



wwPDB EM Validation Summary Report ⓘ

Dec 14, 2024 – 09:45 PM EST

PDB ID : 1Q5C
EMDB ID : EMD-1052
Title : S-S-lambda-shaped TRANS and CIS 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)
Based on initial model : 1L3W

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

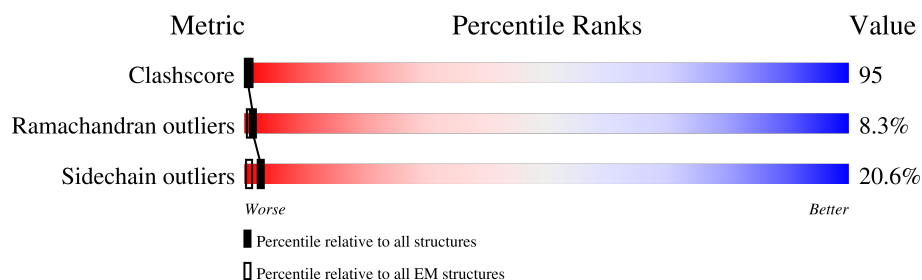
1 Overall quality at a glance

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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

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	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	806	X	-	X	-
2	NAG	A	807	-	-	X	-
2	NAG	A	809	-	-	X	-
2	NAG	A	810	-	-	X	-
2	NAG	A	902	X	-	X	-
2	NAG	A	903	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	902	X	-	X	-
2	NAG	B	903	X	-	-	-
2	NAG	B	904	-	-	X	-
2	NAG	C	801	-	-	X	-
2	NAG	C	805	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	902	X	-	X	-
2	NAG	C	903	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	902	X	-	X	-
2	NAG	D	903	X	-	-	-
2	NAG	D	904	-	-	X	-
3	NDG	A	811	-	-	X	-
3	NDG	B	811	-	-	X	-
3	NDG	D	811	-	-	X	-

2 Entry composition [i](#)

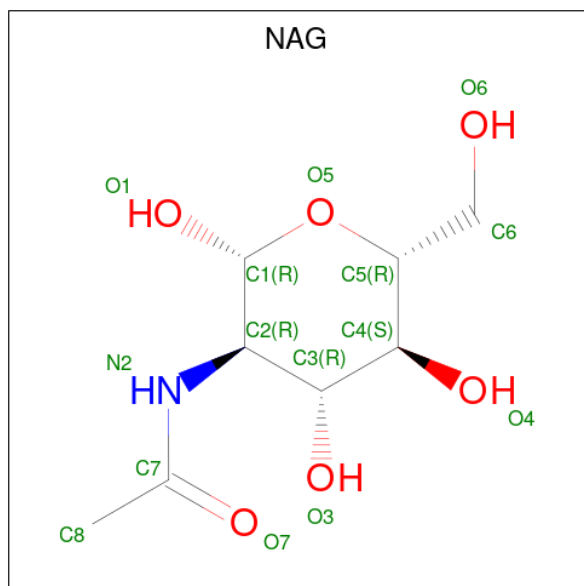
There are 4 unique types of molecules in this entry. The entry contains 17652 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total 14	C 8	N 1	O 5	0
2	A	1	Total 14	C 8	N 1	O 5	0
2	A	1	Total 14	C 8	N 1	O 5	0
2	A	1	Total 14	C 8	N 1	O 5	0
2	A	1	Total 14	C 8	N 1	O 5	0
2	A	1	Total 14	C 8	N 1	O 5	0
2	A	1	Total 14	C 8	N 1	O 5	0
2	A	1	Total 14	C 8	N 1	O 5	0
2	A	1	Total 14	C 8	N 1	O 5	0
2	A	1	Total 14	C 8	N 1	O 5	0
2	A	1	Total 14	C 8	N 1	O 5	0
2	B	1	Total 14	C 8	N 1	O 5	0
2	B	1	Total 14	C 8	N 1	O 5	0
2	B	1	Total 14	C 8	N 1	O 5	0
2	B	1	Total 14	C 8	N 1	O 5	0
2	B	1	Total 14	C 8	N 1	O 5	0
2	B	1	Total 14	C 8	N 1	O 5	0
2	B	1	Total 14	C 8	N 1	O 5	0
2	B	1	Total 14	C 8	N 1	O 5	0
2	B	1	Total 14	C 8	N 1	O 5	0
2	B	1	Total 14	C 8	N 1	O 5	0

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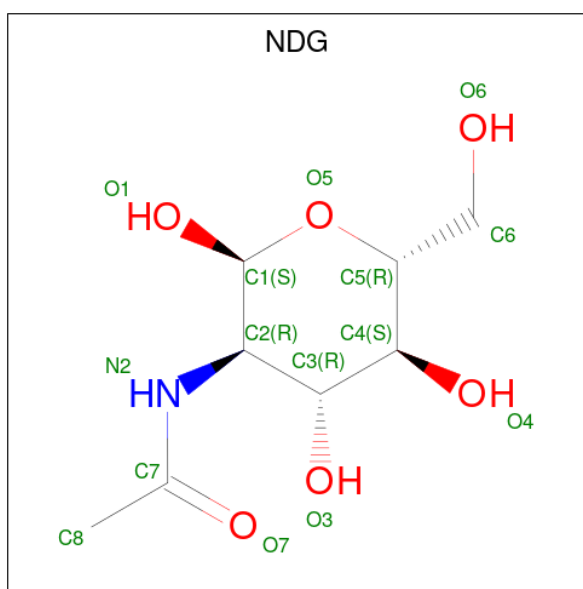
Mol	Chain	Residues	Atoms				AltConf
2	B	1	Total 14	C 8	N 1	O 5	0
2	B	1	Total 14	C 8	N 1	O 5	0
2	B	1	Total 14	C 8	N 1	O 5	0
2	C	1	Total 14	C 8	N 1	O 5	0
2	C	1	Total 14	C 8	N 1	O 5	0
2	C	1	Total 14	C 8	N 1	O 5	0
2	C	1	Total 14	C 8	N 1	O 5	0
2	C	1	Total 14	C 8	N 1	O 5	0
2	C	1	Total 14	C 8	N 1	O 5	0
2	C	1	Total 14	C 8	N 1	O 5	0
2	C	1	Total 14	C 8	N 1	O 5	0
2	C	1	Total 14	C 8	N 1	O 5	0
2	C	1	Total 14	C 8	N 1	O 5	0
2	C	1	Total 14	C 8	N 1	O 5	0
2	C	1	Total 14	C 8	N 1	O 5	0
2	C	1	Total 14	C 8	N 1	O 5	0
2	D	1	Total 14	C 8	N 1	O 5	0
2	D	1	Total 14	C 8	N 1	O 5	0
2	D	1	Total 14	C 8	N 1	O 5	0
2	D	1	Total 14	C 8	N 1	O 5	0
2	D	1	Total 14	C 8	N 1	O 5	0

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Mol	Chain	Residues	Atoms				AltConf
2	D	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 3 is 2-acetamido-2-deoxy- α -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
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	

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

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

LEU	SER	SER	LEU	ASN	SER	ASN	SER	ASN	ASP	GLU	HIS	ASP	TYR	ASN	TYR	LEU	SER	ASP	TRP	GLY	SER	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



MET	GLY	SER	THR	ARG	LEU	ARG	ASN	ALA	SER	VAL	TRP	LEU	CYS	GLY	LEU	CYS	LEU	GLN	VAL	VAL	PRO	SER	ILE	ASN	ALA	ASP	VAL	SER	GLY	CYS	LYS	PRO	GLY	PHE	SER	SER	ALA	ASN	VAL	GLU	TYR	ILE	PHE	SER	VAL	ASN	ARG	ARG	GLU	LEU	LEU	GLU	GLY	LYS	VAL
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ASN	PHE	SER	ASP	THR	THR	ARG	LYS	HIS	GLY	LEU	TYR	ASP	VAL	GLY	ASP	SER	ARG	PHE	ARG	VAL	LEU	PRO	ASP	GLY	THR	VAL	LEU	VAL	LYS	ARG	HIS	VAL	VAL	LYS	LEU	LYS	HIS	ASP	LYS	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	PRO	VAL	LEU	THR	LEU	PHE	PRO	GLU	THR	THR	GLY	LEU	LYS	ARG	LYS	LYS	LYS	ARG	D1	W2	W3	V4	I4	I4	I7	K8	E11	P16	F17	F18	K19	V22	Q23	I24	I27	K28	D29	R30	F31	P32
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K33	V34	V35	V36	S37	I38	T39	G40	G41	G42	N45	P46	P47	Q48	G49	V50	F51	R52	I53	E54	W55	E56	T57	G58	W59	M60	L61	V62	T63	L66	D67	R68	E69	W75	L76	S77	S78	H79	A80	V81	S82	E83	N84	G85	S86	P87	V88	E89	E90	P91	M92	E93	I94	T95	I96	L97	L98	S99	T00
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L0101		L0105	P106	K107	F108	T109	Q110	D111	V112	S116	V117	E118	R119		V127	M128	A129	V130	S131	A132	T133	D134		P137	M138	I139		L142		L146		V150	L151	K152	Q153	D154	P155	E156	E157		P160	M161	L162	F163	T164	L165		T169	G170	V171		L174	L175	G176				R181				F186
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Y187	Y188	Y189	Y190	Y191	Y192	Y193	Y194	Y195	Y196	Y197	Y198	Y199	Y200	Y201	Y202	Y203	Y204	Y205	Y206	Y207	Y208	Y209	Y210	Y211	Y212	Y213	Y214	Y215	Y216	Y217	Y218	Y219	Y220	Y221	Y222	Y223	Y224	Y225	Y226	Y227	Y228	Y229	Y230	Y231	Y232	Y233	Y234	Y235	Y236	Y237	Y238	Y239	Y240	Y241	Y242	Y243	Y244	Y245	Y246	Y247	Y248	Y249	Y250
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P251	T252	P253	A254	W255	P256	A257	T258	W259	P260	T261	P262	T263	T264	G265	G266	G267	P268	T269	T270	T271	T272	T273	T274	T275	E276	S277	T278	Q279	G280	T281	T282	T283	T284	A285	K286	T287	T288	T289	Q290	T291	T292	K293			T296	Q297	T298	Q299	T300	T301			P307	S308	S309	T310	P311	T312			S315	T316
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A317	A318	A319	A320	A321	A322	A323	A324	A327	A330	A331	A332	A333	A334	A335	A336	A337	A338	A339	A340	A341	A342	A343	A344	A345	A346	A347	A348	A349	A350	A351	A352	A353	A354	A355	A356	A357	A358	A359	A360	A361	A362	A363	A364	A365	A366	A367	A368	A369	A370	A371	A372	A373	A374	A375	A376	A377	A378	A379	A380
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V381	K352	K383	K384	K385	G386	K387	V388	K391	K392	K393	K394	K395	K396	K397	K398	K399	K400	K401	K402	K403	K404	K405	K406	K407	K408	K409	K410	K411	K412	K413	K414	K415	K416	K417	K418	K419	K420	K421	K422	K423	K424	K425	K426	K427	K428	K429	K430	K431	K432	K433	K434	K435	K436	K437	K438	K439	K440	K441
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P442
R443
T444
M447
Q448
D449
Q450
M451
P452
L457
T458
L459
Q460
D461
L464
P465
M467
T468
Q469
P470
Y471
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M473
S474
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P476
M477
Q478
S479
D480
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T482
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A485
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Q488
P489
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K503
M504
P505
Q506

Y507	Y508	Y509	Y510	Y511	Y512	Y513	Y514	Y515	Y516	Y517	Y518	Y519	Y520	Y521	Y522	Y523	Y524	Y525	Y526	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	Y703	Y704	Y705	Y706	Y707	Y708	Y709	Y710	Y711	Y712	Y713	Y714	Y715	Y716	Y717	Y718	Y719	Y720	Y721	Y722	Y723	Y724	Y725	Y726	Y727	Y728	Y729	Y730	Y731	Y732	Y733	Y734	Y735	Y736	Y737	Y738	Y739	Y740	Y741	Y742	Y743	Y744	Y745	Y746	Y747	Y748	Y749	Y750	Y751	Y752	Y753	Y754	Y755	Y756	Y757	Y758	Y759	Y760	Y761	Y762	Y763	Y764	Y765	Y766	Y767	Y768	Y769	Y770	Y771	Y772	Y773	Y774	Y775	Y776	Y777	Y778	Y779	Y780	Y781	Y782	Y783	Y784	Y785	Y786	Y787	Y788	Y789	Y790	Y791	Y792	Y793	Y794	Y795	Y796	Y797	Y798	Y799	Y800	Y801	Y802	Y803	Y804	Y805	Y806	Y807	Y808	Y809	Y810	Y811	Y812	Y813	Y814	Y815	Y816	Y817	Y818	Y819	Y820	Y821	Y822	Y823	Y824	Y825	Y826	Y827	Y828	Y829	Y830	Y831	Y832	Y833	Y834	Y835	Y836	Y837	Y838	Y839	Y840	Y841	Y842	Y843	Y844	Y845	Y846	Y847	Y848	Y849	Y850	Y851	Y852	Y853	Y854	Y855	Y856	Y857	Y858	Y859	Y860	Y861	Y862	Y863	Y864	Y865	Y866	Y867	Y868	Y869	Y870	Y871	Y872	Y873	Y874	Y875	Y876	Y877	Y878	Y879	Y880	Y881	Y882	Y883	Y884	Y885	Y886	Y887	Y888	Y889	Y890	Y891	Y892	Y893	Y894	Y895	Y896	Y897	Y898	Y899	Y900	Y901	Y902	Y903	Y904	Y905	Y906	Y907	Y908	Y909	Y910	Y911	Y912	Y913	Y914	Y915	Y916	Y917	Y918	Y919	Y920	Y921	Y922	Y923	Y924	Y925	Y926	Y927	Y928	Y929	Y930	Y931	Y932	Y933	Y934	Y935	Y936	Y937	Y938	Y939	Y940	Y941	Y942	Y943	Y944	Y945	Y946	Y947	Y948	Y949	Y950	Y951	Y952	Y953	Y954	Y955	Y956	Y957	Y958	Y959	Y960	Y961	Y962	Y963	Y964	Y965	Y966	Y967	Y968	Y969	Y970	Y971	Y972	Y973	Y974	Y975	Y976	Y977	Y978	Y979	Y980	Y981	Y982	Y983	Y984	Y985	Y986	Y987	Y988	Y989	Y990	Y991	Y992	Y993	Y994	Y995	Y996	Y997	Y998	Y999	Y1000
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LEU LEU LEU PHE LEU LEU LYS ARG LYS LYS VAL VAL LYS GLU PRO LEU LEU LEU LEU PRO GLU ASP ASP ARG ASN ILE PHE TYR THR ARG ASP GLU GLU GLY GLY GLY GLY GLU GLU GLN ASP ASP TYR TYR ASP ASP LEU SER LEU LEU HIS ARG GLY LEU ASP ASP ARG PRO ASP ILE MET ARG ASN ASD

VAL	VAL	PRO	PRO	THR	LEU	MET	PRO	PRO	PRO	HIS	TYR	ARG	TYR	PRO	PRO	ARG	ARG	PRO	SER	ASN	PRO	ASP	GLU	ILE	GLY	ASN	PHE	ILE	ASP	GLU	ASN	LEU	ASP	ALA	ALA	ASP	ASN	ASP	PRO	THR	PRO	PRO	PRO	TYR	ASP	SER	LEU	LEU	VAL	PHE	ASP	TYR	GLY	GLY	SER	GLU	ALA	ALA	SER	SER	LEU	SER
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SER	LEU	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



SER	GLU	ALA	ALA	ALA	SER	LEU	LEU	PRO	ASP	LEU	Q500	D435	D374	S309	V244	L174	I94	K33	ALA
GLU	ILE	ILE	ILE	ILE	SER	ILE	ILE	ASP	ASP	LEU	Q501	M436	P375	V310	T245	I175	T95	V34	SER
ALA	MET	MET	MET	MET	ARG	ARG	ARG	ILE	ILE	ARG	L502	P437	A376	L312	D246	G176	I96	Y35	ARG
LEU	ASN	ASN	ASN	ASN	ARG	ARG	ARG	PRO	PRO	ARG	K504	P439	W378	L312	L247		N97	Y36	HIS
LEU	ASN	ASN	ASN	ASN	ARG	ARG	ARG	ASP	ASP	ARG	G505	P440	W379	S315	D248		D100	S37	ARG
SER	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	SER	D506	S441	T380	T316	M249	E186	Q101	I38	SER
LEU	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	GLY	F507	R442	T381	A317	G251	Y187		T39	GLY
LEU	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	GLY	R443	R443	T382	T318	T252	T188	G40	G40	GLY
SER	THR	THR	THR	THR	THR	THR	THR	THR	THR	ALA	T446	T446	K383	V319	L189	R105	R105	Q41	ALA
ASN	THR	THR	THR	THR	THR	THR	THR	THR	THR	ALA	Y510	T447	K384	V320	L190	K107	A43	A43	ALA
ASN	MET	MET	MET	MET	MET	MET	MET	MET	MET	LYS	V511	M447	N385	V321	T255	V191	F108	D44	HIS
SER	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	LYS	L512	C448	N386	V322	Q256	Q192	T109	N45	SER
ASN	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	LYS	S514	D449	I387	V323	A257	A193	Q110	P46	ARG
ASP	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	LYS	S515	N451	V388	E324	Y258	T194	D111	P47	SER
GLU	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	VAL	A516	P452	N391	N327	Y259	D195	V112	Q48	SER
HIS	TYR	TYR	TYR	TYR	TYR	TYR	TYR	TYR	TYR	VAL	A517		G392		K260	L196	G49	G49	LYS
ASP	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	LYS	N518	L457	N393	P330	K261	E197	V50	V50	LEU
ASP	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	LYS	N519	T458	L394	F331	R262	G198	F51	F51	PRO
ASN	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	GLU	P520	T459	L395	F332	R263	A199	R52	R52	VAL
TYR	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	GLU	Q521	S460	R396	Y333	N264	G200	E19	E19	VAL
LEU	SER	SER	SER	SER	SER	SER	SER	SER	SER	LEU	L522	D461	E397	P334	G266	L201	E54	E54	THR
SER	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	LEU	T523		S398	A335	G267	V203	W55	W55	PHE
ASP	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	V524	I464	E399	Y336	F268		T57	T57	PRO
TRP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	GLU	V525	P465	Y400	S337	F269	I208	G58	G58	GLU
GLY	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	ASP	N526	P466	V401	R338	N270	Q129	M38	L66	THR
SER	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ASP		M467	K402	Y339	I271	Q210	A132	D67	HIS
ARG	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	V529	T468	N403	R339	I272	Q121	A132	M60	THR
PHE	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	THR	C530	Y469	N404	V341	T273	I211	T133	L61	GLY
ARG	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	ASN	S531	P470	N405	S342	D274	D213	D134	V62	LEU
LYS	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ASN	C532	Y471	Y406	S343	D275	A214	T63	T63	LYS
LEU	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ILE	E533	K472	T407	D344	E276	N215	L66	L66	ARG
ALA	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	PHE	G534	W473	V408	S277	L345	N216	D67	D67	LYS
ASP	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	TYR		S474	I409	S346	N278	N217	R68	R68	ARG
MET	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	TYR	I537	L475	M410	R347	Q279		E69	E69	LYS
TYR	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	GLY	K538	S476	L411	G348	G280	I220	L142	E70	W2
GLY	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	GLY	C539	H477	V412	E349	L281	F221	L146	Y71	V3
GLY	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	GLY	Q540	G478	T413	K350	L282	D222	I4	D72	I4
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	GLY	S479	S479	D414	I351	T283	P223	K73	K73	P6
ASP	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	GLY	LYS	D480	D415	I352	T284	K224	L151	Y74	P6
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	GLY	LEU	L481	G416	S353	T225	K152	V75	I7	I7
GLU	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	GLY	VAL	T482	V417	L354	K286	Y226	L76	K8	K8
GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	VAL	W483	S418		G287	T227	D154	S77	
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ASP	GLY	K494	V419	D388	L288	A228	P155	S78	E11
PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	GLN	PHE	A485	G420	P359	D289	L229	E156	H79	
ASP	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	ASP	ASP	E486	T421	D360	F290	V230	A80	P16	P16
TYR	TYR	TYR	TYR	TYR	TYR	TYR	TYR	TYR	TYR	ASP	LEU	L487	G422	K361	E291	P231	P158	V81	F17
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	PRO	D488	T423	Q362	L292	E232	I159	S82	P18
SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	LEU	ILE	S489	G424	Q363	N233	P160	E83	K19	K19
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	SER	ILE	K490	T425	I364	E234	N161	N84		
LEU	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	LEU	ILE	G491	L426	Q385	L235	L162	G85	V22	V22
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	LEU	VAL	T492	L427	K366	G236	F163	S86	Q23	Q23
PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	HIS	ILE	S493	L428	L367	T237	T164	P87		
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ARG	LEU	M494	H429	S368	E238	I165	V88	N27	N27
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ARG	GLY	L495	Y369	I300	V239		E89	K28	K28
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	SER	L496	F370	T301	Q240	T169	E90	D29	D29
ASP	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ASP	VAL	S497	I371	I371	G372	G170	P91	R30	R30
LEU	SER	SER	SER	SER	SER	SER	SER	SER	SER	LEU	VAL	P498	V433	M92	L242	V171	M92	F31	F31
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ARG	ALA	T499	N434	N373	F308	S243	E93	N32	N32

4 Experimental information

Property	Value	Source
EM reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of tilted images used	Not provided	
Resolution determination method	Not provided	
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 ($e^-/\text{\AA}^2$)	1200	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	500	Depositor
Magnification	68276	Depositor
Image detector	GENERIC GATAN	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: NDG, NAG, CA

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	0.70	8/4276 (0.2%)	1.39	77/5839 (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	311/23356 (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	-8.37	1.34	1.52
1	A	335	ALA	CA-CB	-8.36	1.34	1.52
1	D	335	ALA	CA-CB	-8.34	1.34	1.52
1	C	335	ALA	CA-CB	-8.29	1.35	1.52
1	B	539	CYS	CB-SG	8.15	1.96	1.82

The worst 5 of 311 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	520	PRO	CA-C-N	-13.29	87.95	117.20
1	B	520	PRO	CA-C-N	-13.27	88.00	117.20
1	C	520	PRO	CA-C-N	-13.27	88.00	117.20
1	A	520	PRO	CA-C-N	-13.25	88.04	117.20
1	D	235	ILE	N-CA-C	12.74	145.39	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	4089	796	0
1	B	4191	0	4081	863	0
1	C	4191	0	4078	1116	0
1	D	4191	0	4082	1111	0
2	A	182	0	168	93	0
2	B	182	0	168	90	0
2	C	182	0	169	92	0
2	D	182	0	169	92	0
3	A	28	0	24	9	0
3	B	28	0	24	10	0
3	C	28	0	24	8	0
3	D	28	0	24	9	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	17100	3289	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 95.

The worst 5 of 3289 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:24:ILE:HB	1:D:2:TRP:CE2	1.18	1.70
1:C:87:PRO:HG3	1:D:43:ALA:CB	1.22	1.65
1:C:87:PRO:CG	1:D:43:ALA:CB	1.77	1.61
1:C:87:PRO:HG3	1:D:43:ALA:CA	1.16	1.58
1:D:464:ILE:HD12	1:D:465:PRO:CD	1.29	1.58

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%)	402 (75%)	91 (17%)	45 (8%)	0	9
1	B	538/880 (61%)	401 (74%)	93 (17%)	44 (8%)	1	9
1	C	538/880 (61%)	401 (74%)	92 (17%)	45 (8%)	0	9
1	D	538/880 (61%)	401 (74%)	92 (17%)	45 (8%)	0	9
All	All	2152/3520 (61%)	1605 (75%)	368 (17%)	179 (8%)	1	9

5 of 179 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	6
1	B	480/779 (62%)	381 (79%)	99 (21%)	1	6
1	C	480/779 (62%)	381 (79%)	99 (21%)	1	6
1	D	480/779 (62%)	381 (79%)	99 (21%)	1	6
All	All	1920/3116 (62%)	1524 (79%)	396 (21%)	3	6

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

Mol	Chain	Res	Type
1	C	261	ILE
1	C	492	THR
1	C	284	THR
1	C	382	ASN
1	D	27	ASN

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

Mol	Chain	Res	Type
1	C	278	ASN
1	D	79	HIS
1	C	373	ASN
1	C	467	ASN
1	D	138	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	$\# Z > 2$
3	NDG	D	811	1	14,14,15	0.87	0	17,19,21	1.96	1 (5%)
2	NAG	C	801	1	14,14,15	0.70	0	17,19,21	0.98	1 (5%)
2	NAG	A	903	1	14,14,15	0.55	0	17,19,21	0.79	0
2	NAG	C	808	1	14,14,15	0.67	0	17,19,21	0.70	0
3	NDG	B	811	1	14,14,15	0.86	0	17,19,21	1.96	1 (5%)
2	NAG	D	812	1	14,14,15	0.83	1 (7%)	17,19,21	0.75	1 (5%)
2	NAG	A	807	1	14,14,15	0.64	0	17,19,21	1.19	2 (11%)
2	NAG	A	802	1	14,14,15	0.78	1 (7%)	17,19,21	0.85	0
2	NAG	B	809	1	14,14,15	0.76	0	17,19,21	0.94	0
2	NAG	D	805	1	14,14,15	0.71	0	17,19,21	1.05	1 (5%)
2	NAG	C	902	1	14,14,15	1.13	1 (7%)	17,19,21	1.09	2 (11%)
2	NAG	D	904	1	14,14,15	0.78	1 (7%)	17,19,21	0.70	1 (5%)
2	NAG	C	802	1	14,14,15	0.78	1 (7%)	17,19,21	0.85	0
2	NAG	B	904	1	14,14,15	0.77	1 (7%)	17,19,21	0.69	0
2	NAG	B	903	1	14,14,15	0.56	0	17,19,21	0.79	0
2	NAG	C	806	1	14,14,15	0.57	0	17,19,21	1.39	3 (17%)
2	NAG	D	902	1	14,14,15	1.13	1 (7%)	17,19,21	1.09	1 (5%)
2	NAG	C	903	1	14,14,15	0.55	0	17,19,21	0.78	0
2	NAG	D	806	1	14,14,15	0.55	0	17,19,21	1.38	3 (17%)
2	NAG	D	903	1	14,14,15	0.54	0	17,19,21	0.79	0
3	NDG	A	811	1	14,14,15	0.87	0	17,19,21	1.96	1 (5%)
2	NAG	B	802	1	14,14,15	0.78	1 (7%)	17,19,21	0.85	0
2	NAG	C	807	1	14,14,15	0.64	0	17,19,21	1.19	2 (11%)

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	0.71	0	17,19,21	0.99	1 (5%)
2	NAG	B	807	1	14,14,15	0.65	0	17,19,21	1.20	2 (11%)
2	NAG	C	803	1	14,14,15	1.00	1 (7%)	17,19,21	1.17	2 (11%)
2	NAG	C	904	1	14,14,15	0.77	1 (7%)	17,19,21	0.70	1 (5%)
2	NAG	D	803	1	14,14,15	1.00	1 (7%)	17,19,21	1.16	2 (11%)
2	NAG	B	808	1	14,14,15	0.66	0	17,19,21	0.70	0
3	NDG	A	804	1	14,14,15	0.65	0	17,19,21	0.78	0
3	NDG	B	804	1	14,14,15	0.64	0	17,19,21	0.78	0
3	NDG	C	811	1	14,14,15	0.87	0	17,19,21	1.96	1 (5%)
2	NAG	B	803	1	14,14,15	1.00	1 (7%)	17,19,21	1.17	2 (11%)
2	NAG	A	803	1	14,14,15	1.00	1 (7%)	17,19,21	1.16	2 (11%)
2	NAG	C	809	1	14,14,15	0.77	1 (7%)	17,19,21	0.94	0
2	NAG	C	812	1	14,14,15	0.83	1 (7%)	17,19,21	0.76	1 (5%)
3	NDG	D	804	1	14,14,15	0.64	0	17,19,21	0.78	0
2	NAG	D	809	1	14,14,15	0.77	1 (7%)	17,19,21	0.94	0
2	NAG	B	805	1	14,14,15	0.72	0	17,19,21	1.05	1 (5%)
2	NAG	A	810	1	14,14,15	0.67	0	17,19,21	1.33	4 (23%)
2	NAG	D	801	1	14,14,15	0.70	0	17,19,21	0.98	1 (5%)
2	NAG	B	812	1	14,14,15	0.83	1 (7%)	17,19,21	0.76	1 (5%)
2	NAG	C	810	1	14,14,15	0.66	0	17,19,21	1.33	4 (23%)
2	NAG	B	801	1	14,14,15	0.70	0	17,19,21	0.98	1 (5%)
2	NAG	B	902	1	14,14,15	1.12	1 (7%)	17,19,21	1.09	2 (11%)
2	NAG	A	806	1	14,14,15	0.55	0	17,19,21	1.39	3 (17%)
2	NAG	B	810	1	14,14,15	0.67	0	17,19,21	1.33	4 (23%)
2	NAG	A	812	1	14,14,15	0.84	1 (7%)	17,19,21	0.76	1 (5%)
2	NAG	D	810	1	14,14,15	0.67	0	17,19,21	1.33	4 (23%)
2	NAG	D	807	1	14,14,15	0.65	0	17,19,21	1.19	2 (11%)
2	NAG	A	808	1	14,14,15	0.67	0	17,19,21	0.70	0
2	NAG	A	904	1	14,14,15	0.77	1 (7%)	17,19,21	0.70	1 (5%)
3	NDG	C	804	1	14,14,15	0.64	0	17,19,21	0.78	0
2	NAG	A	809	1	14,14,15	0.77	1 (7%)	17,19,21	0.94	0
2	NAG	D	802	1	14,14,15	0.78	1 (7%)	17,19,21	0.85	0
2	NAG	A	805	1	14,14,15	0.72	0	17,19,21	1.06	1 (5%)
2	NAG	B	806	1	14,14,15	0.56	0	17,19,21	1.39	3 (17%)
2	NAG	D	808	1	14,14,15	0.66	0	17,19,21	0.70	0
2	NAG	A	902	1	14,14,15	1.15	1 (7%)	17,19,21	1.08	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	805	1	14,14,15	0.72	0	17,19,21	1.05	1 (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
3	NDG	D	811	1	-	2/6/23/26	0/1/1/1
2	NAG	C	801	1	-	4/6/23/26	0/1/1/1
2	NAG	A	903	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	C	808	1	-	3/6/23/26	0/1/1/1
3	NDG	B	811	1	-	2/6/23/26	0/1/1/1
2	NAG	D	812	1	-	4/6/23/26	0/1/1/1
2	NAG	D	805	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	A	802	1	-	2/6/23/26	0/1/1/1
2	NAG	A	807	1	-	5/6/23/26	0/1/1/1
2	NAG	B	809	1	-	2/6/23/26	0/1/1/1
2	NAG	C	902	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	D	904	1	-	3/6/23/26	0/1/1/1
2	NAG	C	806	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	D	902	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	B	903	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	B	904	1	-	3/6/23/26	0/1/1/1
2	NAG	C	802	1	-	2/6/23/26	0/1/1/1
2	NAG	C	903	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	D	806	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	D	903	1	1/1/5/7	2/6/23/26	0/1/1/1
3	NDG	A	811	1	-	2/6/23/26	0/1/1/1
2	NAG	B	802	1	-	2/6/23/26	0/1/1/1
2	NAG	C	807	1	-	5/6/23/26	0/1/1/1
2	NAG	A	801	1	-	4/6/23/26	0/1/1/1
2	NAG	B	807	1	-	5/6/23/26	0/1/1/1
2	NAG	C	803	1	-	2/6/23/26	0/1/1/1
2	NAG	C	904	1	-	3/6/23/26	0/1/1/1
2	NAG	D	803	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	808	1	-	3/6/23/26	0/1/1/1
3	NDG	A	804	1	-	0/6/23/26	0/1/1/1
3	NDG	B	804	1	-	0/6/23/26	0/1/1/1
3	NDG	C	811	1	-	2/6/23/26	0/1/1/1
2	NAG	B	803	1	-	2/6/23/26	0/1/1/1
2	NAG	A	803	1	-	2/6/23/26	0/1/1/1
2	NAG	C	809	1	-	2/6/23/26	0/1/1/1
2	NAG	C	812	1	-	4/6/23/26	0/1/1/1
3	NDG	D	804	1	-	0/6/23/26	0/1/1/1
2	NAG	D	809	1	-	2/6/23/26	0/1/1/1
2	NAG	B	805	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	A	810	1	-	3/6/23/26	0/1/1/1
2	NAG	D	801	1	-	4/6/23/26	0/1/1/1
2	NAG	B	812	1	-	4/6/23/26	0/1/1/1
2	NAG	C	810	1	-	3/6/23/26	0/1/1/1
2	NAG	B	801	1	-	4/6/23/26	0/1/1/1
2	NAG	B	902	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	B	810	1	-	3/6/23/26	0/1/1/1
2	NAG	A	805	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	A	812	1	-	4/6/23/26	0/1/1/1
2	NAG	D	810	1	-	3/6/23/26	0/1/1/1
2	NAG	D	807	1	-	5/6/23/26	0/1/1/1
2	NAG	A	808	1	-	3/6/23/26	0/1/1/1
2	NAG	A	904	1	-	3/6/23/26	0/1/1/1
3	NDG	C	804	1	-	0/6/23/26	0/1/1/1
2	NAG	A	809	1	-	2/6/23/26	0/1/1/1
2	NAG	D	802	1	-	2/6/23/26	0/1/1/1
2	NAG	A	806	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	B	806	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	D	808	1	-	3/6/23/26	0/1/1/1
2	NAG	A	902	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	C	805	1	1/1/5/7	2/6/23/26	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	A	902	NAG	C1-C2	3.42	1.57	1.52
2	C	902	NAG	C1-C2	3.37	1.56	1.52
2	B	902	NAG	C1-C2	3.34	1.56	1.52
2	D	902	NAG	C1-C2	3.33	1.56	1.52
2	C	803	NAG	O5-C5	2.65	1.48	1.43

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	811	NDG	C2-N2-C7	-7.43	112.94	122.90
3	A	811	NDG	C2-N2-C7	-7.42	112.95	122.90
3	B	811	NDG	C2-N2-C7	-7.42	112.95	122.90
3	C	811	NDG	C2-N2-C7	-7.41	112.97	122.90
2	B	806	NAG	C2-N2-C7	-3.65	118.01	122.90

5 of 16 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	805	NAG	C1
2	A	806	NAG	C1
2	A	902	NAG	C1
2	A	903	NAG	C1
2	B	805	NAG	C1

5 of 152 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	807	NAG	C3-C2-N2-C7
2	A	808	NAG	C1-C2-N2-C7
2	A	810	NAG	C1-C2-N2-C7
2	A	812	NAG	C1-C2-N2-C7
2	A	902	NAG	C3-C2-N2-C7

There are no ring outliers.

52 monomers are involved in 403 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	811	NDG	7	0
2	C	801	NAG	22	0
2	C	808	NAG	2	0
3	B	811	NDG	8	0
2	D	812	NAG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	807	NAG	17	0
2	B	809	NAG	8	0
2	D	805	NAG	7	0
2	C	902	NAG	8	0
2	D	904	NAG	8	0
2	B	904	NAG	8	0
2	C	806	NAG	10	0
2	D	902	NAG	8	0
2	D	806	NAG	12	0
3	A	811	NDG	7	0
2	C	807	NAG	17	0
2	A	801	NAG	21	0
2	B	807	NAG	16	0
2	C	803	NAG	4	0
2	C	904	NAG	8	0
2	D	803	NAG	4	0
2	B	808	NAG	2	0
3	A	804	NDG	2	0
3	B	804	NDG	2	0
3	C	811	NDG	6	0
2	B	803	NAG	4	0
2	A	803	NAG	4	0
2	C	809	NAG	8	0
2	C	812	NAG	3	0
3	D	804	NDG	2	0
2	D	809	NAG	8	0
2	B	805	NAG	7	0
2	A	810	NAG	13	0
2	D	801	NAG	21	0
2	B	812	NAG	3	0
2	C	810	NAG	13	0
2	B	801	NAG	20	0
2	B	902	NAG	8	0
2	A	806	NAG	12	0
2	B	810	NAG	12	0
2	A	812	NAG	3	0
2	D	810	NAG	12	0
2	D	807	NAG	17	0
2	A	808	NAG	2	0
2	A	904	NAG	8	0
3	C	804	NDG	2	0
2	A	809	NAG	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	805	NAG	7	0
2	B	806	NAG	12	0
2	D	808	NAG	2	0
2	A	902	NAG	8	0
2	C	805	NAG	6	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 Tomogram visualisation

This section contains visualisations of the EMDB entry EMD-1052. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Tomogram analysis

This section contains the results of statistical analysis of the tomogram.

7.1 Map-value distribution

This section was not generated.

8 Map-model fit

This section was not generated.