



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:39 PM BST

PDB ID : 1Q5B
EMDB ID: : EMD-1052
Title : 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

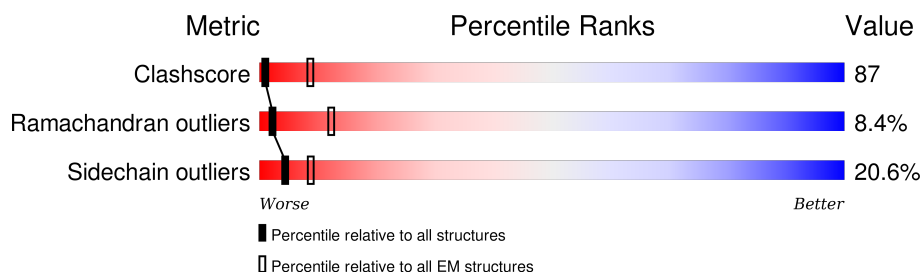
1 Overall quality at a glance

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% 31% 10% . 39%
1	B	880	16% 31% 11% . 39%
1	C	880	16% 31% 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	-
2	NAG	A	807	-	-	X	-
2	NAG	A	809	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-
3	NDG	A	902	-	-	X	-
3	NDG	B	811	-	-	X	-
3	NDG	B	902	-	-	X	-
3	NDG	C	902	-	-	X	-

2 Entry composition [i](#)

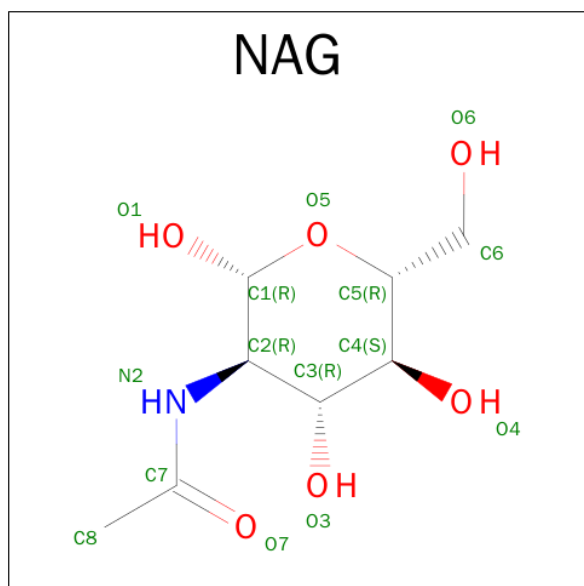
There are 4 unique types of molecules in this entry. The entry contains 13239 atoms, of which 0 are hydrogens and 0 are deuteriums.

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		

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



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

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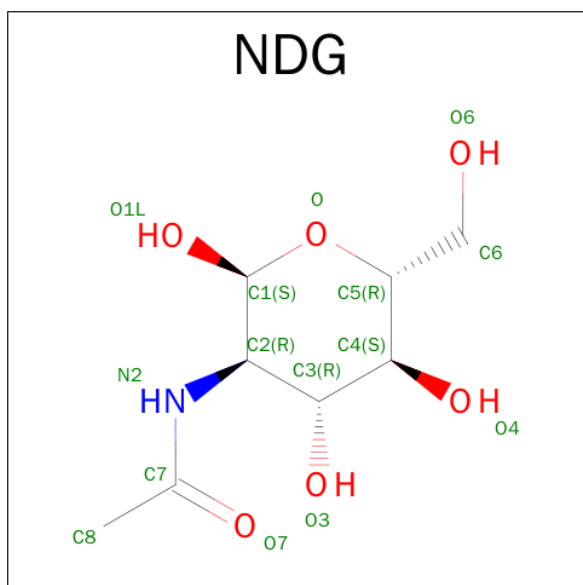
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	B	1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

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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	

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



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

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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	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	

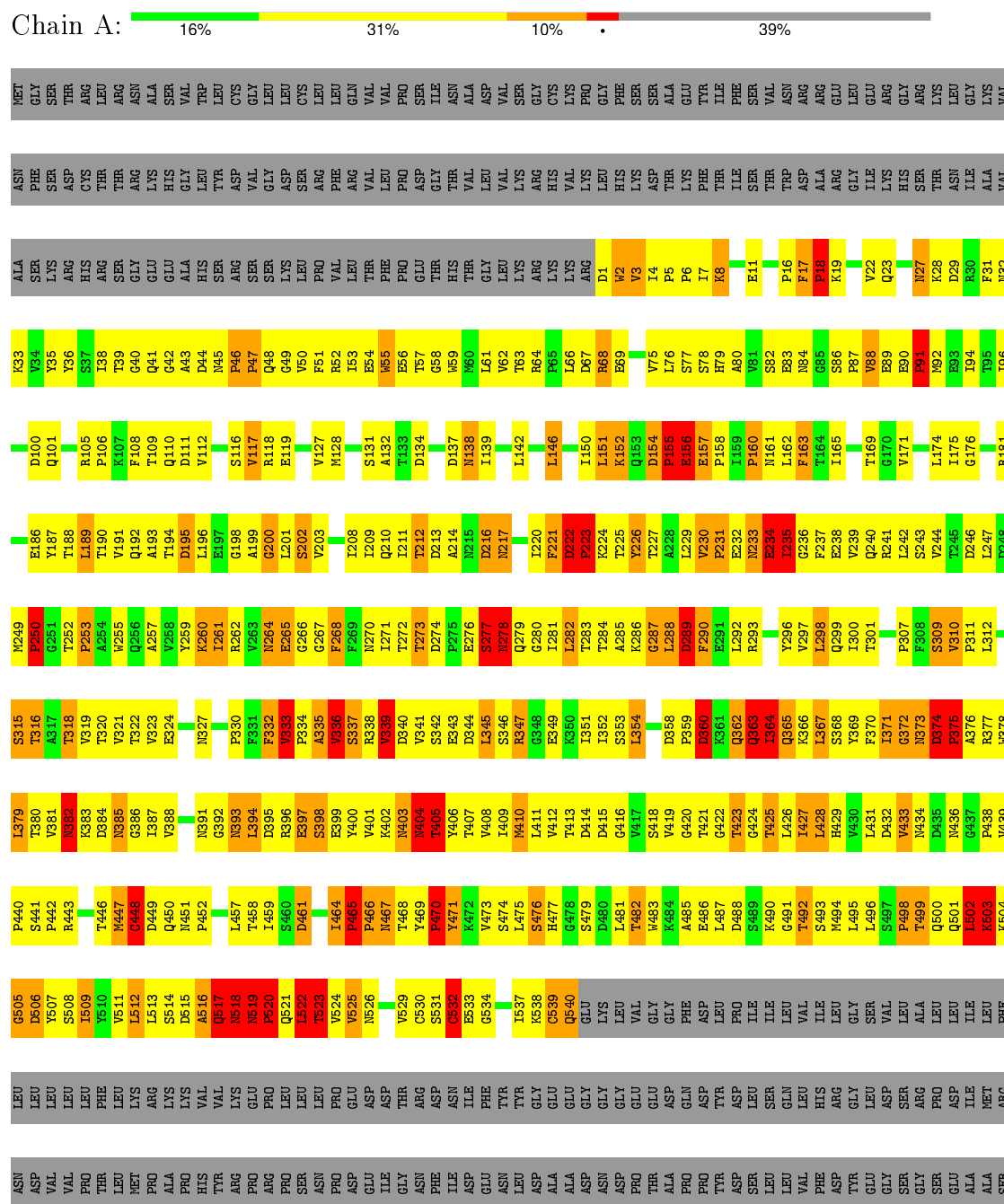
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

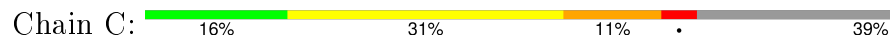
3 Residue-property plots

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



Chain B: 16% 31% 11% • 39%



GLU	ALA	ASP	LEU	Q501	G437	A376	P311	D246	G176	D100	F31	ALA	ASN	MET
ALA	SER	ILE	ILE	L502	P438	R377	L312	L247	G176	Q101	N32	SER	PHE	GLY
SER	ARG	PHE	LEU	R503	P439	L378	S315	D248	R181	Q101	R33	LYS	ASP	SER
LEU	ASN	ARG	LEU	G505	P440	L379	S315	D249	R181	Q101	G34	ARG	THR	THR
SER	ASP	ASN	LEU	G506	P442	T380	T316	G250	E186	R105	Y35	HIS	CYS	ARG
SER	VAL	VAL	LEU	P443	R443	G381	G317	T252	T188	P106	Y36	ARG	THR	LEU
LEU	VAL	VAL	LEU	G444	G444	K383	T318	P253	L189	F107	S37	SER	THR	ARG
ASN	PRO	THR	LEU	F445	T446	D384	T320	A254	L189	F108	L38	GLY	ARG	ASN
SER	THR	THR	PHE	T447	T447	N385	T321	M255	T190	T109	T39	LYS	LYS	ALA
ASN	ASN	MET	LEU	G448	G448	G386	T322	Q256	Q192	Q110	G40	HIS	SER	SER
SER	PRO	PRO	LYS	L512	L512	I387	V323	A257	A193	V112	Q41	ALA	GLY	VAL
ASN	ALA	ALA	ARG	D449	D449	I388	E324	G258	T194	G42	G42	HIS	LEU	TRP
ASP	PRO	PRO	LYS	Q450	Q450	N391	N327	Y259	D195	S116	D44	ARG	ASP	CYS
GLU	GLU	GLU	LYS	P452	P452	G392	G327	K260	L196	V117	N45	SER	VAL	CYS
GLU	GLU	HIS	VAL	A516	A516	N393	G330	L261	G198	R118	P46	SER	GLY	LEU
ASP	ASP	TYR	VAL	Q517	L457	N393	P330	R262	G198	E119	P47	LYS	ASP	LEU
TYR	ASP	ARG	LYS	N518	T458	L394	G331	G263	A199	G48	G48	LEU	SER	CYS
ASN	ASN	PRO	GLU	N519	T459	D395	F332	N264	G200	V127	G49	ARG	ARG	LEU
ASN	ASN	ARG	PRO	P520	I459	R396	F333	E265	L201	M128	V50	VAL	PHE	LEU
LEU	LEU	PRO	PRO	Q521	S460	G397	G334	G266	S202	S131	F51	LEU	ARG	GLN
SER	SER	SER	LEU	L522	D461	S398	A335	G267	G200	A132	I53	VAL	VAL	VAL
ASN	ASN	ASN	LEU	T523	G461	E399	V336	F268	V203	D133	I53	PHE	LEU	VAL
PRO	PRO	PRO	PRO	V524	I464	Y400	S337	F269	T208	T133	E54	VAL	LYS	SER
ASP	ASP	ASP	GLU	V525	P465	V401	R338	N270	T209	D134	R55	ARG	ARG	GLY
GLY	GLY	GLY	ASP	N526	P466	K402	F338	L271	Q210	L146	T63	LYS	VAL	GLY
SER	SER	ILE	ASP	V529	N467	N403	D340	G279	T220	S147	L66	VAL	VAL	LYS
ARG	ARG	GLY	THR	T468	T468	N404	G341	G280	F221	T150	D67	LYS	VAL	PRO
PHE	PHE	ASN	ARG	G530	Y469	T405	S342	T273	D222	L151	R68	HIS	THR	GLY
ARG	ARG	PHE	ASP	S531	P470	Y406	G343	D274	P223	K152	R69	LYS	SER	PHE
LYS	LYS	ILE	ASN	G532	Y471	T407	D344	P275	T225	Q153	V75	ASP	SER	SER
LEU	LEU	ASP	ILE	E533	K472	V408	L345	E276	Y226	P155	L76	LYS	GLU	ALA
ALA	ALA	GLU	PHE	G534	V473	V408	L346	S277	T227	E156	S77	PHE	THR	GLU
ASP	ASP	ASN	TYR	V537	V474	I409	S346	R278	G287	E157	S78	ILE	THR	TYR
MET	MET	LEU	TYR	K538	S474	M410	R347	G280	L288	P158	H79	ILE	THR	PHE
TYR	TYR	GLY	GLY	S476	L475	L411	G348	I281	L229	I159	A80	SER	THR	VAL
GLY	GLY	ALA	GLU	S477	H477	T412	G350	G282	V230	P160	V81	VAL	ASP	ASN
ALA	ALA	ALA	GLU	G539	G478	T413	T351	I283	E232	N161	S82	THR	ASP	ARG
ASP	ASP	ASP	GLY	Q540	S479	D415	I352	T284	E231	L162	E83	ALA	ALA	ARG
ASP	ASP	ASN	GLY	GLU	D480	D416	S353	A285	G291	F163	K19	ARG	ARG	GLU
GLU	GLU	PRO	GLY	VAL	L481	V417	L354	G286	R293	T164	S86	GLY	GLY	LEU
GLU	GLU	THR	GLU	VAL	T482	S418	D358	G287	L235	T164	S87	GLY	GLY	LEU
GLU	GLU	ALA	ASP	GLY	N483	V419	P359	L288	G236	I165	P87	GLY	GLY	LEU
ALA	ALA	PRO	GLN	GLY	K484	G420	R360	D389	L237	N166	V88	ILE	ILE	GLU
PRO	PRO	PRO	ASP	PHE	A485	T421	G361	F290	F237	R167	E89	LYS	LYS	ARG
PRO	PRO	TYR	TYR	ASP	E486	G422	I362	E291	E238	R167	E90	HIS	HIS	ARG
TYR	TYR	TYR	TYR	LEU	L487	T423	Q362	T292	E239	E168	E90	LYS	LYS	ARG
ASP	ASP	ASP	ASP	PRO	D488	G424	Q363	A286	R233	L162	P91	SER	SER	ARG
SER	SER	SER	LEU	ILE	S489	T425	I364	G287	E234	F163	K25	THR	THR	LYS
LEU	LEU	LEU	SER	ILE	K490	L426	Q365	G287	L235	T164	N92	ASN	ASN	LEU
LEU	LEU	LEU	GLN	LEU	G491	I427	K366	Y296	G236	I165	E92	ILE	ILE	GLY
VAL	VAL	VAL	LEU	VAL	T492	L428	I367	T297	F237	N166	V88	ALA	ALA	VAL
PHE	PHE	PHE	HIS	ILE	S493	H429	S368	Q299	E238	R167	E89	LYS	LYS	VAL
ASP	ASP	ASP	ARG	LEU	N494	V430	V369	I300	E239	E168	E90	HIS	HIS	ARG
TYR	TYR	TYR	GLY	GLY	L495	L431	F370	T301	Q240	G170	P91	SER	SER	ARG
GLU	GLU	GLU	LEU	SER	L496	D432	I371	T301	R241	T169	N92	THR	THR	LYS
GLY	GLY	GLY	ASP	VAL	S497	V433	G372	P307	L242	V171	E93	ASN	ASN	LEU
SER	SER	SER	SER	LEU	P498	N434	I373	F308	S243	L174	T95	ILE	ILE	GLY
GLY	GLY	GLY	ARG	ALA	T499	D435	R374	S309	V244	L174	T95	ALA	ALA	VAL
SER	SER	SER	PRO	LEU	Q500	N436	P375	V310	T245	I175	I96	VAL	VAL	VAL

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%)	1.44	81/5839 (1.4%)
1	B	0.70	8/4276 (0.2%)	1.39	79/5839 (1.4%)
1	C	0.70	8/4276 (0.2%)	1.39	79/5839 (1.4%)
All	All	0.70	24/12828 (0.2%)	1.41	239/17517 (1.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	4
1	B	0	4
1	C	0	4
All	All	1	12

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	335	ALA	CA-CB	-8.37	1.34	1.52
1	C	335	ALA	CA-CB	-8.35	1.34	1.52
1	B	335	ALA	CA-CB	-8.33	1.34	1.52
1	C	539	CYS	CB-SG	8.18	1.96	1.82
1	A	539	CYS	CB-SG	8.17	1.96	1.82

The worst 5 of 239 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	490	LYS	N-CA-CB	-28.44	59.41	110.60
1	A	520	PRO	CA-C-N	-13.30	87.95	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	520	PRO	CA-C-N	-13.29	87.97	117.20
1	B	520	PRO	CA-C-N	-13.28	87.99	117.20
1	C	290	PHE	N-CA-C	12.74	145.39	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	490	LYS	CA

5 of 12 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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4191	0	4081	822	0
1	B	4191	0	4087	811	0
1	C	4191	0	4085	858	0
2	A	154	0	143	85	0
2	B	154	0	143	84	0
2	C	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
4	A	12	0	0	0	0
4	B	12	0	0	0	0
4	C	12	0	0	0	0
All	All	13239	0	12838	2266	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 87.

The worst 5 of 2266 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:46:PRO:HB2	1:C:35:TYR:CE2	1.24	1.62
1:B:464:ILE:HD12	1:B:465:PRO:CD	1.30	1.58
1:C:464:ILE:HD12	1:C:465:PRO:CD	1.30	1.56
1:A:464:ILE:HD12	1:A:465:PRO:CD	1.30	1.55
1:A:87:PRO:CG	1:B:89:GLU:HB3	1.16	1.54

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	18
1	B	538/880 (61%)	401 (74%)	92 (17%)	45 (8%)	1	18
1	C	538/880 (61%)	401 (74%)	92 (17%)	45 (8%)	1	18
All	All	1614/2640 (61%)	1203 (74%)	276 (17%)	135 (8%)	2	18

5 of 135 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	10
1	B	480/779 (62%)	381 (79%)	99 (21%)	1	10
1	C	480/779 (62%)	381 (79%)	99 (21%)	1	10
All	All	1440/2337 (62%)	1143 (79%)	297 (21%)	4	10

5 of 297 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	268	PHE
1	B	395	ASP
1	C	427	ILE
1	B	282	LEU
1	B	345	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	122	GLN
1	B	299	GLN
1	C	393	ASN
1	B	138	ASN
1	B	240	GLN

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 81 ligands modelled in this entry, 36 are monoatomic - leaving 45 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	0.64	0	15,19,21	0.88	0
2	NAG	A	802	1	14,14,15	0.71	0	15,19,21	0.82	1 (6%)
2	NAG	A	803	1	14,14,15	0.91	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	0.68	0	15,19,21	1.17	1 (6%)
2	NAG	A	806	1	14,14,15	0.55	0	15,19,21	1.41	2 (13%)
2	NAG	A	807	1	14,14,15	0.64	0	15,19,21	1.14	1 (6%)
2	NAG	A	808	1	14,14,15	0.65	0	15,19,21	0.70	0
2	NAG	A	809	1	14,14,15	0.74	0	15,19,21	0.96	1 (6%)
2	NAG	A	810	1	14,14,15	0.63	0	15,19,21	1.08	2 (13%)
3	NDG	A	811	1	14,14,15	0.83	0	15,19,21	2.16	1 (6%)
2	NAG	A	812	1	14,14,15	0.82	1 (7%)	15,19,21	0.76	1 (6%)
3	NDG	A	902	1	14,14,15	1.07	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	14,14,15	0.75	1 (7%)	15,19,21	0.78	1 (6%)
2	NAG	B	801	1	14,14,15	0.64	0	15,19,21	0.89	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	0.91	1 (7%)	15,19,21	1.19	2 (13%)
3	NDG	B	804	1	14,14,15	0.61	0	15,19,21	0.82	0
2	NAG	B	805	1	14,14,15	0.68	0	15,19,21	1.18	1 (6%)
2	NAG	B	806	1	14,14,15	0.55	0	15,19,21	1.42	2 (13%)
2	NAG	B	807	1	14,14,15	0.63	0	15,19,21	1.14	1 (6%)
2	NAG	B	808	1	14,14,15	0.67	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	0.76	1 (7%)	15,19,21	0.96	1 (6%)
2	NAG	B	810	1	14,14,15	0.63	0	15,19,21	1.09	2 (13%)
3	NDG	B	811	1	14,14,15	0.82	0	15,19,21	2.17	1 (6%)
2	NAG	B	812	1	14,14,15	0.84	1 (7%)	15,19,21	0.75	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	0.51	0	15,19,21	0.64	0
2	NAG	B	904	1	14,14,15	0.76	1 (7%)	15,19,21	0.79	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	0.91	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	1.14	1 (6%)
2	NAG	C	808	1	14,14,15	0.66	0	15,19,21	0.69	0
2	NAG	C	809	1	14,14,15	0.76	1 (7%)	15,19,21	0.97	1 (6%)
2	NAG	C	810	1	14,14,15	0.63	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	0.83	1 (7%)	15,19,21	0.76	1 (6%)
3	NDG	C	902	1	14,14,15	1.08	1 (7%)	15,19,21	0.97	0
3	NDG	C	903	1	14,14,15	0.51	0	15,19,21	0.64	0
2	NAG	C	904	1	14,14,15	0.76	1 (7%)	15,19,21	0.79	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	904	NAG	C1-C2	-2.41	1.49	1.52
2	B	904	NAG	C1-C2	-2.39	1.49	1.52
2	A	904	NAG	C1-C2	-2.37	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	812	NAG	C1-C2	-2.34	1.49	1.52
2	B	812	NAG	C1-C2	-2.33	1.49	1.52

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	811	NDG	C2-N2-C7	-7.83	112.92	123.11
3	A	811	NDG	C2-N2-C7	-7.80	112.95	123.11
3	C	811	NDG	C2-N2-C7	-7.80	112.96	123.11
2	A	806	NAG	C2-N2-C7	-3.89	118.04	123.11
2	B	806	NAG	C2-N2-C7	-3.89	118.05	123.11

5 of 6 chirality outliers are listed below:

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

There are no torsion outliers.

There are no ring outliers.

39 monomers are involved in 300 short contacts:

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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	13	0
3	B	811	NDG	7	0
2	B	812	NAG	3	0
3	B	902	NDG	8	0
2	B	904	NAG	8	0
2	C	801	NAG	20	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	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	7	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.