



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 01:14 AM GMT

PDB ID : 2C6N  
Title : Structure of human somatic angiotensin-I converting enzyme N domain with lisinopril  
Authors : Corradi, H.R.; Schwager, S.L.U.; Nichinda, A.; Sturrock, E.D.; Acharya, K.R.  
Deposited on : 2005-11-10  
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

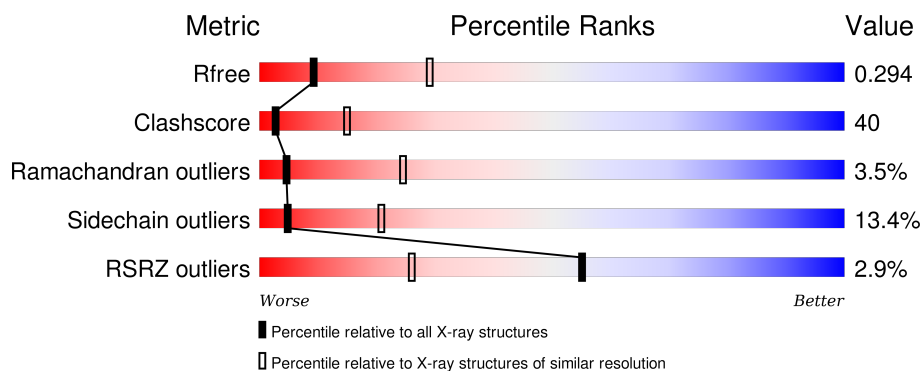
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	612	<div> <div>3%</div> <div>49%</div> <div>41%</div> <div>9%</div> <div>.</div> </div>
1	B	612	<div> <div>3%</div> <div>51%</div> <div>38%</div> <div>9%</div> <div>.</div> </div>

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	691	-	-	-	X
2	NAG	B	696	X	-	-	-
3	NAG	A	695	-	-	-	X
6	LPR	A	705	-	-	-	X
7	GOL	A	2433	-	-	-	X
7	GOL	A	2434	-	-	-	X
8	NDG	B	693	-	-	X	X

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 9621 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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.

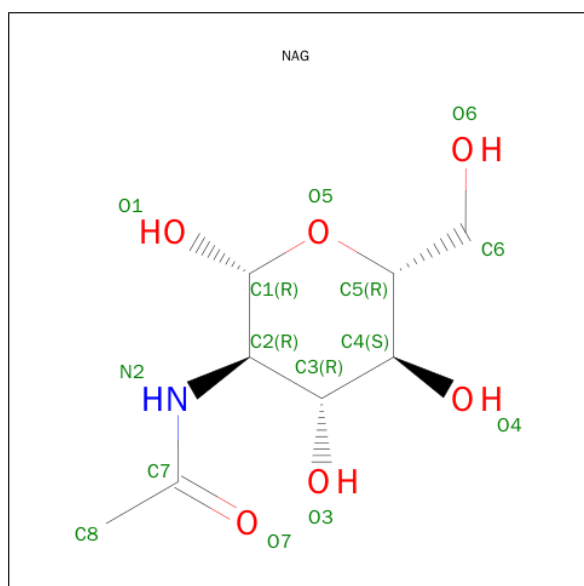
- Molecule 1 is a protein called ANGIOTENSIN-CONVERTING ENZYME, SOMATIC ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	612	Total	C	N	O	S	7	0	0
			4747	3057	811	861	18			
1	B	609	Total	C	N	O	S	9	0	0
			4665	3005	797	845	18			

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

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

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

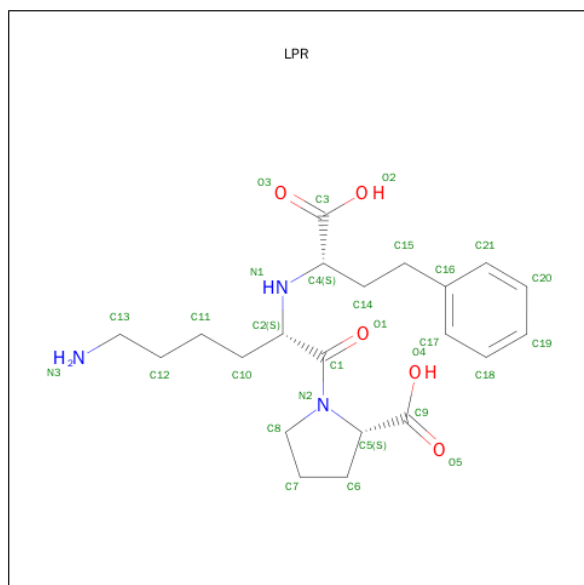
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	0
			1	1		
5	A	1	Total	Cl	0	0
			1	1		

- Molecule 6 is [N2-[(S)-1-CARBOXY-3-PHENYLPROPYL]-L-LYSYL-L-PROLINE (three-letter code: LPR) (formula: C<sub>21</sub>H<sub>31</sub>N<sub>3</sub>O<sub>5</sub>).



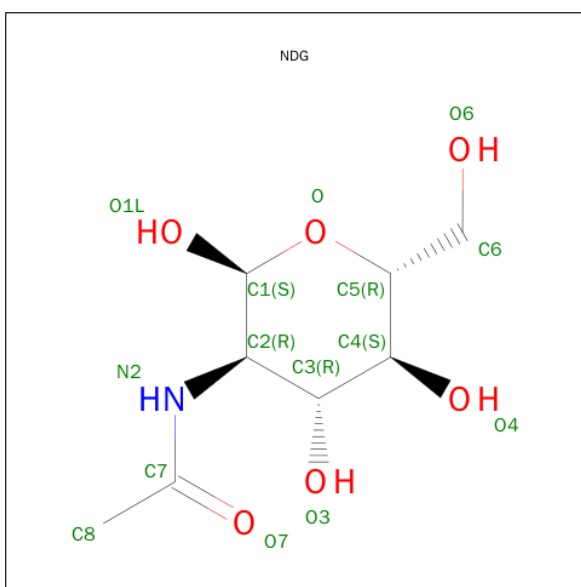
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			29	21	3	5		
6	B	1	Total	C	N	O	0	0
			29	21	3	5		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



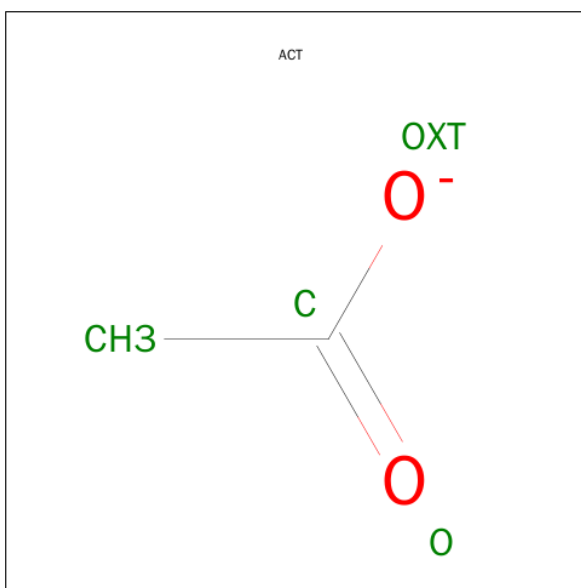
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 9 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 10 is water.

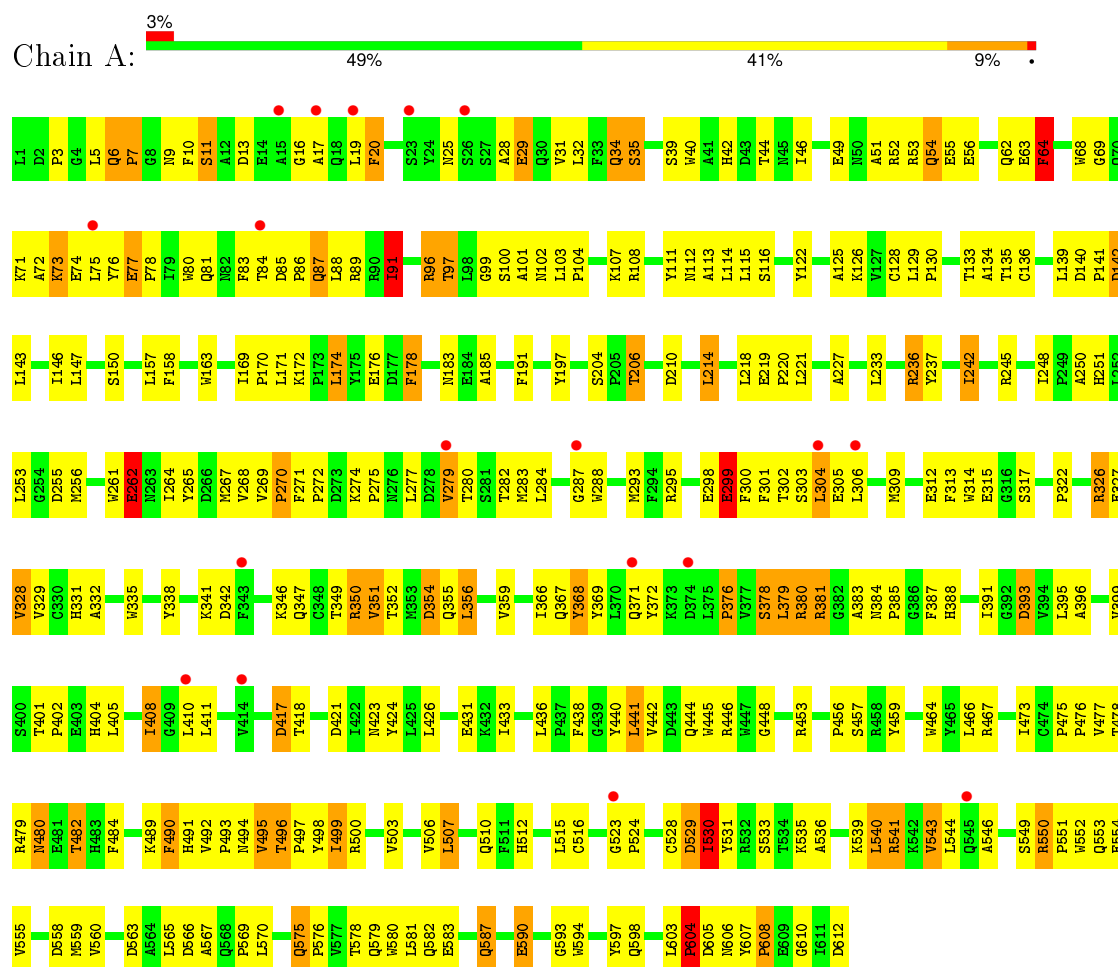
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	8	Total 8	O 8	0	0
10	B	11	Total 11	O 11	0	0



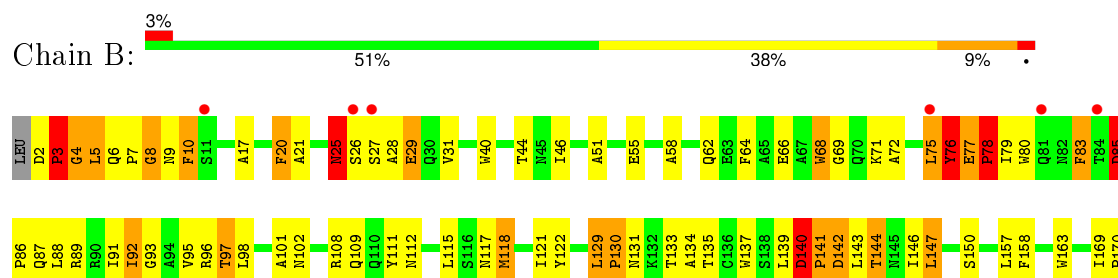
### 3 Residue-property plots

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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: ANGIOTENSIN-CONVERTING ENZYME, SOMATIC ISOFORM



#### • Molecule 1: ANGIOTENSIN-CONVERTING ENZYME, SOMATIC ISOFORM



G589	G590	G593	G594	P595	E596	Y597	Q598	W599	P604	D605	W606	Y607	P608	E609	G610	I611	ASP	L171	K172	P173	L174	N183	E184	A185	Q188	D193	R199	S200	W201	Y202	N203	S204	P205	T206	F207	L211	E212	H213	L214	Y215	Q216	Q217	L218	E219	P220	L221	Y222	L225	Y229	R230	R231	R235	R236	Y241	R245	A250	H251	L252	G254	D255	W256	W257	S260	W261																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
Y501	F502	Y503	S504	L507	Q508	P509	Q510	A514	G520	Y521	E522	G523	C528	D529	I530	Y531	A536	G537	A538	K539	L540	R541	L544	G547	P551	W552	Q553	V560	D563	D566	A567	Q568	P569	L570	L571	F574	Q575	W580	L581	Q582	E583	Q584	R585	Q586	Q587	I588	I284	Y285	D286	L287	V288	W289	A290	T291	H292	Y293	Y294	R295	V296	A297	E298	T302	S303	L304	E305	G306	S307	P308	M309	P310	F313	W314	E315	G316	S317	W318	P322	L253	G254	D255	W256	W257	S260	W261																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
L407	L408	G409	L410	L411	V414	D417	T418	L422	N423	L426	K427	N428	A429	L430	T433	L436	P437	F438	G439	T440	L441	V442	D443	Q444	W445	N460	W464	G472	P475	P476	V477	T478	R479	N480	E481	T482	A486	K489	V492	P493	N494	V495	R498	T499	R500	I284	Y285	D286	L287	V288	W289	A290	T291	H292	Y293	Y294	R295	V296	A297	E298	T302	S303	L304	E305	G306	S307	P308	M309	P310	F313	W314	E315	G316	S317	W318	P322	L253	G254	D255	W256	W257	S260	W261																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
A332	A332	K335	K335	Y338	K339	K340	K341	D342	F343	K346	Q347	C348	T349	K350	Y351	T352	K353	H361	E362	H365	K366	Q367	Y368	Y369	L370	R371	Q372	K373	P376	Y377	S378	L379	K380	K381	G382	A383	K384	F387	K388	A390	T391	G392	D393	V394	L397	S398	D324	P402	E403	H404	K326	E327	V328	Y329	Y330	Y331	Y332	Y333	Y334	Y335	Y336	Y337	Y338	Y339	Y340	Y341	Y342	Y343	Y344	Y345	Y346	Y347	Y348	Y349	Y350	Y351	Y352	Y353	Y354	Y355	Y356	Y357	Y358	Y359	Y360	Y361	Y362	Y363	Y364	Y365	Y366	Y367	Y368	Y369	Y370	Y371	Y372	Y373	Y374	Y375	Y376	Y377	Y378	Y379	Y380	Y381	Y382	Y383	Y384	Y385	Y386	Y387	Y388	Y389	Y390	Y391	Y392	Y393	Y394	Y395	Y396	Y397	Y398	Y399	Y400	Y401	Y402	Y403	Y404	Y405	Y406	Y407	Y408	Y409	Y410	Y411	Y412	Y413	Y414	Y415	Y416	Y417	Y418	Y419	Y420	Y421	Y422	Y423	Y424	Y425	Y426	Y427	Y428	Y429	Y430	Y431	Y432	Y433	Y434	Y435	Y436	Y437	Y438	Y439	Y440	Y441	Y442	Y443	Y444	Y445	Y446	Y447	Y448	Y449	Y450	Y451	Y452	Y453	Y454	Y455	Y456	Y457	Y458	Y459	Y460	Y461	Y462	Y463	Y464	Y465	Y466	Y467	Y468	Y469	Y470	Y471	Y472	Y473	Y474	Y475	Y476	Y477	Y478	Y479	Y480	Y481	Y482	Y483	Y484	Y485	Y486	Y487	Y488	Y489	Y490	Y491	Y492	Y493	Y494	Y495	Y496	Y497	Y498	Y499	Y500	Y501	Y502	Y503	Y504	Y505	Y506	Y507	Y508	Y509	Y510	Y511	Y512	Y513	Y514	Y515	Y516	Y517	Y518	Y519	Y520	Y521	Y522	Y523	Y524	Y525	Y526	Y527	Y528	Y529	Y530	Y531	Y532	Y533	Y534	Y535	Y536	Y537	Y538	Y539	Y540	Y541	Y542	Y543	Y544	Y545	Y546	Y547	Y548	Y549	Y550	Y551	Y552	Y553	Y554	Y555	Y556	Y557	Y558	Y559	Y560	Y561	Y562	Y563	Y564	Y565	Y566	Y567	Y568	Y569	Y570	Y571	Y572	Y573	Y574	Y575	Y576	Y577	Y578	Y579	Y580	Y581	Y582	Y583	Y584	Y585	Y586	Y587	Y588	Y589	Y590	Y591	Y592	Y593	Y594	Y595	Y596	Y597	Y598	Y599	Y600	Y601	Y602	Y603	Y604	Y605	Y606	Y607	Y608	Y609	Y610	Y611	Y612	Y613	Y614	Y615	Y616	Y617	Y618	Y619	Y620	Y621	Y622	Y623	Y624	Y625	Y626	Y627	Y628	Y629	Y630	Y631	Y632	Y633	Y634	Y635	Y636	Y637	Y638	Y639	Y640	Y641	Y642	Y643	Y644	Y645	Y646	Y647	Y648	Y649	Y650	Y651	Y652	Y653	Y654	Y655	Y656	Y657	Y658	Y659	Y660	Y661	Y662	Y663	Y664	Y665	Y666	Y667	Y668	Y669	Y670	Y671	Y672	Y673	Y674	Y675	Y676	Y677	Y678	Y679	Y680	Y681	Y682	Y683	Y684	Y685	Y686	Y687	Y688	Y689	Y690	Y691	Y692	Y693	Y694	Y695	Y696	Y697	Y698	Y699	Y700	Y701	Y702	Y703	Y704	Y705	Y706	Y707	Y708	Y709	Y710	Y711	Y712	Y713	Y714	Y715	Y716	Y717	Y718	Y719	Y720	Y721	Y722	Y723	Y724	Y725	Y726	Y727	Y728	Y729	Y730	Y731	Y732	Y733	Y734	Y735	Y736	Y737	Y738	Y739	Y740	Y741	Y742	Y743	Y744	Y745	Y746	Y747	Y748	Y749	Y750	Y751	Y752	Y753	Y754	Y755	Y756	Y757	Y758	Y759	Y760	Y761	Y762	Y763	Y764	Y765	Y766	Y767	Y768	Y769	Y770	Y771	Y772	Y773	Y774	Y775	Y776	Y777	Y778	Y779	Y780	Y781	Y782	Y783	Y784	Y785	Y786	Y787	Y788	Y789	Y790	Y791	Y792	Y793	Y794	Y795	Y796	Y797	Y798	Y799	Y800	Y801	Y802	Y803	Y804	Y805	Y806	Y807	Y808	Y809	Y810	Y811	Y812	Y813	Y814	Y815	Y816	Y817	Y818	Y819	Y820	Y821	Y822	Y823	Y824	Y825	Y826	Y827	Y828	Y829	Y830	Y831	Y832	Y833	Y834	Y835	Y836	Y837	Y838	Y839	Y840	Y841	Y842	Y843	Y844	Y845	Y846	Y847	Y848	Y849	Y850	Y851	Y852	Y853	Y854	Y855	Y856	Y857	Y858	Y859	Y860	Y861	Y862	Y863	Y864	Y865	Y866	Y867	Y868	Y869	Y870	Y871	Y872	Y873	Y874	Y875	Y876	Y877	Y878	Y879	Y880	Y881	Y882	Y883	Y884	Y885	Y886	Y887	Y888	Y889	Y890	Y891	Y892	Y893	Y894	Y895	Y896	Y897	Y898	Y899	Y900	Y901	Y902	Y903	Y904	Y905	Y906	Y907	Y908	Y909	Y910	Y911	Y912	Y913	Y914	Y915	Y916	Y917	Y918	Y919	Y920	Y921	Y922	Y923	Y924	Y925	Y926	Y927	Y928	Y929	Y930	Y931	Y932	Y933	Y934	Y935	Y936	Y937	Y938	Y939	Y940	Y941	Y942	Y943	Y944	Y945	Y946	Y947	Y948	Y949	Y950	Y951	Y952	Y953	Y954	Y955	Y956	Y957	Y958	Y959	Y960	Y961	Y962	Y963	Y964	Y965	Y966	Y967	Y968	Y969	Y970	Y971	Y972	Y973	Y974	Y975	Y976	Y977	Y978	Y979	Y980	Y981	Y982	Y983	Y984	Y985	Y986	Y987	Y988	Y989	Y990	Y991	Y992	Y993	Y994	Y995	Y996	Y997	Y998	Y999	Y1000

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.30Å 210.90Å 171.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.76 – 3.00 89.76 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.1 (28.76-3.00) 95.0 (89.76-3.00)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.04 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.294 , 0.308 0.287 , 0.294	Depositor DCC
$R_{free}$ test set	1088 reflections (3.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.6	Xtriage
Anisotropy	0.576	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 66.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 35236 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	9621	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, NAG, CL, LPR, NDG, ACT

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	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.60	4/4901 (0.1%)	0.89	23/6707 (0.3%)
1	B	0.58	3/4819 (0.1%)	0.92	26/6608 (0.4%)
All	All	0.59	7/9720 (0.1%)	0.90	49/13315 (0.4%)

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	0	1
1	B	1	8
2	B	1	0
All	All	2	9

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	381	ARG	CB-CG	8.17	1.74	1.52
1	B	25	ASN	CB-CG	-6.37	1.36	1.51
1	B	541	ARG	CB-CG	6.19	1.69	1.52
1	A	381	ARG	CG-CD	6.03	1.67	1.51
1	A	351	VAL	CB-CG1	-5.53	1.41	1.52

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	307	SER	C-N-CD	-10.95	96.50	120.60
1	B	305	GLU	N-CA-C	9.82	137.53	111.00
1	B	77	GLU	C-N-CD	-8.88	101.06	120.60

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	523	GLY	N-CA-C	-8.38	92.16	113.10
1	B	76	TYR	N-CA-C	8.24	133.24	111.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	530	ILE	CB
2	B	696	NAG	C2

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	380	ARG	Mainchain
1	B	76	TYR	Sidechain
1	B	83	PHE	Peptide
1	B	85	ASP	Peptide
1	B	86	PRO	Peptide

## 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	4747	0	4318	390	0
1	B	4665	0	4155	332	0
2	A	28	0	25	2	0
2	B	28	0	25	6	0
3	A	28	0	26	7	0
3	B	14	0	13	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	1	0
6	A	29	0	27	2	0
6	B	29	0	27	0	0
7	A	12	0	14	5	0
8	B	14	0	13	12	0
9	B	4	0	3	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	A	8	0	0	1	0
10	B	11	0	0	1	0
All	All	9621	0	8646	732	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 40.

The worst 5 of 732 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:381:ARG:CG	1:A:381:ARG:CB	1.74	1.63
8:B:693:NDG:C3	8:B:693:NDG:H8C1	1.42	1.39
1:B:482:THR:CG2	2:B:691:NAG:H82	1.56	1.33
1:A:6:GLN:HG3	1:A:7:PRO:CD	1.78	1.11
3:A:693:NAG:O7	3:A:693:NAG:H3	1.48	1.10

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 X-ray entries followed by that with respect to entries of similar resolution.

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	610/612 (100%)	506 (83%)	83 (14%)	21 (3%)	5	25
1	B	605/612 (99%)	514 (85%)	70 (12%)	21 (4%)	4	24
All	All	1215/1224 (99%)	1020 (84%)	153 (13%)	42 (4%)	4	24

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	PRO
1	A	85	ASP

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Mol	Chain	Res	Type
1	B	3	PRO
1	B	130	PRO
1	B	308	PRO

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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	458/526 (87%)	398 (87%)	60 (13%)	5	22
1	B	437/526 (83%)	377 (86%)	60 (14%)	4	20
All	All	895/1052 (85%)	775 (87%)	120 (13%)	5	21

5 of 120 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	582	GLN
1	B	85	ASP
1	B	477	VAL
1	A	587	GLN
1	B	3	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	109	GLN
1	B	183	ASN
1	B	579	GLN
1	B	112	ASN
1	B	188	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 ⓘ

4 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	691	1,2	14,14,15	2.72	3 (21%)	15,19,21	1.81	3 (20%)
2	NAG	A	696	2	14,14,15	2.31	1 (7%)	15,19,21	1.11	2 (13%)
2	NAG	B	691	1,2	14,14,15	0.25	0	15,19,21	0.84	1 (6%)
2	NAG	B	696	2	14,14,15	2.42	1 (7%)	15,19,21	0.87	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	691	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	696	2	-	0/6/23/26	0/1/1/1
2	NAG	B	691	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	696	2	1/1/5/7	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	696	NAG	C8-C7	-8.99	1.32	1.50
2	A	691	NAG	C8-C7	-8.91	1.32	1.50
2	A	696	NAG	C8-C7	-8.45	1.33	1.50
2	A	691	NAG	C4-C3	-2.39	1.46	1.52
2	A	691	NAG	C1-C2	2.53	1.56	1.52

The worst 5 of 7 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	691	NAG	C3-C2-N2	-4.86	98.93	110.56
2	A	691	NAG	C6-C5-C4	-2.91	105.84	113.02
2	A	696	NAG	C1-O5-C5	-2.83	108.66	112.25
2	B	691	NAG	C3-C2-N2	-2.31	105.02	110.56
2	B	696	NAG	C3-C2-N2	-2.29	105.07	110.56

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	696	NAG	C2

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	691	NAG	2	0
2	A	696	NAG	1	0
2	B	691	NAG	6	0

## 5.6 Ligand geometry

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 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	$\# Z  > 2$
7	GOL	A	2433	-	5,5,5	3.39	3 (60%)	5,5,5	2.03	1 (20%)
7	GOL	A	2434	-	5,5,5	3.54	3 (60%)	5,5,5	1.49	1 (20%)
3	NAG	A	693	1	14,14,15	0.25	0	15,19,21	0.84	1 (6%)
3	NAG	A	695	1	14,14,15	0.25	0	15,19,21	0.84	1 (6%)
6	LPR	A	705	4	24,30,30	4.97	14 (58%)	24,39,39	1.55	5 (20%)
8	NDG	B	693	1	14,14,15	0.24	0	15,19,21	0.84	1 (6%)
3	NAG	B	695	1	14,14,15	0.25	0	15,19,21	0.84	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	LPR	B	705	4	24,30,30	5.22	12 (50%)	24,39,39	1.30	5 (20%)
9	ACT	B	710	-	1,3,3	3.42	1 (100%)	0,3,3	0.00	-

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
7	GOL	A	2433	-	-	0/4/4/4	0/0/0/0
7	GOL	A	2434	-	-	0/4/4/4	0/0/0/0
3	NAG	A	693	1	-	0/6/23/26	0/1/1/1
3	NAG	A	695	1	-	0/6/23/26	0/1/1/1
6	LPR	A	705	4	-	0/22/40/40	0/2/2/2
8	NDG	B	693	1	-	0/6/23/26	0/1/1/1
3	NAG	B	695	1	-	0/6/23/26	0/1/1/1
6	LPR	B	705	4	-	0/22/40/40	0/2/2/2
9	ACT	B	710	-	-	0/0/0/0	0/0/0/0

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	705	LPR	C4-N1	-22.07	1.17	1.47
6	A	705	LPR	C4-N1	-20.70	1.19	1.47
7	A	2434	GOL	O2-C2	-6.53	1.24	1.43
6	B	705	LPR	C14-C4	-5.58	1.45	1.53
7	A	2433	GOL	O2-C2	-4.65	1.29	1.43

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2433	GOL	O3-C3-C2	-4.00	90.80	110.18
7	A	2434	GOL	O3-C3-C2	-3.05	95.39	110.18
3	B	695	NAG	C3-C2-N2	-2.32	105.01	110.56
3	A	695	NAG	C3-C2-N2	-2.31	105.02	110.56
3	A	693	NAG	C3-C2-N2	-2.31	105.03	110.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	2433	GOL	3	0
7	A	2434	GOL	2	0
3	A	693	NAG	5	0
3	A	695	NAG	2	0
6	A	705	LPR	2	0
8	B	693	NDG	12	0
3	B	695	NAG	1	0
9	B	710	ACT	1	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.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	612/612 (100%)	0.30	18 (2%)	55 26	5, 39, 64, 72	4 (0%)
1	B	609/612 (99%)	0.28	18 (2%)	54 25	4, 41, 67, 81	4 (0%)
All	All	1221/1224 (99%)	0.29	36 (2%)	55 26	4, 40, 66, 81	8 (0%)

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	520	GLY	3.3
1	A	15	ALA	3.2
1	B	417	ASP	3.1
1	B	376	PRO	3.1
1	B	544	LEU	3.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	A	691	14/15	0.76	0.31	6.57	29,32,35,37	0
2	NAG	B	691	14/15	0.89	0.25	1.71	32,35,37,38	0
2	NAG	A	696	14/15	0.70	0.37	-	100,101,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	B	696	14/15	0.68	0.38	-	90,92,93,94	0

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	GOL	A	2434	6/6	0.87	0.34	5.82	28,29,30,31	0
7	GOL	A	2433	6/6	0.87	0.31	3.92	25,27,27,27	0
6	LPR	A	705	29/29	0.87	0.38	3.13	43,47,49,49	0
3	NAG	A	695	14/15	0.81	0.33	2.57	73,74,75,76	0
8	NDG	B	693	14/15	0.56	0.54	1.86	66,69,70,70	0
6	LPR	B	705	29/29	0.92	0.30	0.25	35,40,43,45	0
3	NAG	A	693	14/15	0.73	0.31	-0.23	69,72,74,75	0
5	CL	A	703	1/1	0.84	0.15	-2.51	31,31,31,31	0
5	CL	B	702	1/1	0.97	0.14	-2.84	25,25,25,25	0
4	ZN	B	701	1/1	0.97	0.09	-	31,31,31,31	0
9	ACT	B	710	4/4	0.83	0.28	-	29,30,30,32	0
3	NAG	B	695	14/15	0.66	0.53	-	77,78,81,83	0
4	ZN	A	701	1/1	0.98	0.08	-	33,33,33,33	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.