



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 08:52 pm GMT

PDB ID : 2C6F  
Title : STRUCTURE OF HUMAN SOMATIC ANGIOTENSIN-I CONVERTING  
ENZYME N DOMAIN  
Authors : Corradi, H.R.; Schwager, S.L.U.; Nichinda, A.; Sturrock, E.D.; Acharya, K.R.  
Deposited on : 2005-11-09  
Resolution : 3.01 Å(reported)

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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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

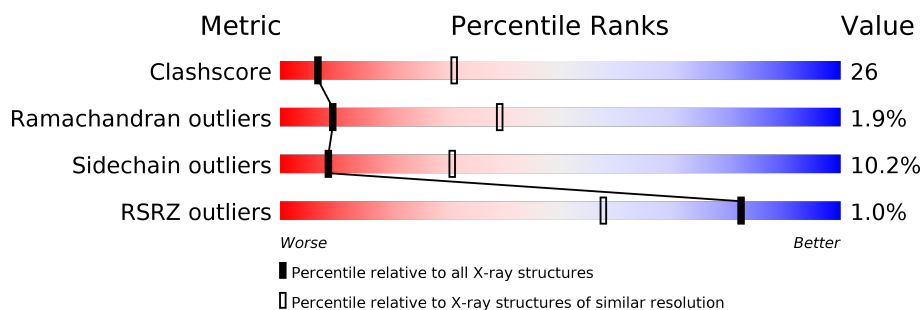
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 3.01 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))
Clashscore	112137	2279 (3.04-3.00)
Ramachandran outliers	110173	2207 (3.04-3.00)
Sidechain outliers	110143	2210 (3.04-3.00)
RSRZ outliers	101464	1948 (3.04-3.00)

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	 58% 36% 6%
1	B	612	 57% 38% 5%

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	691	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	695	-	-	-	X
3	NAG	A	697	-	-	-	X
3	NAG	B	692	-	-	-	X
3	NAG	B	695	-	-	-	X
6	ACT	A	801	-	-	-	X
6	ACT	B	801	-	-	-	X
7	GOL	A	2434	-	-	-	X
7	GOL	B	2433	-	X	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9970 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	6	0	0
			4884	3145	840	880	19			
1	B	611	Total	C	N	O	S	14	0	0
			4852	3124	830	879	19			

- 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	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		
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<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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	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		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

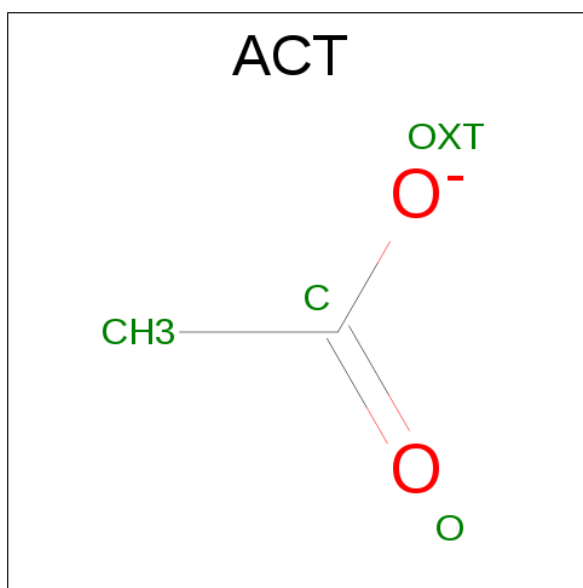
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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).

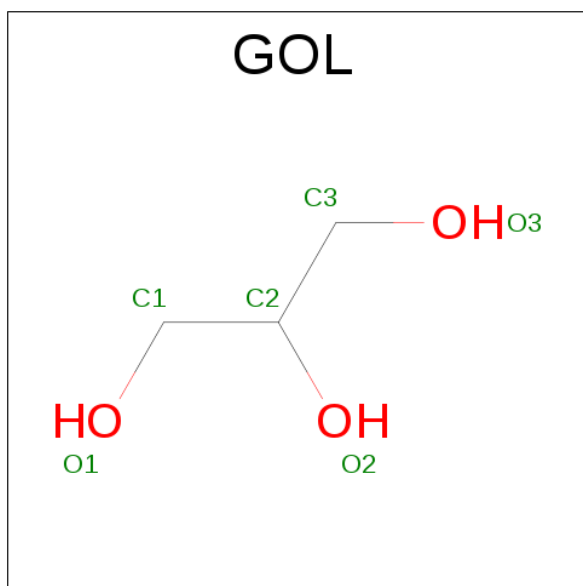
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	0
			1	1		
5	A	1	Total	Cl	0	0
			1	1		

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



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

- 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	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	11	Total	O	0	0
			11	11		
8	B	13	Total	O	0	0
			13	13		





Q553	F271	V440	R350	F569	V279	G561	L356	E362	H292	L562	T282	D563	E362	M283	L571	K373	F294	C382	E299	L304	M309	P310	P311	E312	F313	W314	E315	G316	S317	E320	D324	G325	R326	E327	V328	V329	A332	Y338	M339	K340	K341	D342	F343	R344	I345	K346	Q347	C348	T349
E554	P272	L441	V351	P456	V279	G561	R453	P456	M283	A564	L284	D563	H365	L284	L571	K373	M293	D374	F300	L304	K309	P310	P311	E312	F313	W314	E315	G316	S317	E320	D324	G325	R326	E327	V328	V329	A332	Y338	M339	K340	K341	D342	F343	R344	I345	K346	Q347	C348	T349
K557	K274	D443	M352	Y459	P275	G561	D443	Y459	M293	L565	K283	D566	I366	L284	L571	K373	M293	D374	F300	L304	K309	P310	P311	E312	F313	W314	E315	G316	S317	E320	D324	G325	R326	E327	V328	V329	A332	Y338	M339	K340	K341	D342	F343	R344	I345	K346	Q347	C348	T349
D558	K274	Q444	M353	M460	P275	G561	Q444	M460	M295	L565	K283	D566	I366	L284	L571	K373	M293	D374	F300	L304	K309	P310	P311	E312	F313	W314	E315	G316	S317	E320	D324	G325	R326	E327	V328	V329	A332	Y338	M339	K340	K341	D342	F343	R344	I345	K346	Q347	C348	T349
M559	K274	W445	M355	W464	P275	G561	W445	W464	V296	L566	K283	D566	I366	L284	L571	K373	M293	D374	F300	L304	K309	P310	P311	E312	F313	W314	E315	G316	S317	E320	D324	G325	R326	E327	V328	V329	A332	Y338	M339	K340	K341	D342	F343	R344	I345	K346	Q347	C348	T349
W560	K274	W445	M355	W464	P275	G561	W445	W464	V296	L566	K283	D566	I366	L284	L571	K373	M293	D374	F300	L304	K309	P310	P311	E312	F313	W314	E315	G316	S317	E320	D324	G325	R326	E327	V328	V329	A332	Y338	M339	K340	K341	D342	F343	R344	I345	K346	Q347	C348	T349
G561	P272	R453	V351	P456	V279	G561	R453	P456	M283	L562	T282	D563	H365	L284	L571	K373	M293	D374	F300	L304	K309	P310	P311	E312	F313	W314	E315	G316	S317	E320	D324	G325	R326	E327	V328	V329	A332	Y338	M339	K340	K341	D342	F343	R344	I345	K346	Q347	C348	T349
L562	P272	R453	V351	P456	V279	G561	R453	P456	M283	L562	T282	D563	H365	L284	L571	K373	M293	D374	F300	L304	K309	P310	P311	E312	F313	W314	E315	G316	S317	E320	D324	G325	R326	E327	V328	V329	A332	Y338	M339	K340	K341	D342	F343	R344	I345	K346	Q347	C348	T349
D563	P272	R453	V351	P456	V279	G561	R453	P456	M283	L562	T282	D563	H365	L284	L571	K373	M293	D374	F300	L304	K309	P310	P311	E312	F313	W314	E315	G316	S317	E320	D324	G325	R326	E327	V328	V329	A332	Y338	M339	K340	K341	D342	F343	R344	I345	K346	Q347	C348	T349
A564	P272	R453	V351	P456	V279	G561	R453	P456	M283	L562	T282	D563	H365	L284	L571	K373	M293	D374	F300	L304	K309	P310	P311	E312	F313	W314	E315	G316	S317	E320	D324	G325	R326	E327	V328	V329	A332	Y338	M339	K340	K341	D342	F343	R344	I345	K346	Q347	C348	T349
L565	P272	R453	V351	P456	V279	G561	R453	P456	M283	L562	T282	D563	H365	L284	L571	K373	M293	D374	F300	L304	K309	P310	P311	E312	F313	W314	E315	G316	S317	E320	D324	G325	R326	E327	V328	V329	A332	Y338	M339	K340	K341	D342	F343	R344	I345	K346	Q347	C348	T349
D566	P272	R453	V351	P456	V279	G561	R453	P456	M283	L562	T282	D563	H365	L284	L571	K373	M293	D374	F300	L304	K309	P310	P311	E312	F313	W314	E315	G316	S317	E320	D324	G325	R326	E327	V328	V329	A332	Y338	M339	K340	K341	D342	F343	R344	I345	K346	Q347	C348	T349
A567	P272	R453	V351	P456	V279	G561	R453	P456	M283	L562	T282	D563	H365	L284	L571	K373	M293	D374	F300	L304	K309	P310	P311	E312	F313	W314	E315	G316	S317	E320	D324	G325	R326	E327	V328	V329	A332	Y338	M339	K340	K341	D342	F343	R344	I345	K346	Q347	C348	T349
Q568	P272	R453	V351	P456	V279	G561	R453	P456	M283	L562	T282	D563	H365	L284	L571	K373	M293	D374	F300	L304	K309	P310	P311	E312	F313	W314	E315	G316	S317	E320	D324	G325	R326	E327	V328	V329	A332	Y338	M339	K340	K341	D342	F343	R344	I345	K346	Q347	C348	T349
P569	P272	R453	V351	P456	V279	G561	R453	P456	M283	L562	T282	D563	H365	L284	L571	K373	M293	D374	F300	L304	K309	P310	P311	E312	F313	W314	E315	G316	S317	E320	D324	G325	R326	E327	V328	V329	A332	Y338	M339	K340	K341	D342	F343	R344	I345	K346	Q347	C348	T349
L570	P272	R453	V351	P456	V279	G561	R453	P456	M283	L562	T282	D563	H365	L284	L571	K373	M293	D374	F300	L304	K309	P310	P311	E312	F313	W314	E315	G316	S317	E320	D324	G325	R326	E327	V328	V329	A332	Y338	M339	K340	K341	D342	F343	R344	I345	K346	Q347	C348	T349
L571	P272	R453	V351	P456	V279	G561	R453	P456	M283	L562	T282	D563	H365	L284	L571	K373	M293	D374	F300	L304	K309	P310	P311	E312	F313	W314	E315	G316	S317	E320	D324	G325	R326	E327	V328	V329	A332	Y338	M339	K340	K341	D342	F343	R344	I345	K346	Q347	C348	T349
K572	P272	R453	V351	P456	V279	G561	R453	P456	M283	L562	T282	D563	H365	L284	L571	K373	M293	D374	F300	L304	K309	P310	P311	E312	F313	W314	E315	G316	S317	E320	D324	G325	R326	E327	V328	V329	A332	Y338	M339	K340	K341	D342	F343	R344	I345	K346	Q347	C348	T349
Y573	P272	R453	V351	P456	V279	G561	R453	P456	M283	L562	T282	D563	H365	L284	L571	K373	M293	D374	F300	L304	K309	P310	P311	E312	F313	W314	E315	G316	S317	E320	D324	G325	R326	E327	V328	V329	A332	Y338	M339	K340	K341	D342	F343	R344	I345	K346	Q347	C348	T349
F574	P272	R453	V351	P456	V279	G561	R453	P456	M283	L562	T282	D563	H365	L284	L571	K373	M293	D374	F300	L304	K309	P310	P311	E312	F313	W314	E315	G316	S317	E320	D324	G325	R326	E327	V328	V329	A332	Y338	M339	K340	K341	D342	F343	R344	I345	K346	Q347	C348	T349
Q575	P272	R453	V351	P456	V279	G561	R453	P456	M283	L562	T282	D563	H365	L284	L571	K373	M293	D374	F300	L304	K309	P310	P311	E312	F313	W314	E315	G316	S317	E320	D324	G325	R326	E327	V328	V329	A332	Y338	M339	K340	K341	D342	F343	R344	I345	K346	Q347	C348	T349
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Q584	P272	R453	V351	P456	V279	G561	R453	P456	M283	L562	T282	D563	H365	L284	L571	K373	M293	D374	F300	L304	K309	P310	P311	E312	F313	W314	E315	G316	S317	E320	D324	G325	R326	E327	V328	V329	A332	Y338	M339	K340	K341	D342	F343	R344	I345	K346	Q347	C348	T349
M586	P272	R453	V351	P456	V279	G561	R453	P456	M283	L562	T282	D563	H365	L284	L571	K373	M293	D374	F300	L304	K309	P310	P311	E312	F313	W314	E315	G316	S317	E320	D324	G325	R326	E327	V328	V329	A332	Y338	M339	K340	K341	D342	F343	R344	I345	K346	Q347	C348	T349
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E590	P272	R453	V351	P456	V279	G561	R453	P456	M283	L562	T282	D563	H365	L284	L571	K373	M293	D374	F300	L304	K309	P310	P311	E312	F313	W314	E315	G316	S317	E320	D324	G325	R326	E327	V328	V329	A332	Y338	M339	K340	K341	D342	F343	R344	I345	K346	Q347	C348	T349
G593	P272	R453	V351	P456	V279	G561	R453	P456	M283	L562	T282	D563	H365	L284	L571	K373	M293	D374	F300	L304	K309	P310	P311	E312	F313	W314	E315	G316	S317	E320	D324	G325	R326	E327	V328	V329	A332	Y338	M339	K340	K341	D342	F343	R344	I345	K346	Q347	C348	T349
W594	P272	R453	V351	P456	V279	G561	R453	P456	M283	L562	T282	D563	H365	L284	L571	K373	M293	D374	F300	L304	K309	P310	P311	E312	F313	W314	E315	G316	S317	E320	D324	G325	R326	E327	V328	V329	A332	Y338	M339	K340	K341	D342	F343	R344	I345	K346	Q347	C348	T349
P595	P272	R453	V351	P456	V279	G561	R453	P456	M283	L562	T282	D563	H365	L284	L571	K373	M293	D374	F300	L304	K309	P310	P311	E312	F313	W314	E315	G316	S317	E320	D324	G325	R326	E327	V328	V329	A332	Y338	M339	K340	K341	D342	F343	R344	I345	K346	Q347	C348	T349
E596	P272	R453	V351	P456	V279	G561	R453	P456	M283	L562	T282	D563	H365	L284	L571	K373	M293	D374	F300	L304	K309	P310	P311	E312	F313	W314	E315	G316	S317	E320	D324	G325	R326	E327	V328	V329	A332	Y338	M339	K340	K341	D342	F343	R344	I345	K346	Q347	C348	T349
Y597	P272	R453	V351	P456	V279	G561	R453	P456	M283	L562	T282	D563	H365	L284	L571	K373	M293	D37																															

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.12Å 211.32Å 171.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.91 – 3.01 47.91 – 3.01	Depositor EDS
% Data completeness (in resolution range)	96.7 (47.91-3.01) 96.8 (47.91-3.01)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.33 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.224 , 0.273 0.222 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	45.6	Xtriage
Anisotropy	0.335	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 50.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	9970	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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: GOL, ZN, ACT, NAG, CL

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	0.51	1/5042 (0.0%)	0.74	3/6885 (0.0%)
1	B	0.49	0/5010	0.86	6/6845 (0.1%)
All	All	0.50	1/10052 (0.0%)	0.80	9/13730 (0.1%)

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	3	2
All	All	3	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	117	ASN	CB-CG	-5.47	1.38	1.51

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3	PRO	CA-N-CD	-22.64	79.80	111.50
1	B	608	PRO	CA-N-CD	-18.89	85.05	111.50
1	B	607	TYR	CB-CG-CD1	-9.99	115.01	121.00
1	B	607	TYR	CB-CG-CD2	7.49	125.49	121.00
1	B	409	GLY	N-CA-C	5.92	127.91	113.10

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	79	ILE	CA
1	B	410	LEU	CA
1	B	530	ILE	CB

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	607	TYR	Peptide
1	B	275	PRO	Peptide
1	B	409	GLY	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	4884	0	4582	252	0
1	B	4852	0	4514	243	0
2	A	56	0	50	7	0
2	B	56	0	50	5	0
3	A	42	0	36	4	0
3	B	28	0	23	2	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	8	0	6	0	0
6	B	4	0	3	0	0
7	A	6	0	6	1	0
7	B	6	0	6	1	0
8	A	11	0	0	0	0
8	B	13	0	0	0	0
All	All	9970	0	9276	499	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 26.

The worst 5 of 499 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:B:3:PRO:HD3	1:B:6:GLN:NE2	1.36	1.40
1:B:282:THR:HG21	1:B:410:LEU:CB	1.60	1.31
1:A:279:VAL:HG21	1:A:410:LEU:CD1	1.60	1.29
1:B:282:THR:CG2	1:B:410:LEU:CB	2.18	1.20
1:A:279:VAL:CG1	1:A:410:LEU:HD13	1.73	1.17

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%)	537 (88%)	60 (10%)	13 (2%)	8	36
1	B	609/612 (100%)	526 (86%)	73 (12%)	10 (2%)	11	44
All	All	1219/1224 (100%)	1063 (87%)	133 (11%)	23 (2%)	9	39

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	608	PRO
1	B	3	PRO
1	B	608	PRO
1	A	7	PRO
1	A	250	ALA

### 5.3.2 Protein sidechains [i](#)

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	496/526 (94%)	448 (90%)	48 (10%)	9	34
1	B	489/526 (93%)	437 (89%)	52 (11%)	8	29
All	All	985/1052 (94%)	885 (90%)	100 (10%)	8	31

5 of 100 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	582	GLN
1	B	129	LEU
1	B	553	GLN
1	A	587	GLN
1	B	66	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	6	GLN
1	B	18	GLN
1	B	575	GLN
1	A	545	GLN
1	A	575	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 ⓘ

8 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	0.56	0	15,19,21	0.80	1 (6%)
2	NAG	A	693	1,2	14,14,15	0.57	0	15,19,21	0.79	0
2	NAG	A	694	2	14,14,15	0.49	0	15,19,21	0.72	0
2	NAG	A	696	2	14,14,15	0.49	0	15,19,21	0.72	0
2	NAG	B	691	1,2	14,14,15	0.56	0	15,19,21	0.80	0
2	NAG	B	693	1,2	14,14,15	2.26	1 (7%)	15,19,21	1.06	1 (6%)
2	NAG	B	694	2	14,14,15	2.25	1 (7%)	15,19,21	1.06	1 (6%)
2	NAG	B	696	2	14,14,15	0.50	0	15,19,21	0.71	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	691	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	693	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	694	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	693	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	694	2	-	0/6/23/26	0/1/1/1
2	NAG	B	696	2	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	693	NAG	C8-C7	-8.40	1.32	1.50
2	B	694	NAG	C8-C7	-8.35	1.32	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	693	NAG	C1-C2-N2	-3.21	105.01	110.49
2	B	694	NAG	C1-C2-N2	-3.19	105.04	110.49
2	A	691	NAG	C2-N2-C7	-2.02	120.00	122.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	691	NAG	1	0
2	A	693	NAG	1	0
2	A	694	NAG	6	0
2	B	691	NAG	3	0
2	B	693	NAG	2	0

## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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	2434	-	5,5,5	3.56	3 (60%)	5,5,5	1.78	1 (20%)
3	NAG	A	692	1	14,14,15	3.81	3 (21%)	15,19,21	1.92	4 (26%)
3	NAG	A	695	1	14,14,15	0.57	0	15,19,21	0.79	0
3	NAG	A	697	1	14,14,15	0.57	0	15,19,21	0.80	1 (6%)
6	ACT	A	800	-	1,3,3	3.36	1 (100%)	0,3,3	0.00	-
6	ACT	A	801	-	1,3,3	3.88	1 (100%)	0,3,3	0.00	-
7	GOL	B	2433	-	5,5,5	3.59	3 (60%)	5,5,5	1.95	4 (80%)
3	NAG	B	692	1	14,14,15	3.62	2 (14%)	15,19,21	1.60	3 (20%)
3	NAG	B	695	1	14,14,15	0.56	0	15,19,21	0.80	0
6	ACT	B	801	-	1,3,3	3.38	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	2434	-	-	0/4/4/4	0/0/0/0
3	NAG	A	692	1	-	0/6/23/26	0/1/1/1
3	NAG	A	695	1	-	0/6/23/26	0/1/1/1
3	NAG	A	697	1	-	0/6/23/26	0/1/1/1
6	ACT	A	800	-	-	0/0/0/0	0/0/0/0
6	ACT	A	801	-	-	0/0/0/0	0/0/0/0
7	GOL	B	2433	-	-	0/4/4/4	0/0/0/0
3	NAG	B	692	1	-	0/6/23/26	0/1/1/1
3	NAG	B	695	1	-	0/6/23/26	0/1/1/1
6	ACT	B	801	-	-	0/0/0/0	0/0/0/0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	692	NAG	C8-C7	-13.00	1.22	1.50
3	B	692	NAG	C8-C7	-12.96	1.22	1.50
7	B	2433	GOL	C3-C2	-6.91	1.26	1.52
7	A	2434	GOL	C3-C2	-6.84	1.26	1.52
7	B	2433	GOL	C1-C2	2.38	1.61	1.52

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	692	NAG	C1-O5-C5	-4.31	106.22	112.17
3	B	692	NAG	C1-C2-N2	-3.22	104.99	110.49
3	A	692	NAG	C1-C2-N2	-3.19	105.03	110.49
3	A	692	NAG	O7-C7-N2	-2.82	116.49	121.92
3	B	692	NAG	O7-C7-N2	-2.79	116.55	121.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	2434	GOL	1	0
3	A	692	NAG	3	0
3	A	697	NAG	1	0
7	B	2433	GOL	1	0
3	B	692	NAG	2	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%)	-0.40	3 (0%) 90 73	12, 36, 58, 83	3 (0%)
1	B	611/612 (99%)	-0.28	9 (1%) 74 46	12, 38, 68, 84	6 (0%)
All	All	1223/1224 (99%)	-0.34	12 (0%) 82 57	12, 37, 64, 84	9 (0%)

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	131	ASN	3.1
1	B	612	ASP	3.1
1	B	134	ALA	3.0
1	B	135	THR	2.8
1	B	410	LEU	2.8

### 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	B	691	14/15	0.80	0.33	10.89	55,57,62,69	0
2	NAG	A	691	14/15	0.74	0.34	6.66	56,60,68,72	0
2	NAG	B	693	14/15	0.86	0.24	0.74	61,65,67,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	A	693	14/15	0.90	0.23	-0.07	56,58,60,60	0
2	NAG	B	696	14/15	0.63	0.41	-	86,90,91,91	0
2	NAG	A	696	14/15	0.72	0.37	-	95,96,97,97	0
2	NAG	B	694	14/15	0.78	0.34	-	79,80,81,81	0
2	NAG	A	694	14/15	0.70	0.29	-	69,72,73,75	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
3	NAG	A	697	14/15	0.51	0.87	12.38	116,117,118,119	0
6	ACT	A	801	4/4	0.92	0.39	11.07	32,33,34,35	0
6	ACT	B	801	4/4	0.86	0.41	9.53	52,52,53,53	0
7	GOL	A	2434	6/6	0.91	0.26	5.92	29,31,32,33	0
7	GOL	B	2433	6/6	0.93	0.25	4.59	31,34,35,39	0
3	NAG	A	695	14/15	0.86	0.32	3.89	75,76,79,79	0
3	NAG	B	695	14/15	0.84	0.36	3.81	76,78,80,83	0
3	NAG	B	692	14/15	0.70	0.35	2.29	83,86,86,87	0
3	NAG	A	692	14/15	0.72	0.34	1.16	66,68,70,71	0
5	CL	B	703	1/1	0.95	0.13	-0.64	29,29,29,29	0
5	CL	A	702	1/1	0.95	0.12	-1.86	37,37,37,37	0
4	ZN	B	701	1/1	0.99	0.17	-	29,29,29,29	0
4	ZN	A	701	1/1	1.00	0.12	-	31,31,31,31	0
6	ACT	A	800	4/4	0.76	0.46	-	49,51,52,53	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.