



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 11:05 am GMT

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

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

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

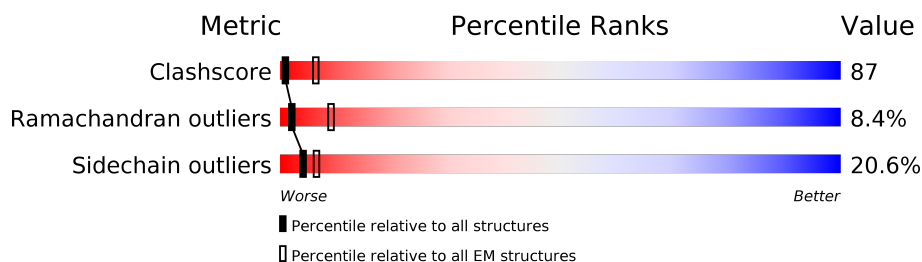
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 30.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	801	-	-	X	-
2	NAG	A	805	X	-	X	-
2	NAG	A	806	X	-	X	-
2	NAG	A	807	-	-	X	-
2	NAG	A	809	-	-	X	-

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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](#)

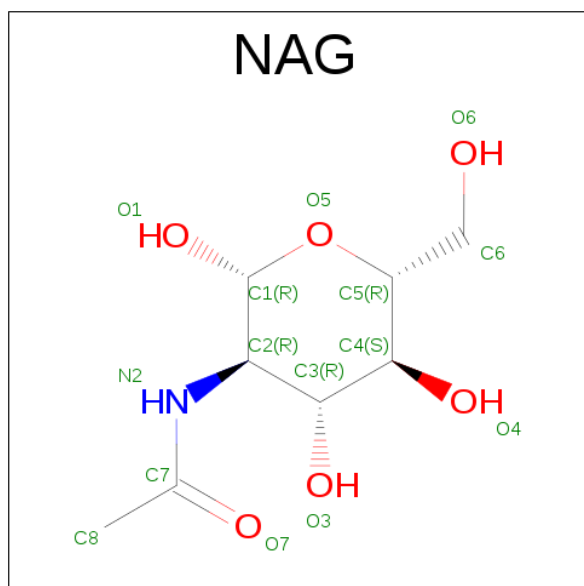
There are 4 unique types of molecules in this entry. The entry contains 13239 atoms, of which 0 are hydrogens and 0 are deuteriums.

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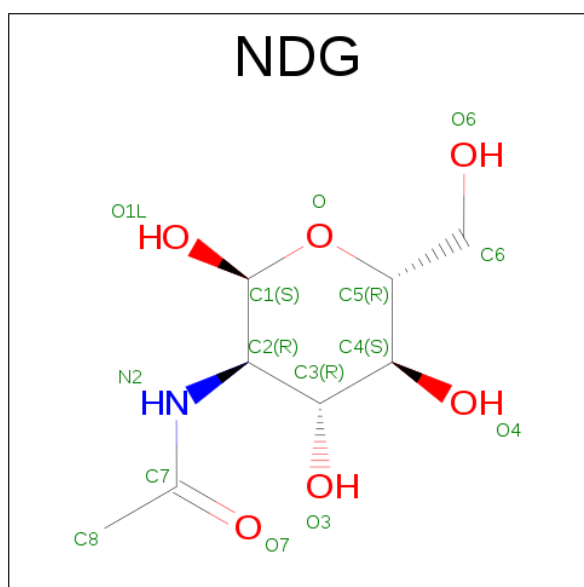
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	B	1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



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	

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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	

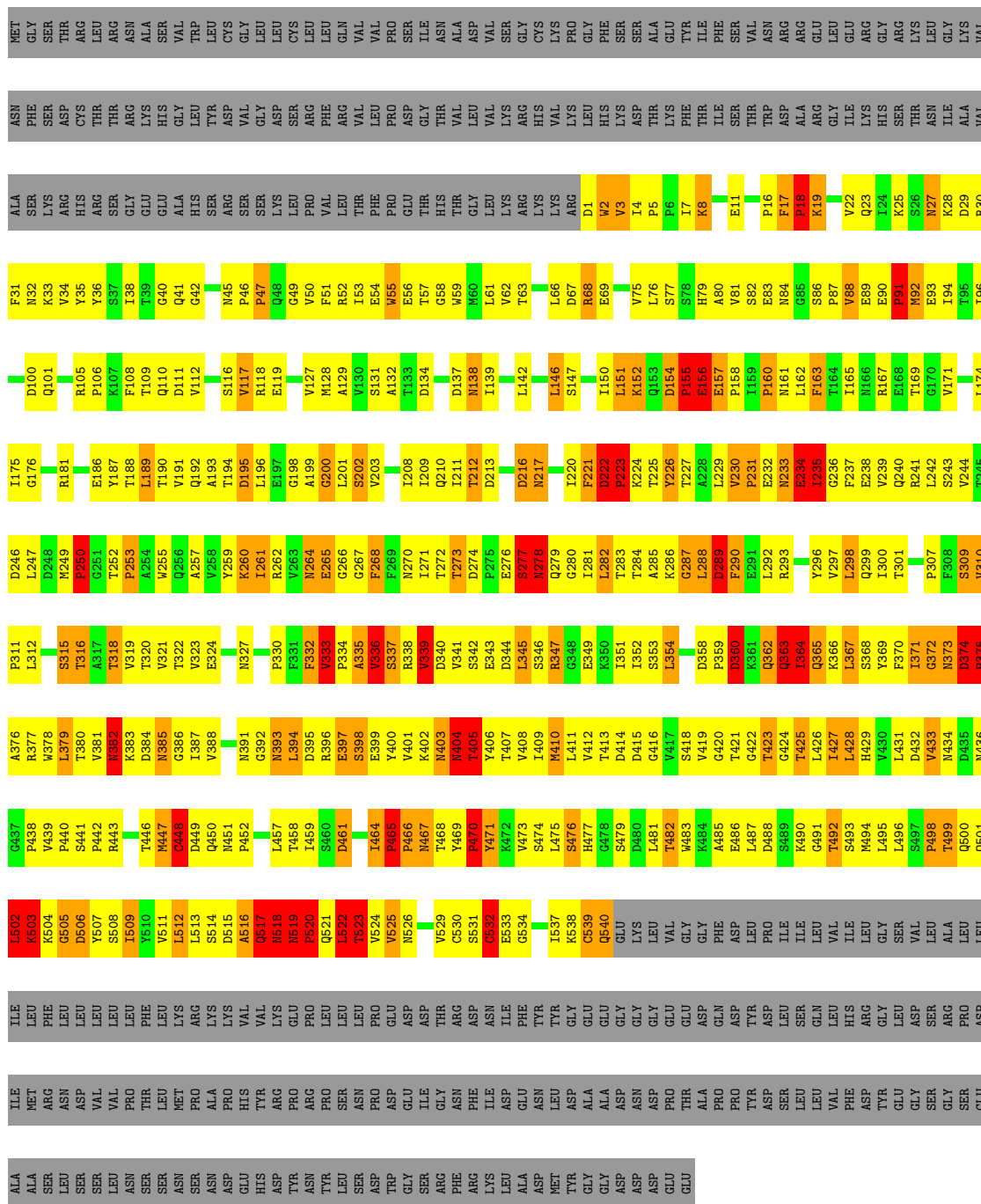
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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	

LEU SER SER SER LEU ASN SER SER ASN ASN ASN ASP GLU HIS ASP TYR ASN TYR LEU SER SER TRP GLY SER SER ARG PHE ARG LYS LEU ALA ASP MET TYR GLY GLY ASP ASP ASP GLU GLU

- Molecule 1: EP-cadherin

Chain B: 



- Molecule 1: EP-cadherin

Chain C:

GLU	ALA	ASP	LEU	Q501	G437	A376	P311	D246	G176			F31	ALA	ASN	MET
ALA	ILE	ILE	ILE	L502	P438	R377	L312	L247	G176			N32	SER	PHE	GLY
SER	PHE	MET	PHE	K503	P439	W378		D248	R181			R33	LYS	ASP	SER
LEU	ASP	ARG	ASP	K504	P440	L379	S315	M249	R181			V34	ARG	THR	THR
LEU	ASP	ASN	LEU	G505	S441	T380	T316	G250	E186			Y35	HIS	CYS	LEU
SER	VAL	ASP	LEU	D506	P442	V381	A317	T252	Y187			Y36	ARG	THR	ARG
LEU	VAL	VAL	LEU	Y507	R443	R382	T318	P253	T188			S37	SER	THR	ARG
LEU	VAL	VAL	LEU	S508	V444	K383	V319	P254	L189			I38	GLY	ARG	ASN
ASN	PRO	THR	LEU	L509	F445	T320	T321	A254	T190			T39	GLU	LYS	ALA
SER	THR	THR	PHE	T446	T446	N385	T321	W255	V191			Q40	GLU	HIS	SER
SER	LEU	LEU	LEU	N447	N447	G386	T322	Q286	Q192			Q41	ALA	GLY	VAL
ASN	LYS	MET	LYS	L512	C448	I387	V323	A257	A193			Q42	HIS	LEU	TRP
SER	ARG	PRO	ARG	L513	D449	V388	E324	V388	T194			A43	SER	TYR	LEU
ASN	LYS	ALA	LYS	Q514	Q450			Y259	D195			D44	ARG	ASP	CYS
ASP	PRO	PRO	LYS	A515	P452	N391	N327	K260	L196			N45	SER	VAL	GLY
GLU	VAL	HIS	VAL	A516				L261	L197			P46	SER	GLY	LEU
ASP	VAL	TYR	VAL	Q517	L457	N393	P330	R262	G198			P47	LYS	ASP	LEU
ASP	VAL	ARG	LYS	N518	T458	L394	F331	V263	A199			Q48	LEU	SER	CYS
TYR	PRO	PRO	GLU	N519	T459	D395	F332	E264	G200			V49	PRO	ARG	LEU
ASN	ARG	ARG	PRO	P520	I459	R396	V333	E265	L201			V50	VAL	PHE	LEU
PRO	PRO	ARG	LEU	Q521	S460	E397	P334	G266	S202			F51	LEU	ARG	GLN
SER	SER	SER	LEU	L522	D461	S398	A335	F268	V203			R52	THR	VAL	VAL
LEU	ASN	ASN	LEU	T523		E399	V336	G267				I53	PHE	VAL	VAL
ASP	PRO	ASP	PRO	V524	I464	Y400	S337	F269	T208			E54	PRO	PRO	PRO
TRP	ASP	ASP	GLU	V525	P465	V401	R338	N270	T209			W55	GLY	ASP	SER
GLY	GLU	GLU	ASP	N526	P466	K402	V339	L271	Q210			E56	THR	GLY	ILE
SER	ILE	ILE	ASP		N467	N403	D340	T272	Q210			T63	VAL	THR	ASN
ARG	GLY	THR	THR	V529	T468	T404	V341	G280	T212			G58	THR	VAL	ALA
PHE	ASN	ASN	ARG	G530	Y469	G540	S342	L281	T213			W59	GLY	LEU	ASP
ARG	PHE	ASP	ASP	S531	P470	Y406	E343	T284	D213			R60	LEU	VAL	VAL
LYS	ILE	ILE	ASN	G532	Y471	T407	D344	G286	A214			L61	LYS	LYS	SER
LEU	ASP	ILE	ILE	E533	K472	V408	L345	S277	D216			V62	ARG	ARG	GLY
ALA	GLU	PHE	PHE	G534	V473	I409	S346	R278	N217			T63	LYS	HIS	CYS
ASP	ASN	TYR	TYR		S474	M410	R347	Q279	T220			L66	VAL	VAL	PRO
LEU	LEU	TYR	GLY	I537	L475	L411	G348	G280	F221			D67	LEU	LEU	GLY
GLY	ALA	GLU	GLU	G538	H476	V412	E349	L282	D222			R68	LEU	HIS	PHE
ALA	ALA	GLU	GLU	G539	H477	T413	K350	L283	P223			E69	LYS	LYS	SER
ASP	ASP	GLY	GLY	Q540	G478	D414	L351	T283	K152				ASP	ASP	SER
ASN	ASN	GLY	GLY	GLU	S479	D415	L352	A285	D154				THR	THR	ALA
ASP	ASP	GLY	GLY	LEU	D480	G416	S353	G287	P155			L76	LYS	PHE	GLY
GLU	PRO	GLU	GLU	VAL	L481	V417	L354	G287	E156			S77	THR	THR	TYR
THR	THR	GLU	GLU	VAL	T482	S418		L288	E157			S78	ILE	ILE	PHE
ALA	ALA	ASP	ASP	GLY	V483	V419	D358	D389	P158			H79	ILE	SER	SER
PRO	PRO	GLN	GLN	PHE	K484	G420	P359	F290	I159			A80	SER	VAL	VAL
PRO	PRO	ASP	ASP	ASP	A485	T421	B360	E291	N160			W81	TRP	ASN	ASN
TYR	TYR	TYR	TYR	LEU	E486	G422	K361	E291	M161			E82	ASP	ASP	ARG
ASP	ASP	ASP	ASP	PRO	D488	T423	Q362	R293	L162			E83	ALA	ALA	ARG
SER	SER	LEU	LEU	ILE	S489	T425	I364		F163				ARG	ARG	GLU
LEU	LEU	SER	SER	ILE	K490	L426	Q365	Y296	T164			S86	GLY	GLY	LEU
LEU	VAL	GLN	GLN	LEU	G491	I427	K366	V297	I165			P87	ILE	ILE	GLU
VAL	VAL	LEU	LEU	VAL	T492	L428	L367	F237	N166			V88	LYS	LYS	GLU
PHE	PHE	HIS	HIS	ILE	S493	H429	S368	Q299	R167			E89	HIS	ARG	ARG
ASP	ASP	ARG	ARG	LEU	N494	V430	Y369	I300	E168			E90	LYS	GLY	GLY
TYR	TYR	GLY	GLY	GLY	L495	L431	F370	T301	T169			P91	SER	LYS	LYS
GLY	GLY	LEU	LEU	SER	L496	D432	T371		G170			N92	THR	ARG	ARG
ASP	ASP	ASP	ASP	VAL	S497	V433	G372	P307	V171			E93	ASN	LEU	LEU
SER	SER	SER	SER	LEU	P498	N434	N373	F308	L174			I94	ILE	GLY	GLY
GLY	GLY	GLY	GLY	ALA	T499	D435	B374	S309	L175			T95	ALA	ALA	LYS
SER	SER	SER	PRO	LEU	Q500	N436	P375	V310	T245			I96	VAL	VAL	VAL

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	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	120000	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	500	Depositor
Magnification	68276	Depositor
Image detector	GATAN 794	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, NAG, NDG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.70	8/4276 (0.2%)	1.44	81/5839 (1.4%)
1	B	0.70	8/4276 (0.2%)	1.39	79/5839 (1.4%)
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	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
All	All	1614/2640 (61%)	1203 (74%)	276 (17%)	135 (8%)	2	15

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	8
1	B	480/779 (62%)	381 (79%)	99 (21%)	1	8
1	C	480/779 (62%)	381 (79%)	99 (21%)	1	8
All	All	1440/2337 (62%)	1143 (79%)	297 (21%)	4	8

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	0.67	0	15,19,21	0.99	1 (6%)
2	NAG	A	802	1	14,14,15	0.73	0	15,19,21	0.92	0
2	NAG	A	803	1	14,14,15	0.94	1 (7%)	15,19,21	1.20	2 (13%)
3	NDG	A	804	1	14,14,15	0.63	0	15,19,21	0.82	0
2	NAG	A	805	1	14,14,15	0.69	0	15,19,21	1.07	1 (6%)
2	NAG	A	806	1	14,14,15	0.55	0	15,19,21	1.44	3 (20%)
2	NAG	A	807	1	14,14,15	0.65	0	15,19,21	1.25	2 (13%)
2	NAG	A	808	1	14,14,15	0.66	0	15,19,21	0.68	0
2	NAG	A	809	1	14,14,15	0.76	1 (7%)	15,19,21	0.86	0
2	NAG	A	810	1	14,14,15	0.65	0	15,19,21	1.40	4 (26%)
3	NDG	A	811	1	14,14,15	0.86	0	15,19,21	1.95	1 (6%)
2	NAG	A	812	1	14,14,15	0.84	1 (7%)	15,19,21	0.75	1 (6%)
3	NDG	A	902	1	14,14,15	1.10	1 (7%)	15,19,21	1.14	1 (6%)
3	NDG	A	903	1	14,14,15	0.52	0	15,19,21	0.80	0
2	NAG	A	904	1	14,14,15	0.77	1 (7%)	15,19,21	0.64	0
2	NAG	B	801	1	14,14,15	0.66	0	15,19,21	1.00	1 (6%)
2	NAG	B	802	1	14,14,15	0.74	0	15,19,21	0.91	0
2	NAG	B	803	1	14,14,15	0.94	1 (7%)	15,19,21	1.21	2 (13%)
3	NDG	B	804	1	14,14,15	0.62	0	15,19,21	0.82	0
2	NAG	B	805	1	14,14,15	0.70	0	15,19,21	1.07	1 (6%)
2	NAG	B	806	1	14,14,15	0.55	0	15,19,21	1.45	3 (20%)
2	NAG	B	807	1	14,14,15	0.64	0	15,19,21	1.25	2 (13%)
2	NAG	B	808	1	14,14,15	0.68	0	15,19,21	0.67	0

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	0.77	1 (7%)	15,19,21	0.86	0
2	NAG	B	810	1	14,14,15	0.64	0	15,19,21	1.40	4 (26%)
3	NDG	B	811	1	14,14,15	0.84	0	15,19,21	1.96	1 (6%)
2	NAG	B	812	1	14,14,15	0.85	1 (7%)	15,19,21	0.75	0
3	NDG	B	902	1	14,14,15	1.09	1 (7%)	15,19,21	1.14	1 (6%)
3	NDG	B	903	1	14,14,15	0.52	0	15,19,21	0.80	0
2	NAG	B	904	1	14,14,15	0.77	1 (7%)	15,19,21	0.65	0
2	NAG	C	801	1	14,14,15	0.66	0	15,19,21	1.00	0
2	NAG	C	802	1	14,14,15	0.74	0	15,19,21	0.92	0
2	NAG	C	803	1	14,14,15	0.94	1 (7%)	15,19,21	1.21	2 (13%)
3	NDG	C	804	1	14,14,15	0.63	0	15,19,21	0.81	0
2	NAG	C	805	1	14,14,15	0.70	0	15,19,21	1.07	1 (6%)
2	NAG	C	806	1	14,14,15	0.55	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	0.66	0	15,19,21	0.67	0
2	NAG	C	809	1	14,14,15	0.78	1 (7%)	15,19,21	0.87	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	0.75	0
3	NDG	C	902	1	14,14,15	1.10	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	0.77	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

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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 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	904	NAG	C1-C2	-2.46	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	812	NAG	C1-C2	-2.38	1.49	1.52
2	B	812	NAG	C1-C2	-2.37	1.49	1.52

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	811	NDG	C2-N2-C7	-6.87	112.92	122.94
3	A	811	NDG	C2-N2-C7	-6.85	112.95	122.94
3	C	811	NDG	C2-N2-C7	-6.84	112.96	122.94
2	A	806	NAG	C2-N2-C7	-3.36	118.04	122.94
2	B	806	NAG	C2-N2-C7	-3.35	118.05	122.94

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.