



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 11:07 am GMT

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/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

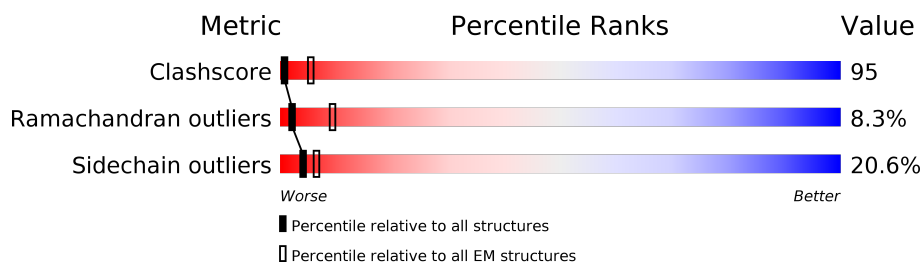
1 Overall quality at a glance

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	
1	D	880	

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

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	807	-	-	X	-
2	NAG	A	809	-	-	X	-
2	NAG	A	810	-	-	X	-
2	NAG	A	904	-	-	X	-
2	NAG	B	801	-	-	X	-
2	NAG	B	805	X	-	X	-
2	NAG	B	806	X	-	X	-
2	NAG	B	807	-	-	X	-
2	NAG	B	809	-	-	X	-
2	NAG	B	810	-	-	X	-
2	NAG	B	904	-	-	X	-
2	NAG	C	801	-	-	X	-
2	NAG	C	805	X	-	-	-
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](#)

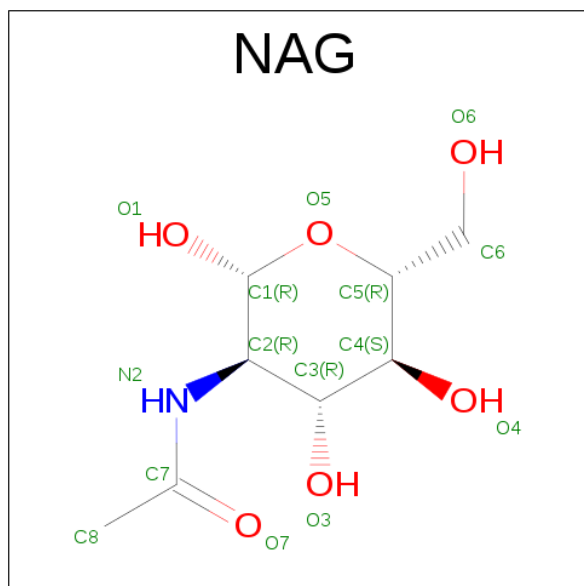
There are 4 unique types of molecules in this entry. The entry contains 17652 atoms, of which 0 are hydrogens and 0 are deuteriums.

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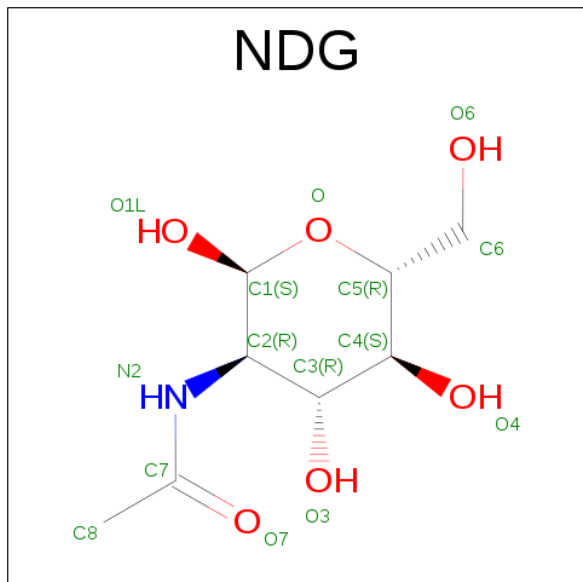
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	B	1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

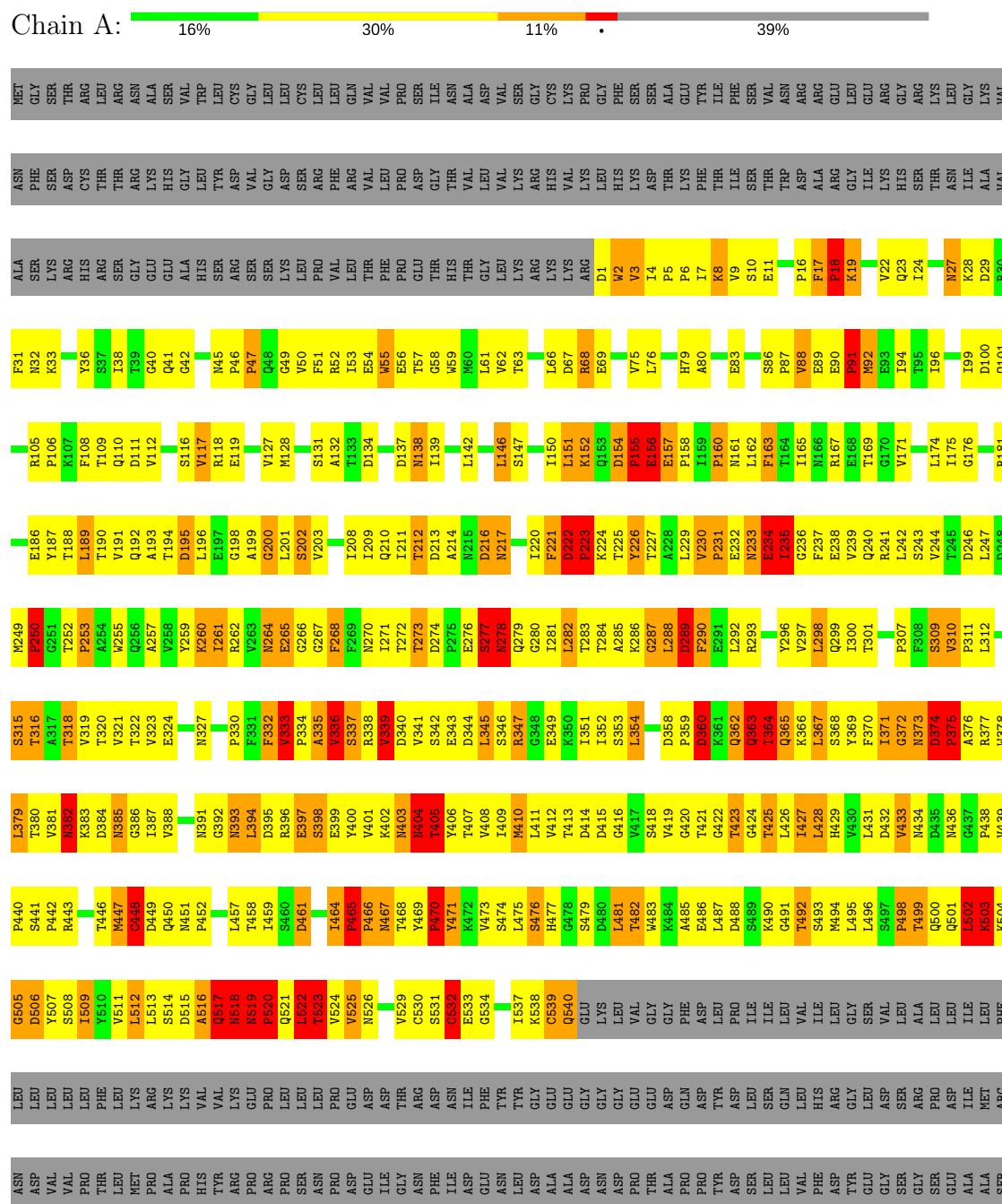
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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	

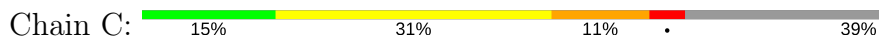
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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%



[illegible]

- Molecule 1: EP-cadherin

Chain D:

Met	Gly	Thr	Arg	Leu	Arg	Asn	Ser	Val	Trp	Leu	Cys	Gly	Val	Leu	Cys	Leu	Leu	Gln	Val	Pro	Ser	Ile	Asn	Ala	Asp	Val	Ser	Gly	Cys	Lys	Pro	Gly	Phe	Ser	Ser	Ala	Glu	Gly	Val	Asn	Arg	Arg	Val	Met
Asn	Phe	Ser	Asp	Thr	Thr	Arg	Lys	His	Gly	Leu	Trp	Val	Gly	Asp	Ser	Arg	Phe	Arg	Val	Leu	Pro	Asp	Gly	Val	Val	Leu	Lys	Arg	His	Val	Lys	Leu	His	Lys	Asp	Ala	Arg	Thr	Ser	Leu	His	Ala	Val	Met

SER	GLU	ALA	ALA	SER	LEU	ASN	SER	LEU	ASP	PRO	LEU	Q500	D435	D374	S309	V244	L174	I94	K33	ALA
GLU	ILE	ALA	ALA	ILE	LEU	ASN	ASP	LEU	ASP	ASP	LEU	Q501	M436	P375	V310	T245	I175	T95	V34	SER
ALA	MET	ALA	ALA	LEU	LEU	ASN	ASP	LEU	ASP	ASP	LEU	L502	P437	A376	F311	D246	G176	I96	V35	ARG
SER	ARG	SER	LEU	PHE	LEU	ASN	ASP	LEU	ASP	ASP	LEU	K504	V439	R377	L312	D248	R181	N97	V36	ARG
LEU	ASN	SER	LEU	LEU	LEU	ASN	ASP	LEU	ASP	ASP	LEU	G505	P440	L379	S315	D249	D100	I38	S37	ARG
SER	ASP	SER	LEU	LEU	LEU	ASN	ASP	LEU	ASP	ASP	LEU	D506	S441	T380	T316	P250	Q101	T39	I38	SER
SER	VAL	SER	LEU	LEU	LEU	ASN	ASP	LEU	ASP	ASP	LEU	Y507	R442	V381	A317	G251	Q101	Q40	T39	SER
VAL	VAL	VAL	LEU	LEU	LEU	ASN	ASP	LEU	ASP	ASP	LEU	S508	R443	R382	T318	T252	R105	Q41	Q40	GLY
ASN	PRO	ASN	LEU	LEU	LEU	ASN	ASP	LEU	ASP	ASP	LEU	I509	P443	K384	T320	P253	L189	Q42	Q42	GLU
SER	THR	SER	LEU	PHE	LEU	ASN	ASP	LEU	ASP	ASP	LEU	Y510	T446	D384	V321	A254	T190	A43	A43	ALA
SER	THR	SER	LEU	PHE	LEU	ASN	ASP	LEU	ASP	ASP	LEU	V511	M447	K385	V321	G255	V191	F108	N45	HIS
ASN	MET	ASN	LEU	LEU	LEU	ASN	ASP	LEU	ASP	ASP	LEU	L512	C448	G386	T322	G256	Q109	N45	N45	SER
SER	PRO	SER	LEU	ARG	LEU	ASN	ASP	LEU	ASP	ASP	LEU	L513	D449	I387	V323	A257	Q110	P46	P46	ARG
ASN	ALA	ASN	LEU	LEU	LEU	ASN	ASP	LEU	ASP	ASP	LEU	S514	Q450	V388	E324	V258	T194	D111	D111	SER
ASP	PRO	ASP	LEU	LEU	LEU	ASN	ASP	LEU	ASP	ASP	LEU	D515	M451	G388	N327	D195	V112	D111	D111	SER
GLU	HIS	GLU	LEU	VAL	VAL	ASN	ASP	LEU	ASP	ASP	LEU	A516	P452	N391	G392	K260	V112	D111	D111	SER
HIS	TYR	HIS	LEU	VAL	VAL	ASN	ASP	LEU	ASP	ASP	LEU	Q517	P452	G392	N327	K260	V112	D111	D111	SER
ASP	ARG	ASP	LEU	VAL	VAL	ASN	ASP	LEU	ASP	ASP	LEU	R518	L457	N393	P330	I261	S116	V50	V50	LEU
TYR	PRO	TYR	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	R519	T458	L394	F331	R262	V117	F51	F51	PRO
ASN	ARG	ASN	LEU	PRO	PRO	ASN	ASP	LEU	ASP	ASP	LEU	P520	T459	L394	F331	R262	V117	F51	F51	PRO
TYR	PRO	TYR	LEU	PRO	PRO	ASN	ASP	LEU	ASP	ASP	LEU	Q521	S460	R396	F332	R263	R118	R52	R52	VAL
LEU	SER	LEU	LEU	LEU	LEU	ASN	ASP	LEU	ASP	ASP	LEU	L522	D461	R397	V333	E265	E119	E53	E53	LEU
SER	SER	SER	LEU	LEU	LEU	ASN	ASP	LEU	ASP	ASP	LEU	T523	P461	E397	F334	G266	V127	E54	E54	THR
ASP	PRO	ASP	LEU	LEU	LEU	ASN	ASP	LEU	ASP	ASP	LEU	V524	T464	S398	A335	G267	M128	E55	E55	PHE
ASP	ASP	ASP	LEU	LEU	LEU	ASN	ASP	LEU	ASP	ASP	LEU	V525	P465	E399	V336	F268	A129	E56	E56	PRO
TRP	GLY	TRP	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	N526	P466	Y400	S337	F269	V130	T57	T57	GLU
GLY	SER	GLY	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	P526	P466	V401	R338	N270	G58	G58	G58	THR
ARG	ARG	ARG	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	V529	N467	K402	V339	I271	M59	M59	M59	HIS
PHE	PHE	PHE	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	C530	T468	K403	D340	I271	M60	M60	M60	THR
ARG	ARG	ARG	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	V469	Y469	R404	V341	T272	L61	L61	L61	GLY
LYS	LYS	LYS	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	S531	P470	T405	S342	D274	D134	V62	V62	LEU
LEU	LEU	LEU	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	C532	R471	Y406	E343	F275	D137	T63	T63	LYS
ALA	ALA	ALA	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	E533	R472	T407	E344	F276	A137	L66	L66	LYS
ASP	ASP	ASP	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	G534	V473	K408	D344	E276	M138	D67	D67	LYS
ASP	ASP	ASP	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	V474	S474	I409	L345	S277	D216	R68	R68	ARG
GLU	GLU	GLU	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	I537	S476	M410	R347	Q279	L142	E69	E69	LYS
GLU	GLU	GLU	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	K538	H477	L411	R348	G280	L146	V70	V70	LYS
GLU	GLU	GLU	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	C539	H477	V412	E349	I281	L146	V71	V71	LYS
GLU	GLU	GLU	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	Q540	G476	T413	K350	L282	L146	V71	V71	LYS
GLU	GLU	GLU	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	GLU	G476	D414	L351	L282	B72	K73	K73	LYS
GLU	GLU	GLU	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	LYS	G476	D415	L352	T283	B72	K73	K73	LYS
GLU	GLU	GLU	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	VAL	L481	G416	S353	A285	Y74	Y74	Y74	LYS
GLU	GLU	GLU	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	VAL	T482	G416	S353	A285	Y75	Y75	Y75	LYS
GLU	GLU	GLU	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	VAL	T482	G416	S353	A285	Y75	Y75	Y75	LYS
GLU	GLU	GLU	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	VAL	T482	G416	S353	A285	Y75	Y75	Y75	LYS
GLU	GLU	GLU	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	VAL	T482	G416	S353	A285	Y75	Y75	Y75	LYS
GLU	GLU	GLU	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	VAL	T482	G416	S353	A285	Y75	Y75	Y75	LYS
GLU	GLU	GLU	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	VAL	T482	G416	S353	A285	Y75	Y75	Y75	LYS
GLU	GLU	GLU	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	VAL	T482	G416	S353	A285	Y75	Y75	Y75	LYS
GLU	GLU	GLU	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	VAL	T482	G416	S353	A285	Y75	Y75	Y75	LYS
GLU	GLU	GLU	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	VAL	T482	G416	S353	A285	Y75	Y75	Y75	LYS
GLU	GLU	GLU	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	VAL	T482	G416	S353	A285	Y75	Y75	Y75	LYS
GLU	GLU	GLU	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	VAL	T482	G416	S353	A285	Y75	Y75	Y75	LYS
GLU	GLU	GLU	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	VAL	T482	G416	S353	A285	Y75	Y75	Y75	LYS
GLU	GLU	GLU	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	VAL	T482	G416	S353	A285	Y75	Y75	Y75	LYS
GLU	GLU	GLU	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	VAL	T482	G416	S353	A285	Y75	Y75	Y75	LYS
GLU	GLU	GLU	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	VAL	T482	G416	S353	A285	Y75	Y75	Y75	LYS
GLU	GLU	GLU	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	VAL	T482	G416	S353	A285	Y75	Y75	Y75	LYS
GLU	GLU	GLU	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	VAL	T482	G416	S353	A285	Y75	Y75	Y75	LYS
GLU	GLU	GLU	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	VAL	T482	G416	S353	A285	Y75	Y75	Y75	LYS
GLU	GLU	GLU	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	VAL	T482	G416	S353	A285	Y75	Y75	Y75	LYS
GLU	GLU	GLU	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	VAL	T482	G416	S353	A285	Y75	Y75	Y75	LYS
GLU	GLU	GLU	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	VAL	T482	G416	S353	A285	Y75	Y75	Y75	LYS
GLU	GLU	GLU	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	VAL	T482	G416	S353	A285	Y75	Y75	Y75	LYS
GLU	GLU	GLU	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	VAL	T482	G416	S353	A285	Y75	Y75	Y75	LYS
GLU	GLU	GLU	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	VAL	T482	G416	S353	A285	Y75	Y75	Y75	LYS
GLU	GLU	GLU	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	VAL	T482	G416	S353	A285	Y75	Y75	Y75	LYS
GLU	GLU	GLU	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	VAL	T482	G416	S353	A285	Y75	Y75	Y75	LYS
GLU	GLU	GLU	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	VAL	T482	G416	S353	A285	Y75	Y75	Y75	LYS
GLU	GLU	GLU	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	VAL	T482	G416	S353	A285	Y75	Y75	Y75	LYS
GLU	GLU	GLU	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	VAL	T482	G416	S353	A285	Y75	Y75	Y75	LYS
GLU	GLU	GLU	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	VAL	T482	G416	S353	A285	Y75	Y75	Y75	LYS
GLU	GLU	GLU	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	VAL	T482	G416	S353	A285	Y75	Y75	Y75	LYS
GLU	GLU	GLU	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	VAL	T482	G416	S353	A285	Y75	Y75	Y75	LYS
GLU	GLU	GLU	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	VAL	T482	G416	S353	A285	Y75	Y75	Y75	LYS
GLU	GLU	GLU	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	VAL	T482	G416	S353	A285	Y75	Y75	Y75	LYS
GLU	GLU	GLU	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	VAL	T482	G416	S353	A285	Y75	Y75	Y75	LYS
GLU	GLU	GLU	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	VAL	T482	G416	S353	A285	Y75	Y75	Y75	LYS
GLU	GLU	GLU	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	VAL	T482	G416	S353	A285	Y75	Y75	Y75	LYS
GLU	GLU	GLU	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	VAL	T482	G416	S353	A285	Y75	Y75	Y75	LYS
GLU	GLU	GLU	LEU	GLU	GLU	ASN	ASP	LEU	ASP	ASP	LEU	VAL	T482	G416	S353	A285	Y75	Y75	Y75	LYS
GL																				

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%)	1.39	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	15
1	B	538/880 (61%)	401 (74%)	93 (17%)	44 (8%)	1	16
1	C	538/880 (61%)	401 (74%)	92 (17%)	45 (8%)	1	15
1	D	538/880 (61%)	401 (74%)	92 (17%)	45 (8%)	1	15
All	All	2152/3520 (61%)	1605 (75%)	368 (17%)	179 (8%)	2	16

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 ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	480/779 (62%)	381 (79%)	99 (21%)	1	8
1	B	480/779 (62%)	381 (79%)	99 (21%)	1	8
1	C	480/779 (62%)	381 (79%)	99 (21%)	1	8
1	D	480/779 (62%)	381 (79%)	99 (21%)	1	8
All	All	1920/3116 (62%)	1524 (79%)	396 (21%)	4	8

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

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

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

Mol	Chain	Res	Type
1	B	455	GLN
1	C	110	GLN
1	D	391	ASN
1	B	467	ASN
1	C	27	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 108 ligands modelled in this entry, 48 are monoatomic - leaving 60 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	A	801	1	14,14,15	0.68	0	15,19,21	1.01	1 (6%)
2	NAG	A	802	1	14,14,15	0.74	1 (7%)	15,19,21	0.91	0
2	NAG	A	803	1	14,14,15	0.95	1 (7%)	15,19,21	1.21	2 (13%)
3	NDG	A	804	1	14,14,15	0.63	0	15,19,21	0.82	0
2	NAG	A	805	1	14,14,15	0.70	0	15,19,21	1.07	1 (6%)
2	NAG	A	806	1	14,14,15	0.54	0	15,19,21	1.45	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	0.68	0	15,19,21	0.67	0
2	NAG	A	809	1	14,14,15	0.78	1 (7%)	15,19,21	0.86	0
2	NAG	A	810	1	14,14,15	0.66	0	15,19,21	1.40	4 (26%)
3	NDG	A	811	1	14,14,15	0.84	0	15,19,21	1.95	1 (6%)
2	NAG	A	812	1	14,14,15	0.85	1 (7%)	15,19,21	0.76	1 (6%)
3	NDG	A	902	1	14,14,15	1.12	1 (7%)	15,19,21	1.13	1 (6%)
3	NDG	A	903	1	14,14,15	0.52	0	15,19,21	0.81	0
2	NAG	A	904	1,2	14,14,15	0.77	1 (7%)	15,19,21	0.65	0
2	NAG	B	801	1	14,14,15	0.67	0	15,19,21	1.00	0
2	NAG	B	802	1	14,14,15	0.74	1 (7%)	15,19,21	0.91	0
2	NAG	B	803	1	14,14,15	0.95	1 (7%)	15,19,21	1.22	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	0.71	0	15,19,21	1.06	1 (6%)
2	NAG	B	806	1	14,14,15	0.54	0	15,19,21	1.45	3 (20%)
2	NAG	B	807	1	14,14,15	0.65	0	15,19,21	1.25	2 (13%)
2	NAG	B	808	1	14,14,15	0.66	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	0.76	1 (7%)	15,19,21	0.86	0
2	NAG	B	810	1	14,14,15	0.66	0	15,19,21	1.40	4 (26%)
3	NDG	B	811	1	14,14,15	0.84	0	15,19,21	1.95	1 (6%)
2	NAG	B	812	1	14,14,15	0.83	1 (7%)	15,19,21	0.75	1 (6%)
3	NDG	B	902	1	14,14,15	1.09	1 (7%)	15,19,21	1.14	2 (13%)
3	NDG	B	903	1	14,14,15	0.53	0	15,19,21	0.80	0
2	NAG	B	904	1,2	14,14,15	0.77	1 (7%)	15,19,21	0.64	0
2	NAG	C	801	1	14,14,15	0.66	0	15,19,21	1.00	1 (6%)
2	NAG	C	802	1	14,14,15	0.74	0	15,19,21	0.91	0
2	NAG	C	803	1	14,14,15	0.95	1 (7%)	15,19,21	1.22	2 (13%)
3	NDG	C	804	1	14,14,15	0.62	0	15,19,21	0.82	0
2	NAG	C	805	1	14,14,15	0.70	0	15,19,21	1.06	1 (6%)
2	NAG	C	806	1	14,14,15	0.55	0	15,19,21	1.44	3 (20%)
2	NAG	C	807	1	14,14,15	0.64	0	15,19,21	1.24	2 (13%)
2	NAG	C	808	1	14,14,15	0.68	0	15,19,21	0.67	0
2	NAG	C	809	1	14,14,15	0.78	1 (7%)	15,19,21	0.86	0
2	NAG	C	810	1	14,14,15	0.64	0	15,19,21	1.40	4 (26%)
3	NDG	C	811	1	14,14,15	0.84	0	15,19,21	1.95	1 (6%)
2	NAG	C	812	1	14,14,15	0.84	1 (7%)	15,19,21	0.76	1 (6%)
3	NDG	C	902	1	14,14,15	1.11	1 (7%)	15,19,21	1.14	1 (6%)
3	NDG	C	903	1	14,14,15	0.53	0	15,19,21	0.80	0
2	NAG	C	904	1	14,14,15	0.77	1 (7%)	15,19,21	0.64	0
2	NAG	D	801	1	14,14,15	0.66	0	15,19,21	1.00	1 (6%)
2	NAG	D	802	1	14,14,15	0.75	1 (7%)	15,19,21	0.92	0
2	NAG	D	803	1	14,14,15	0.95	1 (7%)	15,19,21	1.21	2 (13%)
3	NDG	D	804	1	14,14,15	0.62	0	15,19,21	0.81	0
2	NAG	D	805	1	14,14,15	0.70	0	15,19,21	1.06	1 (6%)
2	NAG	D	806	1	14,14,15	0.54	0	15,19,21	1.44	3 (20%)
2	NAG	D	807	1	14,14,15	0.65	0	15,19,21	1.24	2 (13%)
2	NAG	D	808	1	14,14,15	0.67	0	15,19,21	0.67	0
2	NAG	D	809	1	14,14,15	0.78	1 (7%)	15,19,21	0.87	0
2	NAG	D	810	1	14,14,15	0.65	0	15,19,21	1.39	4 (26%)
3	NDG	D	811	1	14,14,15	0.85	0	15,19,21	1.96	1 (6%)
2	NAG	D	812	1	14,14,15	0.84	1 (7%)	15,19,21	0.75	0
3	NDG	D	902	1	14,14,15	1.10	1 (7%)	15,19,21	1.13	1 (6%)
3	NDG	D	903	1	14,14,15	0.52	0	15,19,21	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	D	904	1	14,14,15	0.78	1 (7%)	15,19,21	0.64	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	801	1	-	0/6/23/26	0/1/1/1
2	NAG	A	802	1	-	0/6/23/26	0/1/1/1
2	NAG	A	803	1	-	0/6/23/26	0/1/1/1
3	NDG	A	804	1	-	0/6/23/26	0/1/1/1
2	NAG	A	805	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	806	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	807	1	-	0/6/23/26	0/1/1/1
2	NAG	A	808	1	-	0/6/23/26	0/1/1/1
2	NAG	A	809	1	-	0/6/23/26	0/1/1/1
2	NAG	A	810	1	-	0/6/23/26	0/1/1/1
3	NDG	A	811	1	-	0/6/23/26	0/1/1/1
2	NAG	A	812	1	-	0/6/23/26	0/1/1/1
3	NDG	A	902	1	-	0/6/23/26	0/1/1/1
3	NDG	A	903	1	-	0/6/23/26	0/1/1/1
2	NAG	A	904	1,2	-	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 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	904	NAG	C1-C2	-2.47	1.49	1.52
2	C	904	NAG	C1-C2	-2.44	1.49	1.52
2	A	904	NAG	C1-C2	-2.44	1.49	1.52
2	B	904	NAG	C1-C2	-2.42	1.49	1.52
2	A	812	NAG	C1-C2	-2.38	1.49	1.52

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	811	NDG	C2-N2-C7	-6.85	112.94	122.94
3	A	811	NDG	C2-N2-C7	-6.85	112.95	122.94
3	B	811	NDG	C2-N2-C7	-6.85	112.95	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	811	NDG	C2-N2-C7	-6.84	112.97	122.94
2	B	806	NAG	C2-N2-C7	-3.38	118.01	122.94

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.