2	NAG	B	807	1	14,14,15	0.65	0	15,19,21	1.24	2 (13%)
2	NAG	B	808	1	14,14,15	0.67	0	15,19,21	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	B	809	1	14,14,15	0.78	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	0.85	0	15,19,21	1.96	1 (6%)
2	NAG	B	812	1	14,14,15	0.84	1 (7%)	15,19,21	0.76	1 (6%)
3	NDG	B	902	1	14,14,15	1.10	1 (7%)	15,19,21	1.13	1 (6%)
3	NDG	B	903	1	14,14,15	0.52	0	15,19,21	0.81	0
2	NAG	B	904	1	14,14,15	0.77	1 (7%)	15,19,21	0.64	0
2	NAG	C	801	1	14,14,15	0.67	0	15,19,21	1.00	1 (6%)
2	NAG	C	802	1	14,14,15	0.74	1 (7%)	15,19,21	0.92	0
2	NAG	C	803	1	14,14,15	0.95	1 (7%)	15,19,21	1.21	2 (13%)
3	NDG	C	804	1	14,14,15	0.62	0	15,19,21	0.82	0
2	NAG	C	805	1	14,14,15	0.70	0	15,19,21	1.06	1 (6%)
2	NAG	C	806	1	14,14,15	0.56	0	15,19,21	1.44	3 (20%)
2	NAG	C	807	1	14,14,15	0.64	0	15,19,21	1.25	2 (13%)
2	NAG	C	808	1	14,14,15	0.67	0	15,19,21	0.67	0
2	NAG	C	809	1	14,14,15	0.77	1 (7%)	15,19,21	0.86	0
2	NAG	C	810	1	14,14,15	0.64	0	15,19,21	1.40	4 (26%)
3	NDG	C	811	1	14,14,15	0.85	0	15,19,21	1.95	1 (6%)
2	NAG	C	812	1	14,14,15	0.84	1 (7%)	15,19,21	0.76	1 (6%)
3	NDG	C	902	1	14,14,15	1.11	1 (7%)	15,19,21	1.13	1 (6%)
3	NDG	C	903	1	14,14,15	0.52	0	15,19,21	0.80	0
2	NAG	C	904	1	14,14,15	0.79	1 (7%)	15,19,21	0.65	0
2	NAG	D	801	1	14,14,15	0.68	0	15,19,21	1.00	0
2	NAG	D	802	1	14,14,15	0.73	0	15,19,21	0.91	0
2	NAG	D	803	1	14,14,15	0.95	1 (7%)	15,19,21	1.21	2 (13%)
3	NDG	D	804	1	14,14,15	0.64	0	15,19,21	0.82	0
2	NAG	D	805	1	14,14,15	0.70	0	15,19,21	1.06	1 (6%)
2	NAG	D	806	1	14,14,15	0.55	0	15,19,21	1.44	3 (20%)
2	NAG	D	807	1	14,14,15	0.65	0	15,19,21	1.24	2 (13%)
2	NAG	D	808	1	14,14,15	0.67	0	15,19,21	0.66	0
2	NAG	D	809	1	14,14,15	0.77	1 (7%)	15,19,21	0.86	0
2	NAG	D	810	1	14,14,15	0.64	0	15,19,21	1.40	4 (26%)
3	NDG	D	811	1	14,14,15	0.85	0	15,19,21	1.96	1 (6%)
2	NAG	D	812	1	14,14,15	0.84	1 (7%)	15,19,21	0.76	1 (6%)
3	NDG	D	902	1	14,14,15	1.11	1 (7%)	15,19,21	1.13	1 (6%)
3	NDG	D	903	1	14,14,15	0.52	0	15,19,21	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	D	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
2	NAG	C	801	1	-	0/6/23/26	0/1/1/1
2	NAG	C	802	1	-	0/6/23/26	0/1/1/1
2	NAG	C	803	1	-	0/6/23/26	0/1/1/1
3	NDG	C	804	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	805	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	C	806	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	C	807	1	-	0/6/23/26	0/1/1/1
2	NAG	C	808	1	-	0/6/23/26	0/1/1/1
2	NAG	C	809	1	-	0/6/23/26	0/1/1/1
2	NAG	C	810	1	-	0/6/23/26	0/1/1/1
3	NDG	C	811	1	-	0/6/23/26	0/1/1/1
2	NAG	C	812	1	-	0/6/23/26	0/1/1/1
3	NDG	C	902	1	-	0/6/23/26	0/1/1/1
3	NDG	C	903	1	-	0/6/23/26	0/1/1/1
2	NAG	C	904	1	-	0/6/23/26	0/1/1/1
2	NAG	D	801	1	-	0/6/23/26	0/1/1/1
2	NAG	D	802	1	-	0/6/23/26	0/1/1/1
2	NAG	D	803	1	-	0/6/23/26	0/1/1/1
3	NDG	D	804	1	-	0/6/23/26	0/1/1/1
2	NAG	D	805	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	D	806	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	D	807	1	-	0/6/23/26	0/1/1/1
2	NAG	D	808	1	-	0/6/23/26	0/1/1/1
2	NAG	D	809	1	-	0/6/23/26	0/1/1/1
2	NAG	D	810	1	-	0/6/23/26	0/1/1/1
3	NDG	D	811	1	-	0/6/23/26	0/1/1/1
2	NAG	D	812	1	-	0/6/23/26	0/1/1/1
3	NDG	D	902	1	-	0/6/23/26	0/1/1/1
3	NDG	D	903	1	-	0/6/23/26	0/1/1/1
2	NAG	D	904	1	-	0/6/23/26	0/1/1/1

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	904	NAG	C1-C2	-2.50	1.49	1.52
2	D	904	NAG	C1-C2	-2.44	1.49	1.52
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	C	812	NAG	C1-C2	-2.37	1.49	1.52

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	811	NDG	C2-N2-C7	-6.88	112.91	122.94
3	D	811	NDG	C2-N2-C7	-6.86	112.94	122.94
3	A	811	NDG	C2-N2-C7	-6.85	112.96	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	811	NDG	C2-N2-C7	-6.83	112.98	122.94
2	C	806	NAG	C2-N2-C7	-3.37	118.03	122.94

5 of 8 chirality outliers are listed below:

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

There are no torsion outliers.

There are no ring outliers.

52 monomers are involved in 398 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	11	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	20	0
2	B	803	NAG	4	0
3	B	804	NDG	2	0
2	B	805	NAG	7	0
2	B	806	NAG	11	0
2	B	807	NAG	17	0
2	B	808	NAG	2	0
2	B	809	NAG	8	0
2	B	810	NAG	13	0
3	B	811	NDG	6	0
2	B	812	NAG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	902	NDG	8	0
2	B	904	NAG	8	0
2	C	801	NAG	21	0
2	C	803	NAG	4	0
3	C	804	NDG	2	0
2	C	805	NAG	7	0
2	C	806	NAG	12	0
2	C	807	NAG	16	0
2	C	808	NAG	2	0
2	C	809	NAG	8	0
2	C	810	NAG	13	0
3	C	811	NDG	6	0
2	C	812	NAG	3	0
3	C	902	NDG	8	0
2	C	904	NAG	8	0
2	D	801	NAG	21	0
2	D	803	NAG	4	0
3	D	804	NDG	2	0
2	D	805	NAG	7	0
2	D	806	NAG	12	0
2	D	807	NAG	16	0
2	D	808	NAG	2	0
2	D	809	NAG	8	0
2	D	810	NAG	13	0
3	D	811	NDG	5	0
2	D	812	NAG	3	0
3	D	902	NDG	8	0
2	D	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.