



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:52 PM BST

PDB ID : 3JAE
EMDB ID: : EMD-6345
Title : Structure of alpha-1 glycine receptor by single particle electron cryo-microscopy, glycine-bound state
Authors : Du, J.; Lu, W.; Wu, S.P.; Cheng, Y.F.; Gouaux, E.
Deposited on : 2015-06-08
Resolution : 3.90 Å(reported)
Based on PDB ID : 3RHW

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

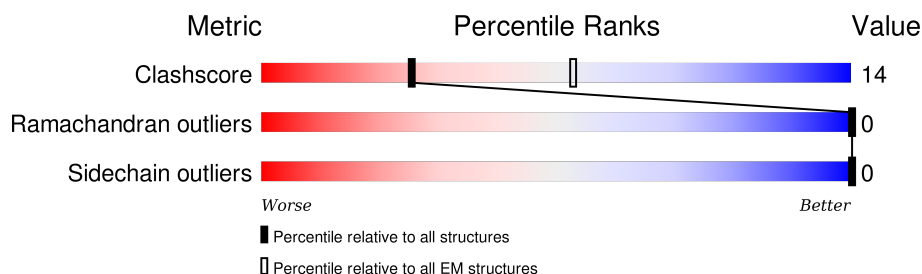
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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	342	75% 24% .
1	B	342	73% 26% .
1	C	342	75% 24% .
1	D	342	73% 25% .
1	E	342	75% 24% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12825 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 Glycine receptor subunit alphaZ1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	338	Total	C	N	O	S	0	0
			2537	1656	424	444	13		
1	B	338	Total	C	N	O	S	0	0
			2537	1656	424	444	13		
1	C	338	Total	C	N	O	S	0	0
			2537	1656	424	444	13		
1	D	338	Total	C	N	O	S	0	0
			2537	1656	424	444	13		
1	E	338	Total	C	N	O	S	0	0
			2537	1656	424	444	13		

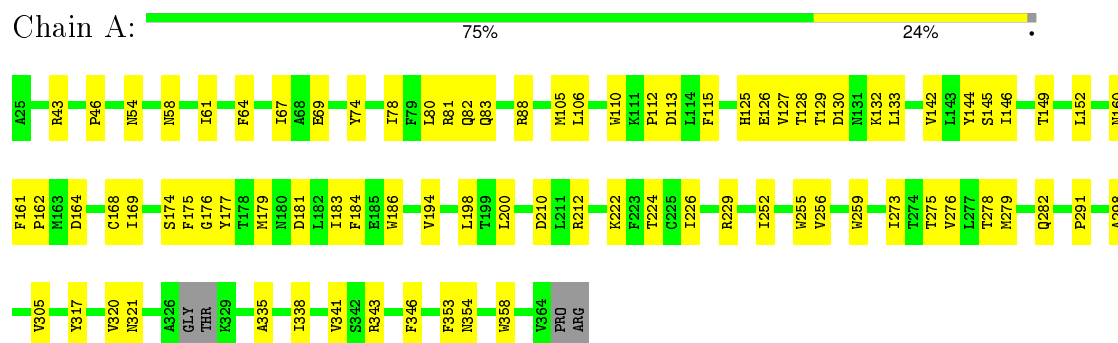
- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				AltConf
2	A	2	Total	C	N	O	0
			28	16	2	10	
2	B	2	Total	C	N	O	0
			28	16	2	10	
2	C	2	Total	C	N	O	0
			28	16	2	10	
2	D	2	Total	C	N	O	0
			28	16	2	10	
2	E	2	Total	C	N	O	0
			28	16	2	10	

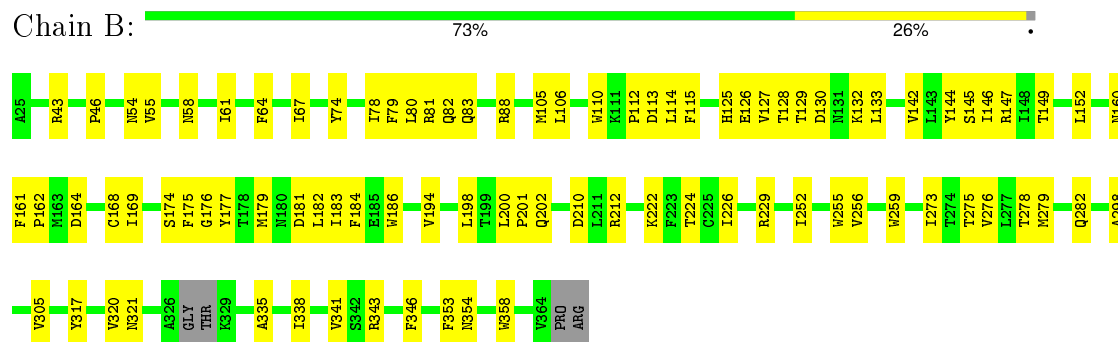
3 Residue-property plots

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.

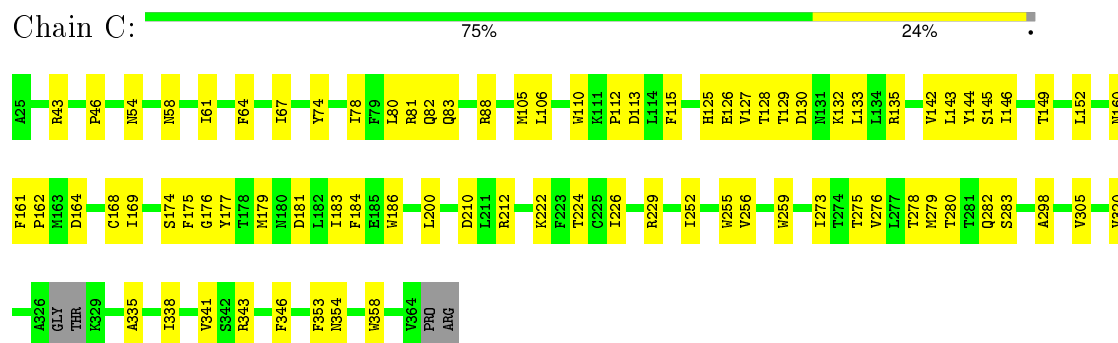
• Molecule 1: Glycine receptor subunit alphaZ1



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A298	A326	A335	A341	A343	A346	F353	F354	F358	F364	L452	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	L481	L482	L483	L484	L485	L486	L200	L210	L211	L212	K222	K223	K224	K225	K226	R229	I252	W255	W256	W259	I273	I274	I275	I276	I277	I278	I279	I280	I281	I282	I283	I284	I285	I286	I287	I288	I289	I290	I291	I292	I293	I294	I295	I296	I297	I298	I299	I300	I301	I302	I303	I304	I305	I306	I307	I308	I309	I310	I311	I312	I313	I314	I315	I316	I317	I318	I319	I320	I321	I322	I323	I324	I325	I326	I327	I328	I329	I330	I331	I332	I333	I334	I335	I336	I337	I338	I339	I340	I341	I342	I343	I344	I345	I346	I347	I348	I349	I350	I351	I352	I353	I354	I355	I356	I357	I358	I359	I360	I361	I362	I363	I364	I365	I366	I367	I368	I369	I370	I371	I372	I373	I374	I375	I376	I377	I378	I379	I380	I381	I382	I383	I384	I385	I386	I387	I388	I389	I390	I391	I392	I393	I394	I395	I396	I397	I398	I399	I400	I401	I402	I403	I404	I405	I406	I407	I408	I409	I410	I411	I412	I413	I414	I415	I416	I417	I418	I419	I420	I421	I422	I423	I424	I425	I426	I427	I428	I429	I430	I431	I432	I433	I434	I435	I436	I437	I438	I439	I440	I441	I442	I443	I444	I445	I446	I447	I448	I449	I450	I451	I452	I453	I454	I455	I456	I457	I458	I459	I460	I461	I462	I463	I464	I465	I466	I467	I468	I469	I470	I471	I472	I473	I474	I475	I476	I477	I478	I479	I480	I481	I482	I483	I484	I485	I486	I487	I488	I489	I490	I491	I492	I493	I494	I495	I496	I497	I498	I499	I500	I501	I502	I503	I504	I505	I506	I507	I508	I509	I510	I511	I512	I513	I514	I515	I516	I517	I518	I519	I520	I521	I522	I523	I524	I525	I526	I527	I528	I529	I530	I531	I532	I533	I534	I535	I536	I537	I538	I539	I540	I541	I542	I543	I544	I545	I546	I547	I548	I549	I550	I551	I552	I553	I554	I555	I556	I557	I558	I559	I560	I561	I562	I563	I564	I565	I566	I567	I568	I569	I570	I571	I572	I573	I574	I575	I576	I577	I578	I579	I580	I581	I582	I583	I584	I585	I586	I587	I588	I589	I590	I591	I592	I593	I594	I595	I596	I597	I598	I599	I600	I601	I602	I603	I604	I605	I606	I607	I608	I609	I610	I611	I612	I613	I614	I615	I616	I617	I618	I619	I620	I621	I622	I623	I624	I625	I626	I627	I628	I629	I630	I631	I632	I633	I634	I635	I636	I637	I638	I639	I640	I641	I642	I643	I644	I645	I646	I647	I648	I649	I650	I651	I652	I653	I654	I655	I656	I657	I658	I659	I660	I661	I662	I663	I664	I665	I666	I667	I668	I669	I670	I671	I672	I673	I674	I675	I676	I677	I678	I679	I680	I681	I682	I683	I684	I685	I686	I687	I688	I689	I690	I691	I692	I693	I694	I695	I696	I697	I698	I699	I700	I701	I702	I703	I704	I705	I706	I707	I708	I709	I710	I711	I712	I713	I714	I715	I716	I717	I718	I719	I720	I721	I722	I723	I724	I725	I726	I727	I728	I729
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- Chain E:  75% 24%

V305	P162	A25
Y317	M163	R43
	D164	
V320	G168	P46
N321	I169	
A326	S174	N54
GLY	F175	V55
THR	G176	N58
K329	Y177	
	T178	I61
A335	M179	
I338	M180	F64
	D181	
V341	L182	I67
S342	I183	
R343	F184	Y74
	E185	
F346	W186	I78
	V194	F79
F353		L80
	L198	R81
V364	T199	Q82
PRO	L200	Q83
ARG	P201	
	Q202	R88
	D210	M105
	L211	L106
	R212	
	K222	W110
	F223	R111
	T224	P112
	C225	D113
	I226	L114
		F115
	R229	H125
		E126
	T252	V127
		T128
	W255	T129
	V256	D130
	W259	H131
		K132
		L133
	T273	V142
	T274	L143
	T275	Y144
	V276	S145
	L277	I146
	T278	
	M279	T149
	Q282	L152
	A298	M160
		F164

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	58188	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	each particle	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	-1500	Depositor
Maximum defocus (nm)	-2500	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 (4k x 4k)	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: NAG

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	0.31	0/2601	0.54	0/3557
1	B	0.32	0/2601	0.54	0/3557
1	C	0.31	0/2601	0.54	0/3557
1	D	0.31	0/2601	0.54	0/3557
1	E	0.32	0/2601	0.54	0/3557
All	All	0.31	0/13005	0.54	0/17785

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2537	0	2391	67	0
1	B	2537	0	2391	70	0
1	C	2537	0	2391	69	0
1	D	2537	0	2391	71	0
1	E	2537	0	2391	68	0
2	A	28	0	25	2	0
2	B	28	0	25	2	0
2	C	28	0	25	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	28	0	25	2	0
2	E	28	0	25	2	0
All	All	12825	0	12080	338	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 14.

All (338) 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:169:ILE:HG21	1:A:229:ARG:HH11	1.36	0.91
1:E:169:ILE:HG21	1:E:229:ARG:HH11	1.36	0.90
1:D:169:ILE:HG21	1:D:229:ARG:HH11	1.36	0.90
1:B:169:ILE:HG21	1:B:229:ARG:HH11	1.36	0.90
1:C:169:ILE:HG21	1:C:229:ARG:HH11	1.36	0.90
1:A:129:THR:HG21	1:E:113:ASP:HB2	1.64	0.79
1:A:113:ASP:HB2	1:B:129:THR:HG21	1.70	0.74
1:B:113:ASP:HB2	1:C:129:THR:HG21	1.69	0.74
1:D:113:ASP:HB2	1:E:129:THR:HG21	1.69	0.74
1:C:113:ASP:HB2	1:D:129:THR:HG21	1.70	0.73
1:D:46:PRO:HA	1:D:88:ARG:HH22	1.55	0.72
1:A:46:PRO:HA	1:A:88:ARG:HH22	1.55	0.71
1:E:46:PRO:HA	1:E:88:ARG:HH22	1.55	0.71
1:B:46:PRO:HA	1:B:88:ARG:HH22	1.55	0.70
1:C:46:PRO:HA	1:C:88:ARG:HH22	1.55	0.70
1:B:212:ARG:NH1	1:B:229:ARG:HE	1.91	0.69
1:D:115:PHE:CE2	1:D:175:PHE:HB2	2.28	0.69
1:C:212:ARG:NH1	1:C:229:ARG:HE	1.91	0.69
1:B:115:PHE:CE2	1:B:175:PHE:HB2	2.28	0.69
1:E:115:PHE:CE2	1:E:175:PHE:HB2	2.28	0.69
1:D:212:ARG:NH1	1:D:229:ARG:HE	1.91	0.68
1:D:74:TYR:HE2	1:D:168:CYS:HB3	1.59	0.68
1:A:74:TYR:HE2	1:A:168:CYS:HB3	1.59	0.68
1:E:74:TYR:HE2	1:E:168:CYS:HB3	1.59	0.68
1:E:212:ARG:NH1	1:E:229:ARG:HE	1.91	0.68
1:C:115:PHE:CE2	1:C:175:PHE:HB2	2.28	0.68
1:C:74:TYR:HE2	1:C:168:CYS:HB3	1.59	0.68
1:A:115:PHE:CE2	1:A:175:PHE:HB2	2.28	0.68
1:B:74:TYR:HE2	1:B:168:CYS:HB3	1.59	0.68
1:A:212:ARG:NH1	1:A:229:ARG:HE	1.91	0.67
1:E:169:ILE:HG21	1:E:229:ARG:NH1	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:ILE:HG21	1:D:229:ARG:NH1	2.09	0.67
1:E:305:VAL:HG11	1:E:353:PHE:CZ	2.31	0.66
1:C:305:VAL:HG11	1:C:353:PHE:CZ	2.31	0.66
1:B:305:VAL:HG11	1:B:353:PHE:CZ	2.31	0.66
1:C:210:ASP:OD2	1:C:212:ARG:NH2	2.29	0.66
1:D:210:ASP:OD2	1:D:212:ARG:NH2	2.29	0.66
1:D:305:VAL:HG11	1:D:353:PHE:CZ	2.31	0.66
1:E:210:ASP:OD2	1:E:212:ARG:NH2	2.29	0.66
1:A:169:ILE:HG21	1:A:229:ARG:NH1	2.09	0.65
1:C:169:ILE:HG21	1:C:229:ARG:NH1	2.09	0.65
1:A:305:VAL:HG11	1:A:353:PHE:CZ	2.31	0.65
1:B:210:ASP:OD2	1:B:212:ARG:NH2	2.29	0.65
1:A:210:ASP:OD2	1:A:212:ARG:NH2	2.29	0.65
1:B:169:ILE:HG21	1:B:229:ARG:NH1	2.09	0.64
1:D:106:LEU:HD22	1:D:132:LYS:HD3	1.80	0.63
1:B:106:LEU:HD22	1:B:132:LYS:HD3	1.80	0.63
1:E:106:LEU:HD22	1:E:132:LYS:HD3	1.80	0.62
1:C:106:LEU:HD22	1:C:132:LYS:HD3	1.80	0.62
1:A:106:LEU:HD22	1:A:132:LYS:HD3	1.80	0.62
1:A:106:LEU:HD13	1:A:132:LYS:HB3	1.83	0.60
1:B:106:LEU:HD13	1:B:132:LYS:HB3	1.83	0.60
1:B:252:ILE:HA	1:B:255:TRP:CE3	2.37	0.60
1:E:252:ILE:HA	1:E:255:TRP:CE3	2.37	0.60
1:D:252:ILE:HA	1:D:255:TRP:CE3	2.37	0.60
1:C:252:ILE:HA	1:C:255:TRP:CE3	2.37	0.59
1:A:252:ILE:HA	1:A:255:TRP:CE3	2.37	0.59
1:E:106:LEU:HD13	1:E:132:LYS:HB3	1.83	0.59
1:D:106:LEU:HD13	1:D:132:LYS:HB3	1.83	0.59
1:C:106:LEU:HD13	1:C:132:LYS:HB3	1.83	0.59
1:B:320:VAL:HG13	1:B:335:ALA:HB1	1.85	0.59
1:E:160:ASN:HA	1:E:298:ALA:HB2	1.84	0.58
1:C:320:VAL:HG13	1:C:335:ALA:HB1	1.85	0.58
1:D:160:ASN:HA	1:D:298:ALA:HB2	1.84	0.58
1:A:160:ASN:HA	1:A:298:ALA:HB2	1.84	0.58
1:C:160:ASN:HA	1:C:298:ALA:HB2	1.84	0.58
1:C:74:TYR:CE2	1:C:168:CYS:HB3	2.39	0.58
1:B:160:ASN:HA	1:B:298:ALA:HB2	1.84	0.58
1:A:320:VAL:HG13	1:A:335:ALA:HB1	1.85	0.57
1:E:133:LEU:HB3	1:E:145:SER:HB3	1.87	0.57
1:A:74:TYR:CE2	1:A:168:CYS:HB3	2.39	0.57
1:B:74:TYR:CE2	1:B:168:CYS:HB3	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:LEU:HD11	1:A:144:TYR:CE1	2.40	0.57
1:C:133:LEU:HB3	1:C:145:SER:HB3	1.87	0.57
1:B:106:LEU:HD11	1:B:144:TYR:CE1	2.40	0.57
1:E:320:VAL:HG13	1:E:335:ALA:HB1	1.85	0.57
1:B:133:LEU:HB3	1:B:145:SER:HB3	1.87	0.57
1:D:133:LEU:HB3	1:D:145:SER:HB3	1.87	0.57
1:A:305:VAL:HG11	1:A:353:PHE:CE2	2.40	0.57
1:C:183:ILE:HA	1:C:224:THR:HG21	1.87	0.56
1:D:320:VAL:HG13	1:D:335:ALA:HB1	1.85	0.56
1:B:305:VAL:HG11	1:B:353:PHE:CE2	2.40	0.56
1:D:106:LEU:HD11	1:D:144:TYR:CE1	2.40	0.56
1:D:183:ILE:HA	1:D:224:THR:HG21	1.87	0.56
1:A:133:LEU:HB3	1:A:145:SER:HB3	1.87	0.56
1:E:305:VAL:HG11	1:E:353:PHE:CE2	2.40	0.56
1:C:305:VAL:HG11	1:C:353:PHE:CE2	2.40	0.56
1:E:183:ILE:HA	1:E:224:THR:HG21	1.87	0.56
1:B:183:ILE:HA	1:B:224:THR:HG21	1.87	0.56
1:E:174:SER:HB2	1:E:184:PHE:HE2	1.71	0.56
1:D:305:VAL:HG11	1:D:353:PHE:CE2	2.40	0.56
1:E:106:LEU:HD11	1:E:144:TYR:CE1	2.40	0.56
1:C:106:LEU:HD11	1:C:144:TYR:CE1	2.40	0.56
1:C:174:SER:HB2	1:C:184:PHE:HE2	1.71	0.56
1:D:174:SER:HB2	1:D:184:PHE:HE2	1.71	0.55
1:D:160:ASN:O	1:D:164:ASP:HB3	2.07	0.55
1:B:160:ASN:O	1:B:164:ASP:HB3	2.07	0.55
1:A:183:ILE:HA	1:A:224:THR:HG21	1.87	0.55
1:C:67:ILE:HG12	1:C:74:TYR:HB3	1.89	0.55
1:A:174:SER:HB2	1:A:184:PHE:HE2	1.71	0.55
1:D:67:ILE:HG12	1:D:74:TYR:HB3	1.89	0.55
1:E:74:TYR:CE2	1:E:168:CYS:HB3	2.39	0.55
1:B:174:SER:HB2	1:B:184:PHE:HE2	1.71	0.55
1:A:160:ASN:O	1:A:164:ASP:HB3	2.07	0.54
1:E:67:ILE:HG12	1:E:74:TYR:HB3	1.89	0.54
1:B:67:ILE:HG12	1:B:74:TYR:HB3	1.89	0.54
1:C:160:ASN:O	1:C:164:ASP:HB3	2.07	0.54
1:D:74:TYR:CE2	1:D:168:CYS:HB3	2.39	0.54
1:C:106:LEU:HD21	1:C:144:TYR:HE1	1.73	0.54
1:A:106:LEU:HD21	1:A:144:TYR:HE1	1.74	0.53
1:E:160:ASN:O	1:E:164:ASP:HB3	2.07	0.53
1:A:179:MET:HG2	1:A:222:LYS:HE3	1.90	0.53
1:A:67:ILE:HG12	1:A:74:TYR:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:LEU:HD21	1:B:144:TYR:HE1	1.73	0.53
1:B:179:MET:HG2	1:B:222:LYS:HE3	1.90	0.53
1:E:179:MET:HG2	1:E:222:LYS:HE3	1.90	0.53
2:A:501:NAG:H83	2:A:501:NAG:H3	1.91	0.53
2:C:501:NAG:H83	2:C:501:NAG:H3	1.91	0.53
1:D:179:MET:HG2	1:D:222:LYS:HE3	1.90	0.53
1:C:179:MET:HG2	1:C:222:LYS:HE3	1.90	0.53
1:D:106:LEU:HD21	1:D:144:TYR:HE1	1.74	0.53
1:D:255:TRP:HE1	1:D:346:PHE:HB3	1.74	0.53
2:E:501:NAG:H3	2:E:501:NAG:H83	1.91	0.53
1:E:106:LEU:HD21	1:E:144:TYR:HE1	1.74	0.52
1:B:255:TRP:HE1	1:B:346:PHE:HB3	1.74	0.52
1:C:255:TRP:HE1	1:C:346:PHE:HB3	1.74	0.52
1:E:255:TRP:HE1	1:E:346:PHE:HB3	1.74	0.52
1:A:255:TRP:HE1	1:A:346:PHE:HB3	1.74	0.52
1:D:162:PRO:HD2	1:D:298:ALA:HB3	1.92	0.52
1:B:259:TRP:CE2	1:B:343:ARG:HD2	2.45	0.52
1:A:162:PRO:HD2	1:A:298:ALA:HB3	1.92	0.52
2:D:501:NAG:H83	2:D:501:NAG:H3	1.91	0.52
1:E:256:VAL:HA	1:E:259:TRP:HD1	1.75	0.52
2:B:501:NAG:H83	2:B:501:NAG:H3	1.91	0.52
1:B:162:PRO:HD2	1:B:298:ALA:HB3	1.92	0.51
1:E:259:TRP:CE2	1:E:343:ARG:HD2	2.45	0.51
1:C:256:VAL:HA	1:C:259:TRP:HD1	1.75	0.51
1:D:259:TRP:CE2	1:D:343:ARG:HD2	2.45	0.51
1:A:259:TRP:CE2	1:A:343:ARG:HD2	2.45	0.51
1:B:256:VAL:HA	1:B:259:TRP:HD1	1.75	0.51
1:D:256:VAL:HA	1:D:259:TRP:HD1	1.75	0.51
1:A:256:VAL:HA	1:A:259:TRP:HD1	1.75	0.51
1:E:162:PRO:HD2	1:E:298:ALA:HB3	1.92	0.51
1:E:126:GLU:HG3	1:E:130:ASP:OD1	2.11	0.51
1:C:259:TRP:CE2	1:C:343:ARG:HD2	2.45	0.50
1:C:162:PRO:HD2	1:C:298:ALA:HB3	1.92	0.50
1:B:126:GLU:HG3	1:B:130:ASP:OD1	2.11	0.50
1:A:106:LEU:HD11	1:A:144:TYR:HE1	1.77	0.50
1:E:125:HIS:CE1	1:E:149:THR:HG1	2.30	0.50
1:C:125:HIS:CE1	1:C:149:THR:HG1	2.30	0.50
1:C:126:GLU:HG3	1:C:130:ASP:OD1	2.11	0.50
1:D:125:HIS:CE1	1:D:149:THR:HG1	2.30	0.50
1:E:106:LEU:HD11	1:E:144:TYR:HE1	1.77	0.50
1:B:125:HIS:CE1	1:B:149:THR:HG1	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:338:ILE:HA	1:E:341:VAL:HG12	1.94	0.50
1:A:125:HIS:CE1	1:A:149:THR:HG1	2.29	0.50
1:D:126:GLU:HG3	1:D:130:ASP:OD1	2.11	0.49
1:A:338:ILE:HA	1:A:341:VAL:HG12	1.94	0.49
1:A:210:ASP:HB3	1:A:229:ARG:HB2	1.95	0.49
1:C:210:ASP:HB3	1:C:229:ARG:HB2	1.95	0.49
1:A:126:GLU:HG3	1:A:130:ASP:OD1	2.11	0.49
1:E:212:ARG:HH12	1:E:229:ARG:HE	1.60	0.49
1:B:106:LEU:HD11	1:B:144:TYR:HE1	1.77	0.49
1:B:210:ASP:HB3	1:B:229:ARG:HB2	1.95	0.49
1:D:106:LEU:HD11	1:D:144:TYR:HE1	1.77	0.49
1:C:106:LEU:HD11	1:C:144:TYR:HE1	1.77	0.49
1:D:338:ILE:HA	1:D:341:VAL:HG12	1.94	0.49
1:D:46:PRO:HD3	1:D:110:TRP:CD2	2.48	0.49
1:A:46:PRO:HD3	1:A:110:TRP:CD2	2.48	0.49
1:C:46:PRO:HD3	1:C:110:TRP:CD2	2.48	0.49
1:E:210:ASP:HB3	1:E:229:ARG:HB2	1.95	0.49
1:D:210:ASP:HB3	1:D:229:ARG:HB2	1.95	0.49
1:D:212:ARG:HH12	1:D:229:ARG:HE	1.61	0.48
1:C:338:ILE:HA	1:C:341:VAL:HG12	1.94	0.48
1:A:127:VAL:O	1:A:128:THR:OG1	2.31	0.48
1:E:46:PRO:HD3	1:E:110:TRP:CD2	2.48	0.48
1:C:127:VAL:O	1:C:128:THR:OG1	2.31	0.48
1:B:46:PRO:HD3	1:B:110:TRP:CD2	2.48	0.48
1:B:338:ILE:HA	1:B:341:VAL:HG12	1.94	0.48
1:D:127:VAL:O	1:D:128:THR:OG1	2.31	0.48
1:C:106:LEU:HD21	1:C:144:TYR:CE1	2.49	0.48
1:E:273:ILE:HA	1:E:276:VAL:HG12	1.96	0.48
1:D:106:LEU:HD21	1:D:144:TYR:CE1	2.49	0.48
1:B:127:VAL:O	1:B:128:THR:OG1	2.31	0.48
1:E:127:VAL:O	1:E:128:THR:OG1	2.31	0.48
1:D:273:ILE:HA	1:D:276:VAL:HG12	1.96	0.48
1:B:106:LEU:HD21	1:B:144:TYR:CE1	2.49	0.48
1:B:125:HIS:HE2	1:B:149:THR:HG1	1.61	0.48
1:A:273:ILE:HA	1:A:276:VAL:HG12	1.96	0.48
1:B:273:ILE:HA	1:B:276:VAL:HG12	1.96	0.48
1:C:179:MET:SD	1:C:224:THR:HG22	2.55	0.47
1:D:179:MET:SD	1:D:224:THR:HG22	2.55	0.47
1:D:82:GLN:NE2	1:D:112:PRO:HG2	2.29	0.47
1:A:212:ARG:HH12	1:A:229:ARG:HE	1.60	0.47
1:A:106:LEU:HD21	1:A:144:TYR:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:179:MET:SD	1:E:224:THR:HG22	2.55	0.47
1:E:106:LEU:HD21	1:E:144:TYR:CE1	2.49	0.47
1:E:82:GLN:NE2	1:E:112:PRO:HG2	2.29	0.47
1:C:273:ILE:HA	1:C:276:VAL:HG12	1.96	0.47
1:A:132:LYS:HG2	1:A:146:ILE:HG22	1.97	0.47
1:A:179:MET:SD	1:A:224:THR:HG22	2.55	0.47
1:E:256:VAL:HA	1:E:259:TRP:CD1	2.50	0.47
1:B:179:MET:SD	1:B:224:THR:HG22	2.55	0.46
1:C:256:VAL:HA	1:C:259:TRP:CD1	2.50	0.46
1:B:82:GLN:NE2	1:B:112:PRO:HG2	2.29	0.46
1:C:212:ARG:HH12	1:C:229:ARG:HE	1.61	0.46
1:E:113:ASP:OD2	1:E:176:GLY:HA3	2.16	0.46
1:D:132:LYS:HG2	1:D:146:ILE:HG22	1.97	0.46
1:B:132:LYS:HG2	1:B:146:ILE:HG22	1.97	0.46
1:D:113:ASP:OD2	1:D:176:GLY:HA3	2.16	0.46
1:C:132:LYS:HG2	1:C:146:ILE:HG22	1.97	0.46
1:A:82:GLN:NE2	1:A:112:PRO:HG2	2.29	0.46
1:C:82:GLN:NE2	1:C:112:PRO:HG2	2.30	0.46
1:B:256:VAL:HA	1:B:259:TRP:CD1	2.50	0.46
1:D:256:VAL:HA	1:D:259:TRP:CD1	2.50	0.46
1:A:74:TYR:HE1	1:A:152:LEU:HD12	1.81	0.46
1:A:256:VAL:HA	1:A:259:TRP:CD1	2.50	0.46
1:E:132:LYS:HG2	1:E:146:ILE:HG22	1.97	0.46
1:A:113:ASP:OD2	1:A:176:GLY:HA3	2.16	0.45
1:D:186:TRP:NE1	1:D:226:ILE:HB	2.32	0.45
1:E:74:TYR:HE1	1:E:152:LEU:HD12	1.81	0.45
1:B:186:TRP:NE1	1:B:226:ILE:HB	2.32	0.45
1:C:186:TRP:NE1	1:C:226:ILE:HB	2.32	0.45
1:E:161:PHE:HB3	1:E:162:PRO:HD3	1.99	0.45
1:A:161:PHE:HB3	1:A:162:PRO:HD3	1.98	0.45
1:E:61:ILE:HG22	1:E:78:ILE:HG22	1.98	0.45
1:E:186:TRP:NE1	1:E:226:ILE:HB	2.32	0.45
1:B:113:ASP:OD2	1:B:176:GLY:HA3	2.16	0.45
1:C:113:ASP:OD2	1:C:176:GLY:HA3	2.16	0.45
1:D:61:ILE:HG22	1:D:78:ILE:HG22	1.98	0.45
1:B:212:ARG:HH12	1:B:229:ARG:HE	1.60	0.45
1:B:161:PHE:HB3	1:B:162:PRO:HD3	1.98	0.45
1:D:161:PHE:HB3	1:D:162:PRO:HD3	1.98	0.45
1:C:74:TYR:HE1	1:C:152:LEU:HD12	1.81	0.44
1:B:74:TYR:HE1	1:B:152:LEU:HD12	1.81	0.44
1:D:74:TYR:HE1	1:D:152:LEU:HD12	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:255:TRP:NE1	1:E:346:PHE:HB3	2.32	0.44
1:D:255:TRP:NE1	1:D:346:PHE:HB3	2.32	0.44
1:E:177:TYR:HB3	1:E:181:ASP:HB2	1.99	0.44
1:C:61:ILE:HG22	1:C:78:ILE:HG22	1.98	0.44
1:B:177:TYR:HB3	1:B:181:ASP:HB2	1.99	0.44
1:A:186:TRP:NE1	1:A:226:ILE:HB	2.32	0.44
1:A:61:ILE:HG22	1:A:78:ILE:HG22	1.98	0.44
1:B:61:ILE:HG22	1:B:78:ILE:HG22	1.98	0.44
1:C:255:TRP:NE1	1:C:346:PHE:HB3	2.32	0.44
1:A:43:ARG:HD2	1:B:105:MET:HG2	2.00	0.44
1:A:125:HIS:HE2	1:A:149:THR:HG1	1.65	0.44
1:E:278:THR:O	1:E:282:GLN:HG2	2.18	0.44
1:C:58:ASN:OD1	1:C:81:ARG:HB2	2.18	0.44
1:A:255:TRP:NE1	1:A:346:PHE:HB3	2.32	0.43
1:A:278:THR:O	1:A:282:GLN:HG2	2.18	0.43
1:D:177:TYR:HB3	1:D:181:ASP:HB2	1.99	0.43
1:B:255:TRP:NE1	1:B:346:PHE:HB3	2.32	0.43
1:A:58:ASN:OD1	1:A:81:ARG:HB2	2.18	0.43
1:D:278:THR:O	1:D:282:GLN:HG2	2.18	0.43
1:C:43:ARG:HD2	1:D:105:MET:HG2	1.99	0.43
1:C:161:PHE:HB3	1:C:162:PRO:HD3	1.99	0.43
1:B:278:THR:O	1:B:282:GLN:HG2	2.18	0.43
1:B:43:ARG:HD2	1:C:105:MET:HG2	2.00	0.43
1:E:58:ASN:OD1	1:E:81:ARG:HB2	2.18	0.43
1:C:278:THR:O	1:C:282:GLN:HG2	2.18	0.43
1:D:125:HIS:NE2	1:D:149:THR:OG1	2.50	0.43
1:A:177:TYR:HB3	1:A:181:ASP:HB2	1.99	0.43
1:A:106:LEU:HD13	1:A:132:LYS:HD3	2.01	0.43
1:A:335:ALA:O	1:A:338:ILE:HG22	2.19	0.43
1:C:106:LEU:HD13	1:C:132:LYS:HD3	2.01	0.43
1:D:335:ALA:O	1:D:338:ILE:HG22	2.19	0.43
1:E:335:ALA:O	1:E:338:ILE:HG22	2.19	0.42
1:B:58:ASN:OD1	1:B:81:ARG:HB2	2.18	0.42
1:B:335:ALA:O	1:B:338:ILE:HG22	2.19	0.42
1:C:335:ALA:O	1:C:338:ILE:HG22	2.19	0.42
1:C:54:ASN:HD21	2:C:501:NAG:C1	2.32	0.42
1:D:54:ASN:HD21	2:D:501:NAG:C1	2.32	0.42
1:C:177:TYR:HB3	1:C:181:ASP:HB2	1.99	0.42
1:D:58:ASN:OD1	1:D:81:ARG:HB2	2.18	0.42
1:E:54:ASN:HD21	2:E:501:NAG:C1	2.32	0.42
1:B:54:ASN:HD21	2:B:501:NAG:C1	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:ARG:HD2	1:E:105:MET:HG2	2.01	0.42
1:A:54:ASN:HD21	2:A:501:NAG:C1	2.32	0.42
1:A:64:PHE:HB2	1:A:200:LEU:CD2	2.50	0.42
1:D:64:PHE:HB2	1:D:200:LEU:CD2	2.50	0.42
1:D:106:LEU:HD13	1:D:132:LYS:HD3	2.01	0.42
1:A:335:ALA:HA	1:A:338:ILE:HG22	2.02	0.42
1:E:125:HIS:NE2	1:E:149:THR:OG1	2.50	0.42
1:B:114:LEU:O	1:C:128:THR:OG1	2.25	0.42
1:A:275:THR:O	1:A:279:MET:HG2	2.20	0.42
1:D:169:ILE:CG2	1:D:229:ARG:HH11	2.20	0.42
1:B:106:LEU:HD13	1:B:132:LYS:HD3	2.01	0.42
1:E:335:ALA:HA	1:E:338:ILE:HG22	2.02	0.42
1:B:354:ASN:OD1	1:B:358:TRP:NE1	2.53	0.42
1:E:106:LEU:HD13	1:E:132:LYS:HD3	2.00	0.42
1:C:64:PHE:HB2	1:C:200:LEU:CD2	2.50	0.42
1:B:275:THR:O	1:B:279:MET:HG2	2.20	0.41
1:C:275:THR:O	1:C:279:MET:HG2	2.20	0.41
1:E:275:THR:O	1:E:279:MET:HG2	2.20	0.41
1:E:64:PHE:HB2	1:E:200:LEU:CD2	2.50	0.41
1:D:335:ALA:HA	1:D:338:ILE:HG22	2.02	0.41
1:C:335:ALA:HA	1:C:338:ILE:HG22	2.02	0.41
1:C:80:LEU:O	1:C:145:SER:HA	2.21	0.41
1:D:275:THR:O	1:D:279:MET:HG2	2.20	0.41
1:D:354:ASN:OD1	1:D:358:TRP:NE1	2.53	0.41
1:D:80:LEU:O	1:D:145:SER:HA	2.21	0.41
1:B:194:VAL:HG13	1:B:198:LEU:HD23	2.02	0.41
1:B:317:TYR:O	1:B:321:ASN:ND2	2.53	0.41
1:E:169:ILE:CG2	1:E:229:ARG:HH11	2.20	0.41
1:E:83:GLN:HA	1:E:142:VAL:O	2.20	0.41
1:B:64:PHE:HB2	1:B:200:LEU:CD2	2.50	0.41
1:A:83:GLN:HA	1:A:142:VAL:O	2.20	0.41
1:A:354:ASN:OD1	1:A:358:TRP:NE1	2.53	0.41
1:C:83:GLN:HA	1:C:142:VAL:O	2.20	0.41
1:E:80:LEU:O	1:E:145:SER:HA	2.21	0.41
1:E:194:VAL:HG13	1:E:198:LEU:HD23	2.02	0.41
1:B:335:ALA:HA	1:B:338:ILE:HG22	2.02	0.41
1:B:55:VAL:HG23	1:B:182:LEU:HD11	2.03	0.41
1:D:83:GLN:HA	1:D:142:VAL:O	2.20	0.41
1:B:80:LEU:O	1:B:145:SER:HA	2.21	0.41
1:A:317:TYR:O	1:A:321:ASN:ND2	2.53	0.41
1:A:105:MET:HG2	1:E:43:ARG:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:GLN:HA	1:B:142:VAL:O	2.21	0.41
1:C:125:HIS:NE2	1:C:149:THR:OG1	2.50	0.40
1:C:125:HIS:HE2	1:C:149:THR:HG1	1.69	0.40
1:E:317:TYR:O	1:E:321:ASN:ND2	2.53	0.40
1:D:55:VAL:HG23	1:D:182:LEU:HD11	2.03	0.40
1:C:354:ASN:OD1	1:C:358:TRP:NE1	2.53	0.40
1:C:175:PHE:O	1:D:133:LEU:HD12	2.21	0.40
1:D:135:ARG:HG2	1:D:143:LEU:HB3	2.03	0.40
1:A:69:GLU:CB	1:A:291:PRO:HD3	2.52	0.40
1:C:135:ARG:HG2	1:C:143:LEU:HB3	2.03	0.40
1:A:80:LEU:O	1:A:145:SER:HA	2.21	0.40
1:E:201:PRO:O	1:E:202:GLN:HB2	2.22	0.40
1:D:317:TYR:O	1:D:321:ASN:ND2	2.53	0.40
1:A:194:VAL:HG13	1:A:198:LEU:HD23	2.02	0.40
1:B:201:PRO:O	1:B:202:GLN:HB2	2.22	0.40
1:E:55:VAL:HG23	1:E:182:LEU:HD11	2.03	0.40
1:D:69:GLU:CB	1:D:291:PRO:HD3	2.52	0.40
1:B:79:PHE:CE1	1:B:147:ARG:HD2	2.57	0.40
1:D:280:THR:O	1:D:283:SER:OG	2.30	0.40
1:C:280:THR:O	1:C:283:SER:OG	2.30	0.40

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	334/342 (98%)	331 (99%)	3 (1%)	0	100	100
1	B	334/342 (98%)	331 (99%)	3 (1%)	0	100	100
1	C	334/342 (98%)	331 (99%)	3 (1%)	0	100	100
1	D	334/342 (98%)	331 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	334/342 (98%)	331 (99%)	3 (1%)	0	100	100
All	All	1670/1710 (98%)	1655 (99%)	15 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	246/304 (81%)	246 (100%)	0	100	100
1	B	246/304 (81%)	246 (100%)	0	100	100
1	C	246/304 (81%)	246 (100%)	0	100	100
1	D	246/304 (81%)	246 (100%)	0	100	100
1	E	246/304 (81%)	246 (100%)	0	100	100
All	All	1230/1520 (81%)	1230 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	160	ASN
1	B	54	ASN
1	B	160	ASN
1	C	54	ASN
1	C	160	ASN
1	D	54	ASN
1	D	160	ASN
1	E	54	ASN
1	E	160	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 ⓘ

10 carbohydrates are modelled in this entry.

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	501	2	14,14,15	0.38	0	15,19,21	1.32	1 (6%)
2	NAG	A	502	2	14,14,15	0.61	0	15,19,21	0.58	0
2	NAG	B	501	2	14,14,15	0.38	0	15,19,21	1.32	1 (6%)
2	NAG	B	502	2	14,14,15	0.61	0	15,19,21	0.58	0
2	NAG	C	501	2	14,14,15	0.37	0	15,19,21	1.33	1 (6%)
2	NAG	C	502	2	14,14,15	0.60	0	15,19,21	0.58	0
2	NAG	D	501	2	14,14,15	0.39	0	15,19,21	1.32	1 (6%)
2	NAG	D	502	2	14,14,15	0.60	0	15,19,21	0.58	0
2	NAG	E	501	2	14,14,15	0.38	0	15,19,21	1.32	1 (6%)
2	NAG	E	502	2	14,14,15	0.62	0	15,19,21	0.58	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	501	2	-	0/6/23/26	0/1/1/1
2	NAG	A	502	2	-	0/6/23/26	0/1/1/1
2	NAG	B	501	2	-	0/6/23/26	0/1/1/1
2	NAG	B	502	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	501	2	-	0/6/23/26	0/1/1/1
2	NAG	C	502	2	-	0/6/23/26	0/1/1/1
2	NAG	D	501	2	-	0/6/23/26	0/1/1/1
2	NAG	D	502	2	-	0/6/23/26	0/1/1/1
2	NAG	E	501	2	-	0/6/23/26	0/1/1/1
2	NAG	E	502	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	NAG	C2-N2-C7	4.51	128.97	123.11
2	A	501	NAG	C2-N2-C7	4.51	128.97	123.11
2	E	501	NAG	C2-N2-C7	4.51	128.97	123.11
2	D	501	NAG	C2-N2-C7	4.52	128.98	123.11
2	C	501	NAG	C2-N2-C7	4.55	129.02	123.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NAG	2	0
2	B	501	NAG	2	0
2	C	501	NAG	2	0
2	D	501	NAG	2	0
2	E	501	NAG	2	0

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.