



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 07:48 AM GMT

PDB ID : 3NXQ  
Title : Angiotensin Converting Enzyme N domain glycosylation mutant (Ndom389)  
in complex with RXP407  
Authors : Anthony, C.S.; Corradi, H.R.; Schwager, S.L.U.; Redelinghuys, P.; Georgiadis,  
D.; Dive, V.; Acharya, K.R.; Sturrock, E.D.  
Deposited on : 2010-07-14  
Resolution : 1.99 Å(reported)

This is a full wwPDB validation 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/ValidationPDFNotes.html>

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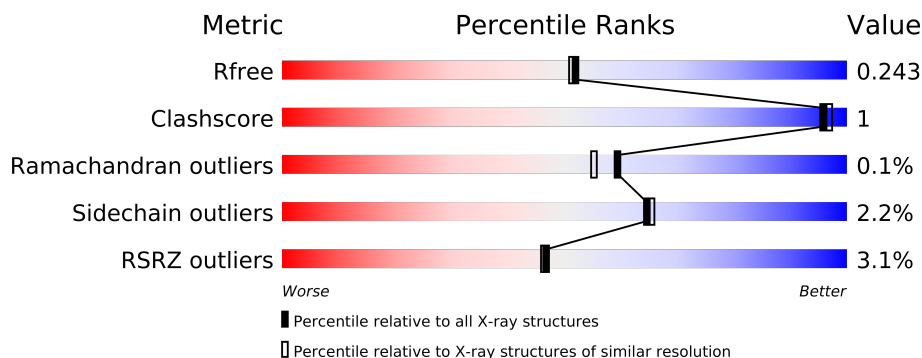
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.99 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))
$R_{free}$	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	629	
1	B	629	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
7	P6G	B	709	-	X
9	PEG	B	710	-	X

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 10796 atoms, of which 0 are hydrogen and 0 are deuterium.

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-convertingenzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	607	Total	C	N	O	S	0	6	0
			4955	3189	850	897	19			
1	B	610	Total	C	N	O	S	0	3	0
			4935	3181	841	894	19			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	GLN	ASN	ENGINEERED MUTATION	UNP P12821
A	25	GLN	ASN	ENGINEERED MUTATION	UNP P12821
A	82	GLN	ASN	ENGINEERED MUTATION	UNP P12821
A	117	GLN	ASN	ENGINEERED MUTATION	UNP P12821
A	131	GLN	ASN	ENGINEERED MUTATION	UNP P12821
A	289	GLN	ASN	ENGINEERED MUTATION	UNP P12821
A	545	ARG	GLN	ENGINEERED MUTATION	UNP P12821
A	576	LEU	PRO	ENGINEERED MUTATION	UNP P12821
A	629	LEU	ARG	ENGINEERED MUTATION	UNP P12821
B	9	GLN	ASN	ENGINEERED MUTATION	UNP P12821
B	25	GLN	ASN	ENGINEERED MUTATION	UNP P12821
B	82	GLN	ASN	ENGINEERED MUTATION	UNP P12821
B	117	GLN	ASN	ENGINEERED MUTATION	UNP P12821
B	131	GLN	ASN	ENGINEERED MUTATION	UNP P12821
B	289	GLN	ASN	ENGINEERED MUTATION	UNP P12821
B	545	ARG	GLN	ENGINEERED MUTATION	UNP P12821
B	576	LEU	PRO	ENGINEERED MUTATION	UNP P12821
B	629	LEU	ARG	ENGINEERED MUTATION	UNP P12821

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

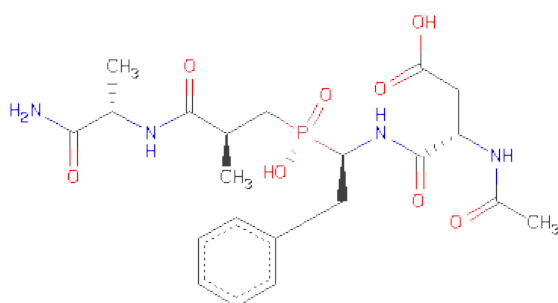
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is N 2 -ACETYL-N-{(1R)-1-[(S)-[(2S)-3-{[(2S)-1-AMINO-1-OXOPROPAN-2-YL]AMINO}-2-METHYL-3-OXOPROPYL](HYDROXY)PHOSPHORYL]-2-PHENYLETHYL}-L-ALPHA-ASPARAGINE (three-letter code: RX4) (formula: C<sub>21</sub>H<sub>31</sub>N<sub>4</sub>O<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			34	21	4	8	1		
3	B	1	Total	C	N	O	P	0	0
			34	21	4	8	1		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			24	14	1	9		
4	B	2	Total	C	N	O	0	0
			24	14	1	9		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	GLN	ASN	ENGINEERED MUTATION	UNP P12821
A	25	GLN	ASN	ENGINEERED MUTATION	UNP P12821

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Chain	Residue	Modelled	Actual	Comment	Reference
A	82	GLN	ASN	ENGINEERED MUTATION	UNP P12821
A	117	GLN	ASN	ENGINEERED MUTATION	UNP P12821
A	131	GLN	ASN	ENGINEERED MUTATION	UNP P12821
A	289	GLN	ASN	ENGINEERED MUTATION	UNP P12821
A	545	ARG	GLN	ENGINEERED MUTATION	UNP P12821
A	576	LEU	PRO	ENGINEERED MUTATION	UNP P12821
A	629	LEU	ARG	ENGINEERED MUTATION	UNP P12821
B	9	GLN	ASN	ENGINEERED MUTATION	UNP P12821
B	25	GLN	ASN	ENGINEERED MUTATION	UNP P12821
B	82	GLN	ASN	ENGINEERED MUTATION	UNP P12821
B	117	GLN	ASN	ENGINEERED MUTATION	UNP P12821
B	131	GLN	ASN	ENGINEERED MUTATION	UNP P12821
B	289	GLN	ASN	ENGINEERED MUTATION	UNP P12821
B	545	ARG	GLN	ENGINEERED MUTATION	UNP P12821
B	576	LEU	PRO	ENGINEERED MUTATION	UNP P12821
B	629	LEU	ARG	ENGINEERED MUTATION	UNP P12821

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

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

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	GLN	ASN	ENGINEERED MUTATION	UNP P12821
A	25	GLN	ASN	ENGINEERED MUTATION	UNP P12821
A	82	GLN	ASN	ENGINEERED MUTATION	UNP P12821
A	117	GLN	ASN	ENGINEERED MUTATION	UNP P12821
A	131	GLN	ASN	ENGINEERED MUTATION	UNP P12821
A	289	GLN	ASN	ENGINEERED MUTATION	UNP P12821
A	545	ARG	GLN	ENGINEERED MUTATION	UNP P12821
A	576	LEU	PRO	ENGINEERED MUTATION	UNP P12821
A	629	LEU	ARG	ENGINEERED MUTATION	UNP P12821
B	9	GLN	ASN	ENGINEERED MUTATION	UNP P12821
B	25	GLN	ASN	ENGINEERED MUTATION	UNP P12821
B	82	GLN	ASN	ENGINEERED MUTATION	UNP P12821
B	117	GLN	ASN	ENGINEERED MUTATION	UNP P12821
B	131	GLN	ASN	ENGINEERED MUTATION	UNP P12821

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Chain	Residue	Modelled	Actual	Comment	Reference
B	289	GLN	ASN	ENGINEERED MUTATION	UNP P12821
B	545	ARG	GLN	ENGINEERED MUTATION	UNP P12821
B	576	LEU	PRO	ENGINEERED MUTATION	UNP P12821
B	629	LEU	ARG	ENGINEERED MUTATION	UNP P12821

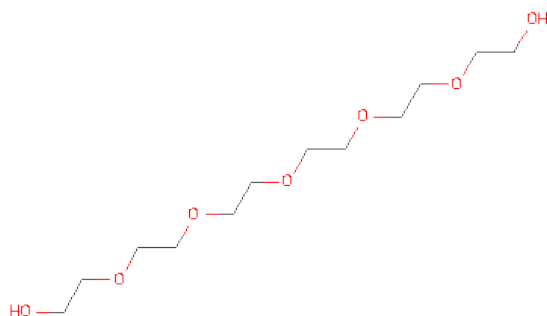
- Molecule 6 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	4	Total	C	N	O	0	0
			49	28	2	19		
6	B	4	Total	C	N	O	0	0
			49	28	2	19		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	GLN	ASN	ENGINEERED MUTATION	UNP P12821
A	25	GLN	ASN	ENGINEERED MUTATION	UNP P12821
A	82	GLN	ASN	ENGINEERED MUTATION	UNP P12821
A	117	GLN	ASN	ENGINEERED MUTATION	UNP P12821
A	131	GLN	ASN	ENGINEERED MUTATION	UNP P12821
A	289	GLN	ASN	ENGINEERED MUTATION	UNP P12821
A	545	ARG	GLN	ENGINEERED MUTATION	UNP P12821
A	576	LEU	PRO	ENGINEERED MUTATION	UNP P12821
A	629	LEU	ARG	ENGINEERED MUTATION	UNP P12821
B	9	GLN	ASN	ENGINEERED MUTATION	UNP P12821
B	25	GLN	ASN	ENGINEERED MUTATION	UNP P12821
B	82	GLN	ASN	ENGINEERED MUTATION	UNP P12821
B	117	GLN	ASN	ENGINEERED MUTATION	UNP P12821
B	131	GLN	ASN	ENGINEERED MUTATION	UNP P12821
B	289	GLN	ASN	ENGINEERED MUTATION	UNP P12821
B	545	ARG	GLN	ENGINEERED MUTATION	UNP P12821
B	576	LEU	PRO	ENGINEERED MUTATION	UNP P12821
B	629	LEU	ARG	ENGINEERED MUTATION	UNP P12821

- Molecule 7 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C<sub>12</sub>H<sub>26</sub>O<sub>7</sub>).

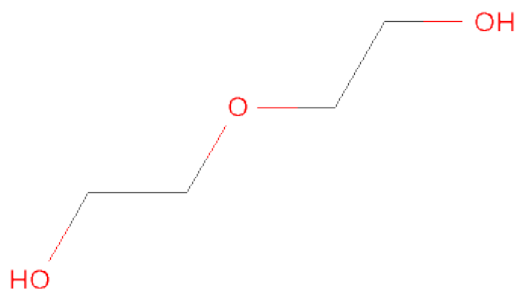


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			13	8	5		
7	B	1	Total	C	O	0	0
			19	12	7		

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

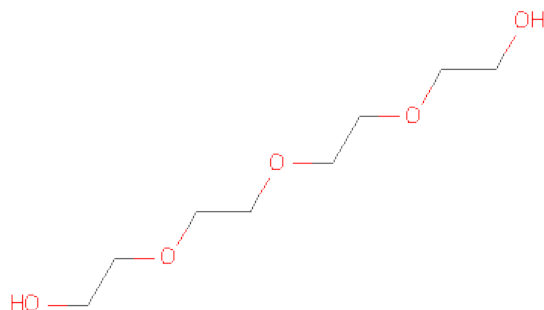
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Cl	0	0
			1	1		
8	A	1	Total	Cl	0	0
			1	1		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			7	4	3		
9	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 10 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			10	6	4		
10	B	1	Total	C	O	0	0
			13	8	5		



- Molecule 11 is water.

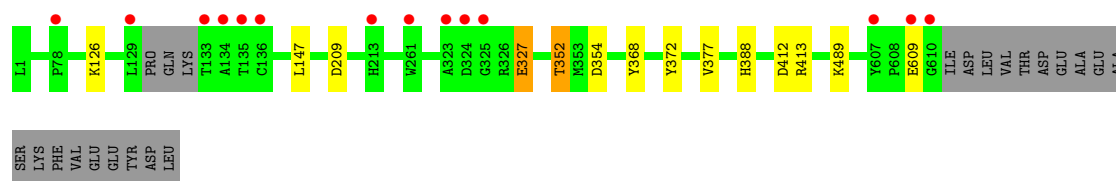
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	303	Total 303	O 303	0	0
11	B	260	Total 260	O 260	0	0

### 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.

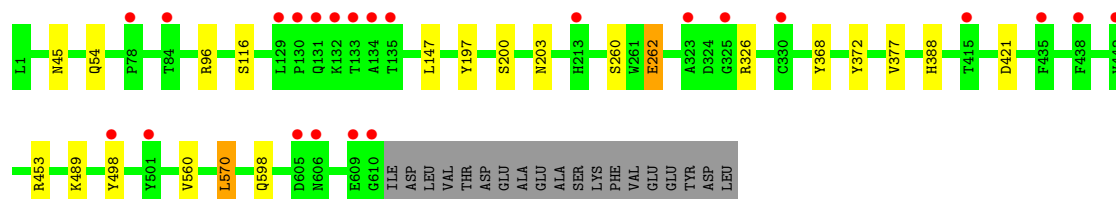
- Molecule 1: Angiotensin-convertingenzyme

Chain A: 



- Molecule 1: Angiotensin-convertingenzyme

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.88Å 76.69Å 82.65Å 88.63° 64.17° 75.70°	Depositor
Resolution (Å)	40.81 – 1.99 40.81 – 1.99	Depositor EDS
% Data completeness (in resolution range)	95.6 (40.81-1.99) 95.6 (40.81-1.99)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.42 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.194 , 0.237 0.202 , 0.243	Depositor DCC
$R_{free}$ test set	1025 reflections (1.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.3	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 30.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 101705 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10796	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.29% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, BMA, NAG, CL, PG4, FUC, P6G, PEG, RX4

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	0.39	0/5129	0.51	0/6989
1	B	0.39	0/5101	0.51	1/6959 (0.0%)
All	All	0.39	0/10230	0.51	1/13948 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	570	LEU	CB-CG-CD1	5.66	120.62	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4955	0	0	4	0
1	B	4935	0	0	7	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	34	0	29	2	0
3	B	34	0	29	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	24	0	22	0	0
4	B	24	0	22	1	0
5	A	28	0	25	0	0
5	B	28	0	25	0	0
6	A	49	0	43	0	0
6	B	49	0	43	0	0
7	A	13	0	17	0	0
7	B	19	0	26	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	A	7	0	10	0	0
9	B	7	0	10	0	0
10	B	23	0	31	1	0
11	A	303	0	0	0	0
11	B	260	0	0	3	0
All	All	10796	0	332	13	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 1.

All (13) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:54:GLN:NE2	11:B:829:HOH:O	2.24	0.69
1:B:489:LYS:NZ	3:B:700:RX4:HAD2	2.00	0.59
1:B:260:SER:OG	1:B:262:GLU:OE1	2.22	0.58
1:A:412:ASP:O	1:A:413:ARG:C	2.46	0.54
1:A:352:THR:CG2	1:A:354:ASP:OD2	2.60	0.50
1:A:126:LYS:NZ	1:A:327:GLU:OE2	2.45	0.50
1:A:489:LYS:NZ	3:A:700:RX4:HAD2	2.10	0.49
4:B:631:FUC:H5	11:B:706:HOH:O	2.19	0.43
1:B:197:TYR:O	1:B:200:SER:OG	2.36	0.42
1:B:498:TYR:OH	3:B:700:RX4:NAD	2.52	0.42
1:B:598:GLN:NE2	11:B:779:HOH:O	2.52	0.42
1:B:453:ARG:NH2	10:B:704:PG4:O5	2.54	0.41
3:A:700:RX4:HBF	3:A:700:RX4:HAA1	1.75	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	609/629 (97%)	598 (98%)	11 (2%)	0	100	100
1	B	611/629 (97%)	596 (98%)	14 (2%)	1 (0%)	56	51
All	All	1220/1258 (97%)	1194 (98%)	25 (2%)	1 (0%)	59	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	45	ASN

### 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	515/541 (95%)	506 (98%)	9 (2%)	73	75
1	B	508/541 (94%)	495 (97%)	13 (3%)	59	58
All	All	1023/1082 (94%)	1001 (98%)	22 (2%)	64	65

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	147	LEU
1	A	209	ASP
1	A	327	GLU
1	A	352	THR
1	A	368	TYR
1	A	372	TYR
1	A	377	VAL
1	A	388	HIS

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Mol	Chain	Res	Type
1	A	609	GLU
1	B	96	ARG
1	B	116	SER
1	B	147	LEU
1	B	203	ASN
1	B	262	GLU
1	B	326	ARG
1	B	368	TYR
1	B	372	TYR
1	B	377	VAL
1	B	388	HIS
1	B	421	ASP
1	B	560	VAL
1	B	570	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

16 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	$\# Z  > 2$
4	NAG	A	630	1,4	12,14,15	0.57	0	15,19,21	1.67	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	FUC	A	631	4	9,10,11	0.77	0	10,14,16	0.87	0
5	NAG	A	632	1,5	12,14,15	0.65	0	15,19,21	0.68	0
5	NAG	A	633	5	12,14,15	0.57	0	15,19,21	0.92	1 (6%)
6	NAG	A	634	1,6	12,14,15	0.71	1 (8%)	15,19,21	0.89	0
6	NAG	A	635	6	12,14,15	0.67	0	15,19,21	0.94	1 (6%)
6	BMA	A	636	6	10,11,12	0.44	0	11,15,17	0.93	0
6	FUC	A	637	6	9,10,11	0.75	0	10,14,16	0.44	0
4	NAG	B	630	1,4	12,14,15	0.52	0	15,19,21	1.42	2 (13%)
4	FUC	B	631	4	9,10,11	0.72	0	10,14,16	0.81	0
5	NAG	B	632	1,5	12,14,15	0.77	1 (8%)	15,19,21	0.71	0
5	NAG	B	633	5	12,14,15	0.56	0	15,19,21	0.74	0
6	NAG	B	634	1,6	12,14,15	0.67	0	15,19,21	0.67	0
6	NAG	B	635	6	12,14,15	0.64	0	15,19,21	0.87	1 (6%)
6	BMA	B	636	6	10,11,12	0.48	0	11,15,17	1.01	1 (9%)
6	FUC	B	637	6	9,10,11	0.51	0	10,14,16	0.53	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
4	NAG	A	630	1,4	-	0/6/23/26	0/1/1/1
4	FUC	A	631	4	-	0/0/17/20	0/1/1/1
5	NAG	A	632	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	633	5	-	0/6/23/26	0/1/1/1
6	NAG	A	634	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	635	6	-	0/6/23/26	0/1/1/1
6	BMA	A	636	6	-	0/2/19/22	0/1/1/1
6	FUC	A	637	6	-	0/0/17/20	0/1/1/1
4	NAG	B	630	1,4	-	0/6/23/26	0/1/1/1
4	FUC	B	631	4	-	0/0/17/20	0/1/1/1
5	NAG	B	632	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	633	5	-	0/6/23/26	0/1/1/1
6	NAG	B	634	1,6	-	0/6/23/26	0/1/1/1
6	NAG	B	635	6	-	0/6/23/26	0/1/1/1
6	BMA	B	636	6	-	0/2/19/22	0/1/1/1
6	FUC	B	637	6	-	0/0/17/20	0/1/1/1

All (2) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	632	NAG	O5-C5	-2.29	1.41	1.45
6	A	634	NAG	O5-C5	-2.11	1.41	1.45

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	630	NAG	O5-C5-C6	5.55	112.81	106.98
4	B	630	NAG	O5-C5-C6	3.47	110.63	106.98
6	B	635	NAG	O5-C5-C6	2.42	109.52	106.98
5	A	633	NAG	O5-C5-C6	2.39	109.49	106.98
4	B	630	NAG	C3-C2-N2	-2.30	108.25	111.76
6	A	635	NAG	O5-C5-C6	2.30	109.39	106.98
6	B	636	BMA	C4-C3-C2	2.09	113.31	110.50
4	A	630	NAG	C3-C2-N2	-2.01	108.69	111.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	$\# Z  > 2$
3	RX4	A	700	2	34,34,34	0.83	1 (2%)	47,47,47	1.27	2 (4%)
9	PEG	A	706	-	6,6,6	0.41	0	5,5,5	0.35	0
7	P6G	A	708	-	12,12,18	0.59	0	11,11,17	0.57	0
3	RX4	B	700	2	34,34,34	0.89	3 (8%)	47,47,47	1.46	4 (8%)
10	PG4	B	704	-	9,9,12	0.62	0	8,8,11	0.65	0
10	PG4	B	705	-	12,12,12	0.45	0	11,11,11	0.31	0
7	P6G	B	709	-	18,18,18	0.51	0	17,17,17	0.28	0
9	PEG	B	710	-	6,6,6	0.41	0	5,5,5	0.35	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
3	RX4	A	700	2	-	1/43/43/43	0/1/1/1
9	PEG	A	706	-	-	0/4/4/4	0/0/0/0
7	P6G	A	708	-	-	0/10/10/16	0/0/0/0
3	RX4	B	700	2	-	1/43/43/43	0/1/1/1
10	PG4	B	704	-	-	0/7/7/10	0/0/0/0
10	PG4	B	705	-	-	0/10/10/10	0/0/0/0
7	P6G	B	709	-	-	0/16/16/16	0/0/0/0
9	PEG	B	710	-	-	0/4/4/4	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	700	RX4	P1-O4	-2.72	1.50	1.55
3	B	700	RX4	P1-CBG	-2.44	1.81	1.83
3	B	700	RX4	P1-O4	-2.30	1.51	1.55
3	B	700	RX4	P1-CAT	2.28	1.81	1.79

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	700	RX4	CAS-CBG-NAW	-7.67	105.00	112.02
3	A	700	RX4	CAS-CBG-NAW	-6.18	106.36	112.02
3	B	700	RX4	O3-P1-CBG	-2.87	107.66	112.22
3	B	700	RX4	CBC-CAS-CBG	-2.71	108.86	113.47
3	A	700	RX4	CAR-CBF-NAU	-2.68	105.10	110.61
3	B	700	RX4	CAR-CBF-NAU	-2.35	105.78	110.61

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	700	RX4	CAT-P1-CBG-NAW
3	A	700	RX4	CAT-P1-CBG-NAW

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	607/629 (96%)	0.11	14 (2%) 57 57	19, 31, 43, 66	0
1	B	610/629 (96%)	0.22	23 (3%) 38 38	21, 33, 51, 66	0
All	All	1217/1258 (96%)	0.16	37 (3%) 47 47	19, 31, 48, 66	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	130	PRO	8.1
1	A	610	GLY	5.9
1	B	135	THR	5.9
1	A	323	ALA	5.1
1	A	135	THR	4.5
1	A	134	ALA	4.5
1	B	134	ALA	4.4
1	B	325	GLY	4.4
1	B	609	GLU	4.4
1	B	131	GLN	4.2
1	B	129	LEU	4.2
1	A	325	GLY	4.2
1	B	323	ALA	3.5
1	B	133	THR	3.3
1	A	133	THR	3.3
1	B	78	PRO	3.2
1	B	415	THR	3.2
1	B	84	THR	3.2
1	B	605	ASP	3.1
1	B	438	PHE	3.1
1	A	324	ASP	3.0
1	A	136	CYS	3.0
1	A	213[A]	HIS	2.8
1	B	610	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	132	LYS	2.7
1	A	607	TYR	2.5
1	A	129	LEU	2.4
1	B	606	ASN	2.4
1	B	213	HIS	2.3
1	A	78	PRO	2.3
1	B	442	VAL	2.2
1	A	261	TRP	2.1
1	B	498	TYR	2.1
1	B	330	CYS	2.1
1	A	609	GLU	2.1
1	B	435	PHE	2.1
1	B	501	TYR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	FUC	B	631	10/11	0.40	16.39	58,60,60,60	0
5	NAG	A	633	14/15	0.27	13.14	51,53,56,56	0
6	FUC	B	637	10/11	0.31	6.36	63,63,64,64	0
6	NAG	B	635	14/15	0.29	4.01	62,64,65,65	0
4	FUC	A	631	10/11	0.35	3.78	56,58,59,59	0
6	FUC	A	637	10/11	0.18	2.31	53,55,55,56	0
6	NAG	B	634	14/15	0.19	1.71	52,56,59,62	0
4	NAG	B	630	14/15	0.14	1.30	40,46,49,54	0
5	NAG	B	632	14/15	0.23	1.26	38,44,47,51	0
6	NAG	A	634	14/15	0.14	1.00	43,47,51,51	0
6	NAG	A	635	14/15	0.19	0.39	54,56,57,60	0
4	NAG	A	630	14/15	0.13	0.32	38,45,48,52	0
5	NAG	A	632	14/15	0.15	0.06	39,43,45,48	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	BMA	A	636	11/12	0.26	-	61,62,63,63	0
6	BMA	B	636	11/12	0.35	-	66,67,67,67	0
5	NAG	B	633	14/15	0.44	-	55,58,59,60	0

## 6.4 Ligands

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
9	PEG	B	710	7/7	0.28	4.03	66,67,67,67	0
7	P6G	B	709	19/19	0.20	2.69	60,60,61,61	0
7	P6G	A	708	13/19	0.18	1.78	46,47,49,49	0
10	PG4	B	705	13/13	0.11	1.24	52,53,54,55	0
10	PG4	B	704	10/13	0.14	0.84	52,52,52,53	0
3	RX4	A	700	34/34	0.15	0.64	20,26,35,39	0
9	PEG	A	706	7/7	0.13	0.52	51,52,52,52	0
3	RX4	B	700	34/34	0.17	0.43	19,23,37,38	0
2	ZN	A	650	1/1	0.11	-1.00	23,23,23,23	0
2	ZN	B	650	1/1	0.11	-1.18	21,21,21,21	0
8	CL	A	900	1/1	0.09	-1.22	23,23,23,23	0
8	CL	B	900	1/1	0.09	-1.65	28,28,28,28	0

## 6.5 Other polymers

There are no such residues in this entry.