



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:38 PM BST

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)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

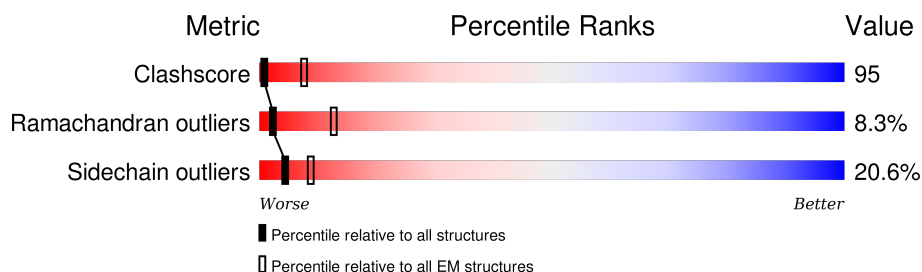
1 Overall quality at a glance

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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	16% 30% 11% • 39%
1	B	880	16% 31% 11% • 39%
1	C	880	15% 31% 11% • 39%
1	D	880	15% 32% 11% • 39%

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	-	-	-
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	811	-	-	X	-
3	NDG	B	902	-	-	X	-
3	NDG	C	902	-	-	X	-
3	NDG	D	811	-	-	X	-
3	NDG	D	902	-	-	X	-

2 Entry composition [i](#)

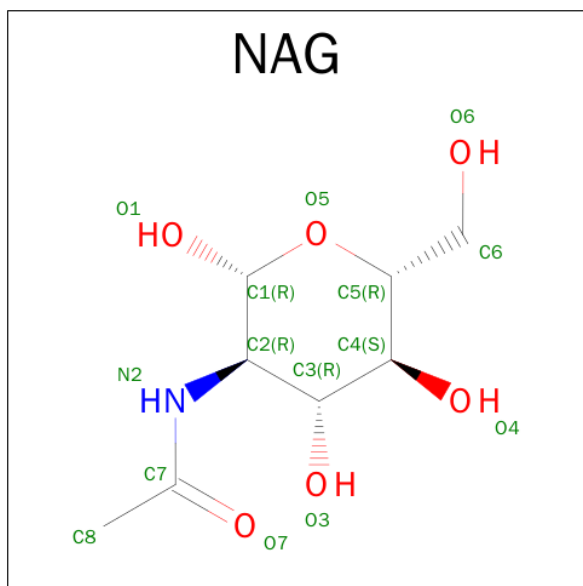
There are 4 unique types of molecules in this entry. The entry contains 17652 atoms, of which 0 are hydrogens and 0 are deuteriums.

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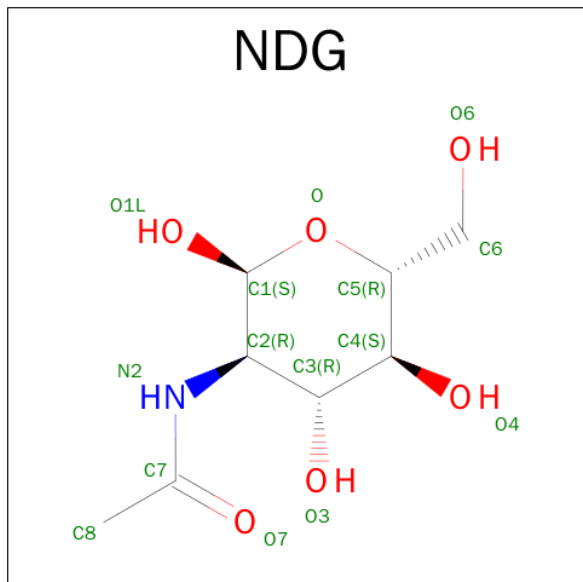
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	B	1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

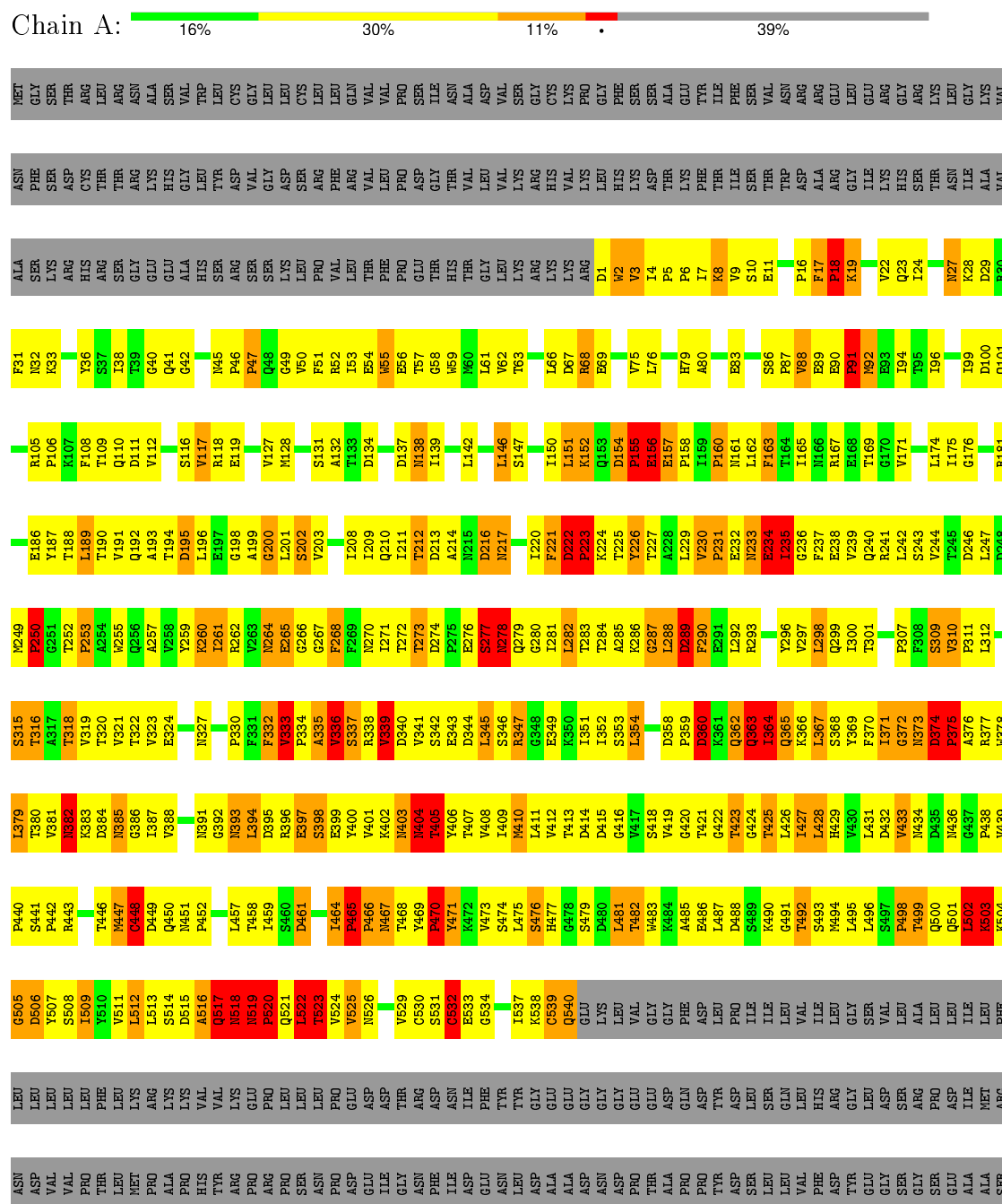
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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	

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: EP-cadherin



- Molecule 1: EP-cadherin

Chain D:

[illegible]

SER	GLU	PRO	LEU	Q500	D435	D374	S309	V244	L174	I94	K33	ALA
GLU	ILE	ASP	LEU	Q501	M436	P375	V310	T245	I175	T95	V34	SER
ALA	LEU	ILE	LEU	L502	G437	A376	P311	D246	G176	I96	V35	LYS
ALA	LEU	MET	LEU	K503	P438	R377	L312	L247		N97	T36	ARG
SER	LEU	ARG	PHE	K504	V439	M378	S315	D248	R181	D100	S37	HIS
LEU	LEU	ASN	LEU	G505	P440	L379	L316	M249		Q101	I38	ARG
SER	LEU	ASP	LEU	D506	S441	T380	T316	P250	E186		T39	SER
SER	LEU	VAL	LEU	P442	R443	V381	A317	T251	T187		Q40	GLY
LEU	LEU	VAL	LEU	R443		M382	T318	T252	T188		Q41	GLU
ASN	PRO	PRO	PHE	L509		K383	T319	P253	L189	R105	Q42	GLU
SER	SER	THR	PHE	Y510	T446	D384	V320	A254	T190	K107	A43	ALA
SER	SER	LEU	LEU	V511	M447	N385	V321	T255	V191	F108	D44	HIS
ASN	ASN	MET	LYS	L512	C448	N386	T322	Q256	Q192	T109	N45	SER
SER	SER	PRO	ARG	L513	D449	I387	V323	A257	A193	Q110	P46	ARG
ASN	ASN	ALA	LYS	S514	Q450	V388	E324	V258	T194		P47	SER
ASP	ASP	PRO	LYS	D515	M451			T259	D195	V112	Q48	SER
GLU	GLU	HIS	VAL	A516	P452	N391	N327	T260	L196		Q49	LYS
HIS	TYR	TYR	VAL	Q517		G392		I261	E197	S116	V50	LEU
ASP	ASP	ARG	LYS	M518	L457	N393	P330	R262	G198	V117	F51	PRO
TYR	TYR	PRO	GLU	M519	T458	L394	F331	V263	A199	R118	R52	VAL
ASN	ASN	ARG	PRO	P520	T459	D395	P332	R264	G200	E119	E54	LEU
TYR	TYR	PRO	LEU	Q521	S460	R396	V333	E265	L201		P55	THR
LEU	LEU	SER	LEU	L522	D461	E397	P334	G266	S202	V127		PHE
SER	SER	ASN	LEU	T523		S398	A335	G267	V203	M128	E56	PRO
ASP	ASP	PRO	PRO	V524	L464	E399	V336	F268		A129	T57	GLU
TRP	TRP	ASP	GLU	V525	P465	Y400	S337	F269	T208	V130	G58	THR
GLY	GLY	GLU	ASP	N526	P466	V401	R338		I209		R59	HIS
SER	SER	ILE	ASP		M467	K402	V339	E276	Q210	A132	L66	THR
ARG	ARG	GLY	THR	V529	T468	N403	D340	T271	T212	T133	L61	GLY
PHE	PHE	ASN	THR	C530	Y469	M404	V341	T272	T211		V62	LEU
ARG	ARG	PHE	ASN	S531	P470	T405	S342	D274	D213	D134	T63	LYS
LYS	LYS	ILE	ASN	G532	Y471	Y406	E343	F275	A214	D137		ARG
LEU	LEU	ASP	ILE	E533	T472	T407	D344	E276	R215	M138	L66	LYS
ALA	ALA	GLU	PHE	G534	Y473	V408	L345	S277	D216	I139	D67	LYS
ASP	ASP	ASN	TYR		S474	Y409	S346	T278	N217		R68	ARG
ASP	ASP	LEU	TYR	I537	S475	M410	R347	Q279		L142	E69	
GLU	GLU	PRO	GLY	K538	S476	L411	G348	G280	I220		V2	
GLU	GLU	ASP	GLU	G539	H477	V412	E349	I281	F221	L146	V3	
GLY	GLY	ALA	ALA	Q540	G478	T413	R350	T282	D222		I4	
ASP	ASP	ALA	GLY		S479	D414	L351	T283	P223	I150	P6	
ASP	ASP	ASN	GLY	LYS	D480	D415	L352	T284	K224	L151	P6	
ASP	ASP	ASP	GLY	LEU	L481	G416	S353	A285	T225	K152	V74	
GLU	GLU	PRO	GLU	VAL	T482	V417	L354	G286	K286	Q153	V75	
GLU	GLU	THR	GLU	GLY	M483	S418		G287	T227	D154	L76	
THR	THR	ALA	ASP	GLY	K484	V419	D358	L288	A228	P155	S77	
ALA	ALA	PRO	GLN	PHE	A485	G420	P359	D289	L229	E156	S78	
PRO	PRO	PRO	ASP	ASP	E486	T421	D360		V230	E157	R79	
TYR	TYR	TYR	TYR	LEU	L487	G422	L361	E291	P231	P158	V81	
ASP	ASP	ASP	ASP	PRO	D488	T423	D362	L292	E232	I159	S82	
SER	SER	SER	LEU	ILE	S489	G424	D363	R293	N233	P160	E83	
LEU	LEU	LEU	SER	ILE	K490	T425	L364		E234	N161	R84	
LEU	LEU	LEU	GLN	LEU	G491	L426	D365	Y296	I235	L162	G85	
VAL	VAL	VAL	LEU	VAL	T492	I427	K366	V297	G236	F163	S86	
PHE	PHE	HIS	HIS	ILE	S493	L428	L367	L298	F237	T164	P87	
ASP	ASP	ARG	ARG	LEU	M494	A429	S368	Q299	E238	I165	V88	
TYR	TYR	TYR	GLY	GLY	L495	V430	Y369	I300	V239		E89	
GLU	GLU	GLU	LEU	GLY	L496	L431	F370	T301	Q240	T169	E90	
GLY	GLY	GLY	ASP	VAL	S497	D432	I371		R241	G170	F91	
SER	SER	SER	SER	LEU	P498	V433	G372	P307	L242	V171	M92	
GLY	GLY	GLY	ARG	ALA	T499	M434	N373	F308	S243		E93	

4 Experimental information

Property	Value	Source
Reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	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	50000	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	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	794	0
1	B	4191	0	4081	861	0
1	C	4191	0	4078	1114	0
1	D	4191	0	4082	1110	0
2	A	154	0	142	84	0
2	B	154	0	142	81	0
2	C	154	0	143	83	0
2	D	154	0	143	83	0
3	A	56	0	52	16	0
3	B	56	0	52	17	0
3	C	56	0	52	15	0
3	D	56	0	52	17	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	17108	3282	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 3282 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%)	1	18
1	B	538/880 (61%)	401 (74%)	93 (17%)	44 (8%)	1	18
1	C	538/880 (61%)	401 (74%)	92 (17%)	45 (8%)	1	18
1	D	538/880 (61%)	401 (74%)	92 (17%)	45 (8%)	1	18
All	All	2152/3520 (61%)	1605 (75%)	368 (17%)	179 (8%)	2	18

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	10
1	B	480/779 (62%)	381 (79%)	99 (21%)	1	10
1	C	480/779 (62%)	381 (79%)	99 (21%)	1	10
1	D	480/779 (62%)	381 (79%)	99 (21%)	1	10
All	All	1920/3116 (62%)	1524 (79%)	396 (21%)	4	10

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 [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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	0.65	0	15,19,21	0.89	0
2	NAG	A	802	1	14,14,15	0.72	0	15,19,21	0.82	1 (6%)
2	NAG	A	803	1	14,14,15	0.92	1 (7%)	15,19,21	1.19	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	1.17	1 (6%)
2	NAG	A	806	1	14,14,15	0.54	0	15,19,21	1.41	2 (13%)
2	NAG	A	807	1	14,14,15	0.63	0	15,19,21	1.14	1 (6%)
2	NAG	A	808	1	14,14,15	0.67	0	15,19,21	0.70	0
2	NAG	A	809	1	14,14,15	0.76	1 (7%)	15,19,21	0.96	1 (6%)
2	NAG	A	810	1	14,14,15	0.64	0	15,19,21	1.09	1 (6%)
3	NDG	A	811	1	14,14,15	0.82	0	15,19,21	2.16	1 (6%)
2	NAG	A	812	1	14,14,15	0.83	1 (7%)	15,19,21	0.76	1 (6%)
3	NDG	A	902	1	14,14,15	1.09	1 (7%)	15,19,21	0.96	0
3	NDG	A	903	1	14,14,15	0.51	0	15,19,21	0.64	0
2	NAG	A	904	1,2	14,14,15	0.76	1 (7%)	15,19,21	0.79	1 (6%)
2	NAG	B	801	1	14,14,15	0.64	0	15,19,21	0.88	0
2	NAG	B	802	1	14,14,15	0.72	0	15,19,21	0.82	1 (6%)
2	NAG	B	803	1	14,14,15	0.92	1 (7%)	15,19,21	1.20	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	0.69	0	15,19,21	1.17	1 (6%)
2	NAG	B	806	1	14,14,15	0.54	0	15,19,21	1.42	2 (13%)
2	NAG	B	807	1	14,14,15	0.64	0	15,19,21	1.15	1 (6%)
2	NAG	B	808	1	14,14,15	0.66	0	15,19,21	0.70	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	0.75	0	15,19,21	0.96	1 (6%)
2	NAG	B	810	1	14,14,15	0.64	0	15,19,21	1.09	2 (13%)
3	NDG	B	811	1	14,14,15	0.81	0	15,19,21	2.16	1 (6%)
2	NAG	B	812	1	14,14,15	0.82	1 (7%)	15,19,21	0.76	1 (6%)
3	NDG	B	902	1	14,14,15	1.07	1 (7%)	15,19,21	0.96	0
3	NDG	B	903	1	14,14,15	0.52	0	15,19,21	0.65	0
2	NAG	B	904	1,2	14,14,15	0.75	1 (7%)	15,19,21	0.77	1 (6%)
2	NAG	C	801	1	14,14,15	0.64	0	15,19,21	0.88	0
2	NAG	C	802	1	14,14,15	0.72	0	15,19,21	0.82	1 (6%)
2	NAG	C	803	1	14,14,15	0.92	1 (7%)	15,19,21	1.20	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	0.69	0	15,19,21	1.17	1 (6%)
2	NAG	C	806	1	14,14,15	0.55	0	15,19,21	1.41	2 (13%)
2	NAG	C	807	1	14,14,15	0.63	0	15,19,21	1.13	1 (6%)
2	NAG	C	808	1	14,14,15	0.67	0	15,19,21	0.70	0
2	NAG	C	809	1	14,14,15	0.76	1 (7%)	15,19,21	0.96	1 (6%)
2	NAG	C	810	1	14,14,15	0.62	0	15,19,21	1.09	2 (13%)
3	NDG	C	811	1	14,14,15	0.82	0	15,19,21	2.16	1 (6%)
2	NAG	C	812	1	14,14,15	0.82	1 (7%)	15,19,21	0.76	1 (6%)
3	NDG	C	902	1	14,14,15	1.08	1 (7%)	15,19,21	0.96	0
3	NDG	C	903	1	14,14,15	0.52	0	15,19,21	0.64	0
2	NAG	C	904	1	14,14,15	0.76	1 (7%)	15,19,21	0.78	1 (6%)
2	NAG	D	801	1	14,14,15	0.64	0	15,19,21	0.88	0
2	NAG	D	802	1	14,14,15	0.73	0	15,19,21	0.82	1 (6%)
2	NAG	D	803	1	14,14,15	0.92	1 (7%)	15,19,21	1.20	2 (13%)
3	NDG	D	804	1	14,14,15	0.62	0	15,19,21	0.82	0
2	NAG	D	805	1	14,14,15	0.69	0	15,19,21	1.16	1 (6%)
2	NAG	D	806	1	14,14,15	0.54	0	15,19,21	1.40	2 (13%)
2	NAG	D	807	1	14,14,15	0.64	0	15,19,21	1.13	1 (6%)
2	NAG	D	808	1	14,14,15	0.66	0	15,19,21	0.70	0
2	NAG	D	809	1	14,14,15	0.76	1 (7%)	15,19,21	0.96	1 (6%)
2	NAG	D	810	1	14,14,15	0.63	0	15,19,21	1.08	1 (6%)
3	NDG	D	811	1	14,14,15	0.82	0	15,19,21	2.17	1 (6%)
2	NAG	D	812	1	14,14,15	0.83	1 (7%)	15,19,21	0.75	1 (6%)
3	NDG	D	902	1	14,14,15	1.07	1 (7%)	15,19,21	0.96	0
3	NDG	D	903	1	14,14,15	0.51	0	15,19,21	0.63	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	0.78	1 (6%)

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	1,2	-	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	1,2	-	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 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	904	NAG	C1-C2	-2.43	1.49	1.52
2	C	904	NAG	C1-C2	-2.40	1.49	1.52
2	A	904	NAG	C1-C2	-2.39	1.49	1.52
2	B	904	NAG	C1-C2	-2.38	1.49	1.52
2	A	812	NAG	C1-C2	-2.34	1.49	1.52

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	811	NDG	C2-N2-C7	-7.81	112.94	123.11
3	A	811	NDG	C2-N2-C7	-7.81	112.95	123.11
3	B	811	NDG	C2-N2-C7	-7.80	112.95	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	811	NDG	C2-N2-C7	-7.80	112.97	123.11
2	B	806	NAG	C2-N2-C7	-3.92	118.01	123.11

5 of 8 chirality outliers are listed below:

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

There are no torsion outliers.

There are no ring outliers.

52 monomers are involved in 396 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	NAG	20	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	19	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
2	B	810	NAG	12	0
3	B	811	NDG	7	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	6	0
2	C	806	NAG	10	0
2	C	807	NAG	17	0
2	C	808	NAG	2	0
2	C	809	NAG	8	0
2	C	810	NAG	13	0
3	C	811	NDG	5	0
2	C	812	NAG	3	0
3	C	902	NDG	8	0
2	C	904	NAG	8	0
2	D	801	NAG	20	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	17	0
2	D	808	NAG	2	0
2	D	809	NAG	8	0
2	D	810	NAG	12	0
3	D	811	NDG	7	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.