



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:49 AM GMT

PDB ID : 3Q3T  
Title : Alkyl Amine Renin Inhibitors: Filling S1 from S3  
Authors : Wu, Z.; McKeever, B.  
Deposited on : 2010-12-22  
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure 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/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

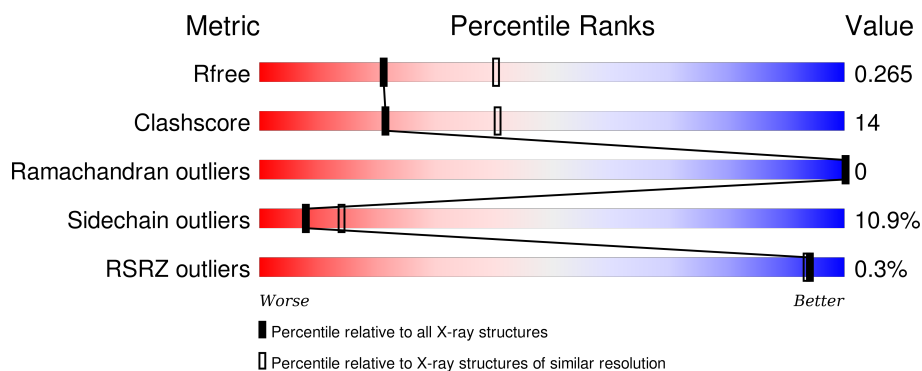
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	340	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>%</span> <div style="width: 66%; height: 10px; background-color: green;"></div> <div style="width: 30%; height: 10px; background-color: yellow;"></div> <div style="width: 4%; height: 10px; background-color: orange;"></div> <div style="width: 4%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>66%</span> <span>30%</span> <span>..</span> </div> </div>
1	B	340	<div> <div style="width: 65%; height: 10px; background-color: green;"></div> <div style="width: 28%; height: 10px; background-color: yellow;"></div> <div style="width: 4%; height: 10px; background-color: orange;"></div> <div style="width: 4%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>65%</span> <span>28%</span> <span>..</span> </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
4	GOL	A	502	-	-	-	X
5	NAG	B	600	-	-	-	X

## 2 Entry composition [i](#)

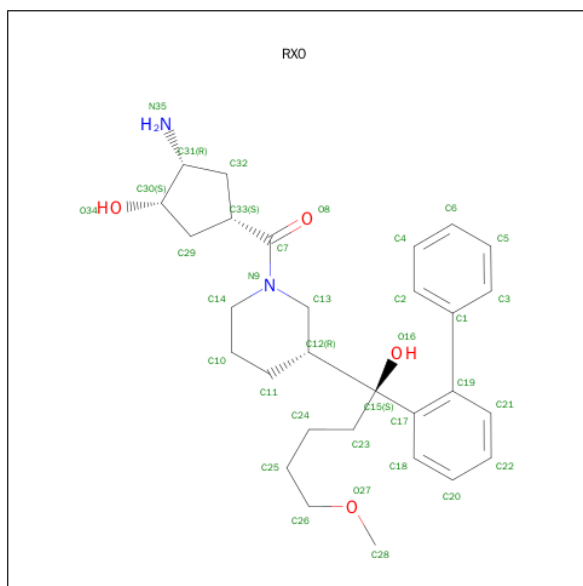
There are 6 unique types of molecules in this entry. The entry contains 5428 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Renin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	0	0
			2598	1656	421	507	14			
1	B	333	Total	C	N	O	S	0	0	0
			2566	1639	415	498	14			

- Molecule 2 is [(1S,3R,4S)-3-AMINO-4-HYDROXYCYCLOPENTYL]{(3R)-3-[(1S)-1-(BIPHENYL-2-YL)-1-HYDROXY-5-METHOXY-PENTYL]PIPERIDIN-1-YL}METHANONE (three-letter code: RX0) (formula: C<sub>29</sub>H<sub>40</sub>N<sub>2</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			35	29	2	4		
2	B	1	Total	C	N	O	0	0
			35	29	2	4		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

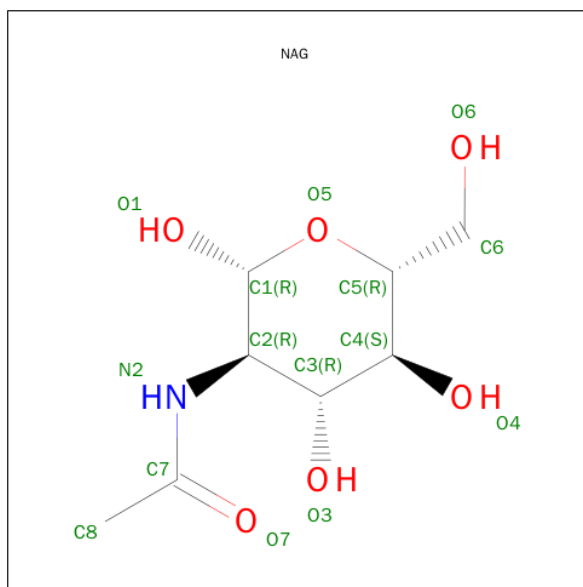
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

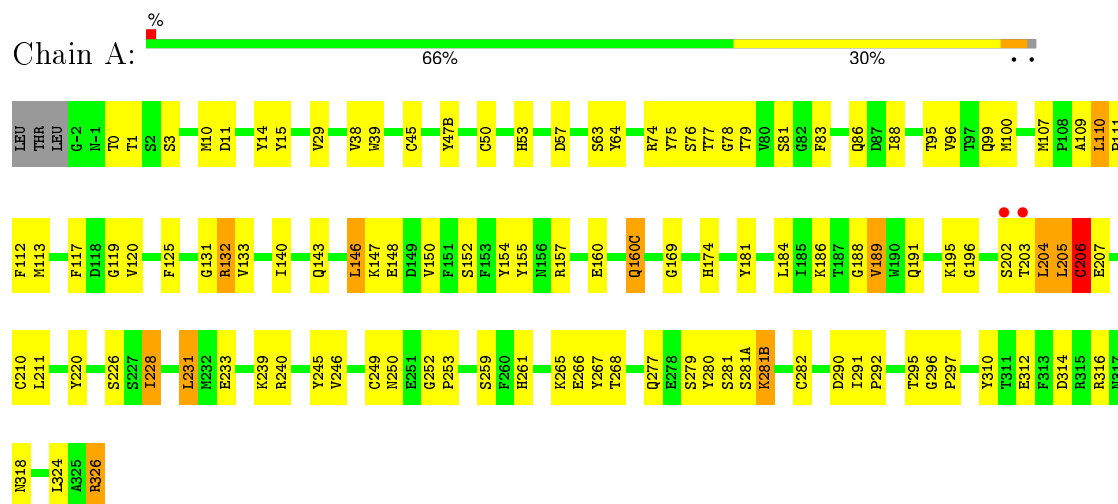
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	65	Total	O	0	0
			65	65		
6	B	75	Total	O	0	0
			75	75		

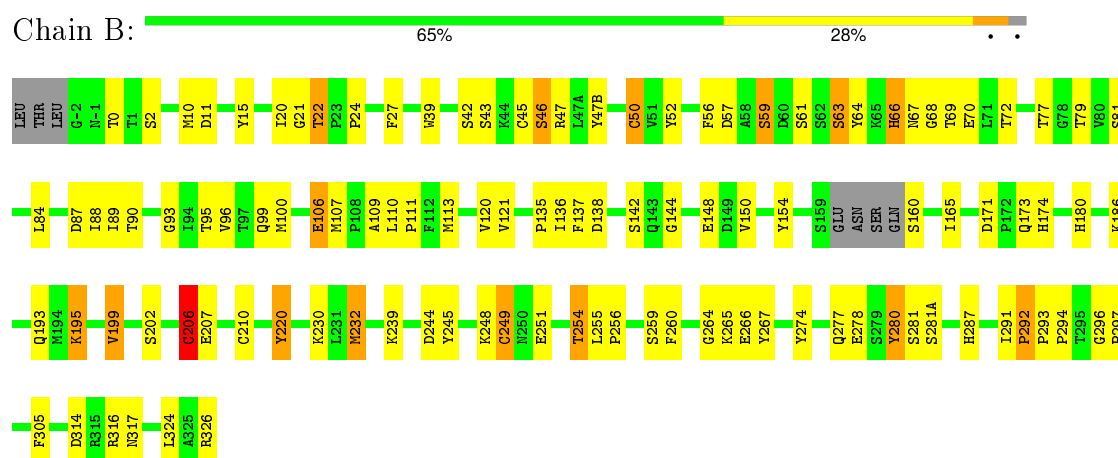
### 3 Residue-property plots

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: Renin



#### • Molecule 1: Renin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.25Å 97.58Å 148.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.36 – 2.60 46.36 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.9 (46.36-2.60) 99.0 (46.36-2.60)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.05 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.200 , 0.268 0.209 , 0.265	Depositor DCC
$R_{free}$ test set	1263 reflections (5.38%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.7	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 39.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 24724 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5428	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAG, RX0

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	1.96	23/2658 (0.9%)	0.90	1/3604 (0.0%)
1	B	1.89	21/2625 (0.8%)	0.93	0/3558
All	All	1.93	44/5283 (0.8%)	0.92	1/7162 (0.0%)

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	50	CYS	CB-SG	-12.28	1.61	1.82
1	A	206	CYS	CB-SG	-10.59	1.64	1.82
1	B	50	CYS	CB-SG	-10.05	1.65	1.82
1	B	199	VAL	CB-CG1	-8.11	1.35	1.52
1	A	45	CYS	CB-SG	-8.03	1.68	1.82
1	B	210	CYS	CB-SG	-7.99	1.68	1.82
1	B	206	CYS	CB-SG	-7.87	1.68	1.82
1	A	210	CYS	CB-SG	-7.32	1.69	1.82
1	B	220	TYR	CD1-CE1	-6.99	1.28	1.39
1	B	220	TYR	CD2-CE2	-6.90	1.29	1.39
1	B	15	TYR	CD1-CE1	-6.67	1.29	1.39
1	B	249	CYS	CB-SG	-6.27	1.71	1.82
1	B	154	TYR	CD1-CE1	-6.18	1.30	1.39
1	B	280	TYR	CE1-CZ	-6.17	1.30	1.38
1	B	280	TYR	CD2-CE2	-6.10	1.30	1.39
1	A	14	TYR	CD2-CE2	-6.04	1.30	1.39
1	A	233	GLU	CG-CD	-6.03	1.43	1.51
1	A	312	GLU	CD-OE1	-5.81	1.19	1.25
1	A	47(B)	TYR	CD1-CE1	-5.75	1.30	1.39
1	A	154	TYR	CD1-CE1	-5.73	1.30	1.39
1	B	45	CYS	CB-SG	-5.71	1.72	1.81
1	B	154	TYR	CD2-CE2	-5.68	1.30	1.39
1	B	280	TYR	CD1-CE1	-5.61	1.30	1.39
1	A	38	VAL	CB-CG2	-5.59	1.41	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	15	TYR	CD2-CE2	-5.59	1.30	1.39
1	A	220	TYR	CD2-CE2	-5.58	1.30	1.39
1	B	274	TYR	CD1-CE1	-5.56	1.31	1.39
1	B	274	TYR	CD2-CE2	-5.56	1.31	1.39
1	A	15	TYR	CD2-CE2	-5.50	1.31	1.39
1	A	83	PHE	CD1-CE1	-5.50	1.28	1.39
1	A	155	TYR	CD2-CE2	-5.49	1.31	1.39
1	B	267	TYR	CD1-CE1	-5.48	1.31	1.39
1	B	199	VAL	CB-CG2	-5.46	1.41	1.52
1	A	117	PHE	CD2-CE2	-5.46	1.28	1.39
1	A	155	TYR	CD1-CE1	-5.43	1.31	1.39
1	A	133	VAL	CB-CG2	-5.41	1.41	1.52
1	A	181	TYR	CD1-CE1	-5.40	1.31	1.39
1	A	14	TYR	CD1-CE1	-5.29	1.31	1.39
1	B	305	PHE	CD1-CE1	-5.24	1.28	1.39
1	A	181	TYR	CE2-CZ	-5.24	1.31	1.38
1	A	47(B)	TYR	CE1-CZ	-5.21	1.31	1.38
1	A	64	TYR	CD1-CE1	-5.14	1.31	1.39
1	A	267	TYR	CD1-CE1	-5.03	1.31	1.39
1	B	260	PHE	CG-CD1	-5.00	1.31	1.38

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	ASP	CB-CG-OD1	5.54	123.28	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2598	0	2525	74	0
1	B	2566	0	2499	69	0
2	A	35	0	40	2	0
2	B	35	0	40	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	28	0	25	0	0
4	A	12	0	16	0	0
5	B	14	0	13	3	0
6	A	65	0	0	3	0
6	B	75	0	0	3	0
All	All	5428	0	5158	147	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 (147) 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:22:THR:OG1	1:B:63:SER:OG	1.65	1.12
1:A:77:THR:HG23	1:A:78:GLY:N	1.51	1.12
1:A:1:THR:HG22	1:A:1:THR:O	1.53	1.06
1:A:77:THR:CG2	1:A:78:GLY:N	2.19	1.05
1:A:160(C):GLN:HA	1:A:160(C):GLN:NE2	1.68	1.05
1:A:77:THR:CG2	1:A:78:GLY:H	1.71	1.00
1:A:259:SER:OG	1:A:268:THR:OG1	1.84	0.95
1:A:202:SER:OG	1:A:204:LEU:HD21	1.69	0.92
1:B:206:CYS:SG	1:B:206:CYS:O	2.36	0.84
1:B:27:PHE:CZ	1:B:56:PHE:HB2	2.13	0.82
1:B:266:GLU:OE1	6:B:364:HOH:O	2.00	0.80
1:A:160(C):GLN:CA	1:A:160(C):GLN:NE2	2.43	0.79
1:A:202:SER:OG	1:A:204:LEU:CD2	2.32	0.78
1:B:100:MET:HE1	5:B:600:NAG:O5	1.82	0.78
1:A:160(C):GLN:HA	1:A:160(C):GLN:HE21	1.50	0.76
1:A:77:THR:HG23	1:A:78:GLY:H	1.24	0.76
1:B:27:PHE:HZ	1:B:56:PHE:HB2	1.50	0.75
1:B:180:HIS:CD2	1:B:265:LYS:HE3	2.22	0.75
1:A:206:CYS:O	1:A:206:CYS:SG	2.44	0.74
1:B:180:HIS:NE2	1:B:265:LYS:HE3	2.02	0.74
1:A:95:THR:O	1:A:143:GLN:NE2	2.21	0.74
1:B:20:ILE:HG12	1:B:89:ILE:HG12	1.71	0.72
1:B:39:TRP:NE1	1:B:120:VAL:HG13	2.06	0.71
1:B:248:LYS:HB2	1:B:251:GLU:HG3	1.72	0.71
1:A:174:HIS:HA	1:A:326:ARG:OXT	1.90	0.71
1:A:160(C):GLN:HE21	1:A:160(C):GLN:CA	2.03	0.70
1:B:232:MET:HG3	1:B:245:TYR:CD1	2.25	0.70
1:A:53:HIS:HE1	1:A:112:PHE:O	1.75	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:CYS:O	1:A:277:GLN:NE2	2.25	0.69
1:B:232:MET:HG3	1:B:245:TYR:CE1	2.28	0.69
1:B:67:ASN:OD1	1:B:67:ASN:C	2.32	0.67
1:B:70:GLU:O	6:B:378:HOH:O	2.12	0.67
1:A:77:THR:HG22	1:A:78:GLY:H	1.60	0.65
2:B:500:RX0:C2	2:B:500:RX0:H23	2.27	0.65
1:B:69:THR:HB	1:B:84:LEU:HD12	1.78	0.64
1:B:66:HIS:ND1	1:B:66:HIS:C	2.51	0.64
1:A:203:THR:O	1:A:203:THR:HG22	1.97	0.64
2:B:500:RX0:H23	2:B:500:RX0:H2	1.80	0.63
1:B:87:ASP:OD1	1:B:88:ILE:N	2.26	0.61
1:B:277:GLN:HG2	1:B:280:TYR:CE1	2.34	0.61
1:B:174:HIS:HA	1:B:326:ARG:OXT	2.01	0.59
1:A:125:PHE:CB	1:A:188:GLY:HA2	2.33	0.59
1:A:202:SER:O	1:A:204:LEU:HD23	2.04	0.58
1:B:88:ILE:CG2	1:B:95:THR:HG22	2.33	0.58
1:A:202:SER:HG	1:A:204:LEU:HD21	1.68	0.58
1:B:2:SER:HB2	1:B:93:GLY:H	1.70	0.57
1:A:140:ILE:O	1:A:143:GLN:HB2	2.06	0.56
1:A:250:ASN:OD1	1:A:281(A):SER:HA	2.05	0.56
1:A:125:PHE:CG	1:A:188:GLY:HA2	2.40	0.56
1:A:291:ILE:O	1:A:296:GLY:HA3	2.06	0.56
1:A:110:LEU:HG	1:A:110:LEU:O	2.06	0.56
1:B:88:ILE:CG2	1:B:95:THR:CG2	2.85	0.55
1:B:64:TYR:OH	1:B:66:HIS:HB2	2.06	0.55
1:A:277:GLN:HG2	1:A:280:TYR:CE1	2.42	0.55
1:B:66:HIS:ND1	1:B:67:ASN:N	2.55	0.55
1:A:246:VAL:HA	1:A:282:CYS:O	2.07	0.55
1:A:205:LEU:HD11	1:A:231:LEU:HB2	1.89	0.55
1:A:268:THR:HB	6:A:365:HOH:O	2.07	0.54
1:B:67:ASN:OD1	1:B:69:THR:N	2.36	0.54
1:A:10:MET:O	1:A:11:ASP:HB2	2.08	0.54
1:B:46:SER:OG	1:B:47:ARG:N	2.38	0.53
1:B:195:LYS:NZ	1:B:264:GLY:H	2.06	0.53
1:A:204:LEU:N	1:A:204:LEU:HD23	2.23	0.53
1:B:57:ASP:OD1	1:B:59:SER:N	2.40	0.53
1:A:207:GLU:N	1:A:207:GLU:OE1	2.30	0.52
1:B:67:ASN:OD1	1:B:68:GLY:N	2.42	0.52
1:A:150:VAL:HG12	1:A:314:ASP:HA	1.91	0.52
1:B:255:LEU:HB3	1:B:256:PRO:HD2	1.91	0.52
1:B:150:VAL:HG12	1:B:314:ASP:HA	1.91	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:LYS:HG3	1:A:245:TYR:CE1	2.44	0.52
1:B:106:GLU:O	1:B:106:GLU:CG	2.58	0.52
1:A:246:VAL:HG12	1:A:282:CYS:O	2.10	0.51
1:A:316:ARG:NH1	6:A:391:HOH:O	2.43	0.51
1:B:220:TYR:HB2	1:B:287:HIS:HD2	1.75	0.51
1:A:189:VAL:HG22	1:A:191:GLN:HB2	1.93	0.51
1:A:109:ALA:O	1:A:113:MET:HB2	2.12	0.50
1:A:160(C):GLN:HE21	1:A:160(C):GLN:N	2.09	0.50
1:B:67:ASN:CG	5:B:600:NAG:O7	2.51	0.49
1:A:88:ILE:CG2	1:A:95:THR:CG2	2.91	0.49
1:A:88:ILE:CG2	1:A:95:THR:HG23	2.43	0.49
1:A:184:LEU:HG	1:A:318:ASN:O	2.13	0.49
1:B:296:GLY:HA2	1:B:297:PRO:C	2.32	0.49
1:A:152:SER:OG	1:A:169:GLY:O	2.22	0.49
1:B:249:CYS:HB2	1:B:281:SER:O	2.13	0.49
1:B:66:HIS:CE1	1:B:67:ASN:O	2.67	0.48
1:A:53:HIS:CE1	1:A:112:PHE:O	2.61	0.48
1:B:21:GLY:O	1:B:24:PRO:HA	2.14	0.48
1:A:110:LEU:HA	1:A:111:PRO:HA	1.59	0.47
1:B:135:PRO:HD2	1:B:138:ASP:OD2	2.13	0.47
1:A:0:THR:O	1:A:146:LEU:HA	2.13	0.47
1:A:228:ILE:HA	1:A:228:ILE:HD12	1.67	0.47
1:A:148:GLU:HA	1:A:148:GLU:OE1	2.14	0.47
2:A:500:RX0:H13	2:A:500:RX0:H33	1.62	0.47
1:B:99:GLN:OE1	1:B:136:ILE:HA	2.15	0.47
1:A:281:SER:C	1:A:281(B):LYS:H	2.17	0.47
1:A:99:GLN:HG3	1:A:100:MET:N	2.28	0.47
1:A:196:GLY:O	1:A:261:HIS:HD2	1.98	0.46
1:A:152:SER:HB2	1:A:310:TYR:CE1	2.51	0.46
1:B:259:SER:HB3	1:B:266:GLU:HG3	1.98	0.46
1:A:261:HIS:CE1	1:A:266:GLU:HG2	2.51	0.46
1:B:39:TRP:HE1	1:B:120:VAL:HG13	1.81	0.46
1:A:29:VAL:HA	1:A:119:GLY:O	2.16	0.45
2:A:500:RX0:H12	2:A:500:RX0:C1	2.46	0.45
1:B:110:LEU:HA	1:B:111:PRO:HA	1.69	0.45
1:B:22:THR:O	1:B:61:SER:HA	2.17	0.45
1:B:171:ASP:OD1	1:B:173:GLN:HB2	2.17	0.45
1:A:252:GLY:N	1:A:253:PRO:CD	2.79	0.45
1:A:77:THR:HG21	1:A:111:PRO:HG3	1.99	0.45
1:B:57:ASP:OD1	1:B:59:SER:HB2	2.17	0.44
1:A:131:GLY:C	1:A:132:ARG:HG3	2.37	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:ARG:OXT	1:B:326:ARG:CG	2.65	0.44
1:B:316:ARG:HH11	1:B:317:ASN:HD21	1.65	0.44
1:B:136:ILE:HG23	1:B:137:PHE:N	2.33	0.44
1:A:261:HIS:CE1	1:A:266:GLU:CG	3.01	0.43
1:A:296:GLY:HA2	1:A:297:PRO:C	2.38	0.43
1:B:293:PRO:HA	1:B:294:PRO:C	2.39	0.43
1:A:204:LEU:N	1:A:204:LEU:CD2	2.82	0.43
1:A:204:LEU:HD23	1:A:204:LEU:H	1.83	0.43
1:B:100:MET:HE1	5:B:600:NAG:C5	2.48	0.43
1:B:195:LYS:HE3	1:B:195:LYS:HB2	1.77	0.43
1:A:39:TRP:NE1	1:A:120:VAL:HG13	2.34	0.43
1:A:239:LYS:HG3	1:A:245:TYR:CZ	2.53	0.43
1:B:220:TYR:HB2	1:B:287:HIS:CD2	2.54	0.42
1:B:199:VAL:O	1:B:199:VAL:HG12	2.18	0.42
1:B:72:THR:HG23	1:B:79:THR:HG23	2.01	0.42
1:B:121:VAL:HG12	1:B:121:VAL:O	2.19	0.42
1:A:196:GLY:C	1:A:261:HIS:HD2	2.23	0.42
1:B:254:THR:HG23	1:B:254:THR:H	1.59	0.42
1:A:75:TYR:C	1:A:77:THR:N	2.71	0.42
1:A:246:VAL:HG12	1:A:282:CYS:C	2.39	0.42
1:A:96:VAL:HG13	1:A:96:VAL:O	2.20	0.42
1:B:248:LYS:CB	1:B:251:GLU:HG3	2.47	0.41
1:B:239:LYS:HD3	1:B:245:TYR:CZ	2.54	0.41
1:B:142:SER:C	1:B:144:GLY:N	2.69	0.41
1:B:106:GLU:O	1:B:106:GLU:HG2	2.21	0.41
1:B:47(B):TYR:CE2	1:B:106:GLU:HA	2.55	0.41
1:A:86:GLN:NE2	6:A:362:HOH:O	2.21	0.41
1:B:109:ALA:O	1:B:113:MET:HB2	2.20	0.41
1:B:10:MET:O	1:B:11:ASP:HB2	2.20	0.41
1:A:250:ASN:HB3	1:A:280:TYR:O	2.19	0.41
1:B:291:ILE:HA	1:B:292:PRO:HD3	1.82	0.41
1:A:291:ILE:HA	1:A:292:PRO:HD3	1.87	0.41
1:B:244:ASP:HB2	6:B:396:HOH:O	2.21	0.41
1:A:196:GLY:HA2	1:A:206:CYS:O	2.21	0.40
1:B:88:ILE:HG22	1:B:95:THR:CG2	2.52	0.40
1:B:148:GLU:OE1	1:B:148:GLU:HA	2.22	0.40
1:A:75:TYR:O	1:A:76:SER:C	2.59	0.40

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	335/340 (98%)	330 (98%)	5 (2%)	0	100	100
1	B	329/340 (97%)	322 (98%)	7 (2%)	0	100	100
All	All	664/680 (98%)	652 (98%)	12 (2%)	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 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	287/290 (99%)	256 (89%)	31 (11%)	8	15
1	B	283/290 (98%)	252 (89%)	31 (11%)	8	14
All	All	570/580 (98%)	508 (89%)	62 (11%)	8	14

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	63	SER
1	A	74	ARG
1	A	79	THR
1	A	81	SER
1	A	107	MET
1	A	110	LEU
1	A	132	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	146	LEU
1	A	147	LYS
1	A	157	ARG
1	A	160	GLU
1	A	160(C)	GLN
1	A	186	LYS
1	A	189	VAL
1	A	195	LYS
1	A	204	LEU
1	A	205	LEU
1	A	206	CYS
1	A	211	LEU
1	A	226	SER
1	A	228	ILE
1	A	231	LEU
1	A	240	ARG
1	A	265	LYS
1	A	279	SER
1	A	281(B)	LYS
1	A	290	ASP
1	A	295	THR
1	A	324	LEU
1	A	326	ARG
1	B	0	THR
1	B	22	THR
1	B	42	SER
1	B	43	SER
1	B	46	SER
1	B	50	CYS
1	B	52	TYR
1	B	59	SER
1	B	63	SER
1	B	66	HIS
1	B	77	THR
1	B	81	SER
1	B	90	THR
1	B	96	VAL
1	B	106	GLU
1	B	107	MET
1	B	160	SER
1	B	165	ILE
1	B	186	LYS

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	193	GLN
1	B	195	LYS
1	B	202	SER
1	B	206	CYS
1	B	207	GLU
1	B	230	LYS
1	B	232	MET
1	B	254	THR
1	B	278	GLU
1	B	281(A)	SER
1	B	292	PRO
1	B	324	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	HIS
1	A	128	GLN
1	A	160(C)	GLN
1	A	183	ASN
1	A	191	GLN
1	A	287	HIS
1	B	86	GLN
1	B	261	HIS
1	B	317	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 ⓘ

2 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
3	NAG	A	600	1,3	14,14,15	0.56	0	15,19,21	1.71	4 (26%)
3	NAG	A	601	3	14,14,15	0.59	0	15,19,21	1.04	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
3	NAG	A	600	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	601	3	-	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(°)
3	A	600	NAG	O7-C7-C8	-2.21	118.00	122.06
3	A	600	NAG	O7-C7-N2	2.29	126.53	121.86
3	A	601	NAG	O5-C5-C6	2.33	112.39	107.35
3	A	600	NAG	O5-C5-C6	2.83	113.47	107.35
3	A	600	NAG	C2-N2-C7	3.95	128.12	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.6 Ligand geometry ⓘ

5 ligands 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	GOL	A	341	-	5,5,5	0.49	0	5,5,5	0.99	0
2	RX0	A	500	-	37,38,38	1.01	2 (5%)	38,53,53	1.77	10 (26%)
4	GOL	A	502	-	5,5,5	0.31	0	5,5,5	0.51	0
2	RX0	B	500	-	37,38,38	1.10	2 (5%)	38,53,53	1.78	9 (23%)
5	NAG	B	600	1	14,14,15	0.60	0	15,19,21	1.47	2 (13%)

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	GOL	A	341	-	-	0/4/4/4	0/0/0/0
2	RX0	A	500	-	-	0/31/53/53	0/4/4/4
4	GOL	A	502	-	-	0/4/4/4	0/0/0/0
2	RX0	B	500	-	-	0/31/53/53	0/4/4/4
5	NAG	B	600	1	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	RX0	C33-C7	-2.01	1.48	1.51
2	A	500	RX0	C13-N9	3.13	1.50	1.46
2	A	500	RX0	C7-N9	3.29	1.39	1.34
2	B	500	RX0	C7-N9	4.48	1.41	1.34

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	RX0	O16-C15-C23	-4.56	98.75	108.98
2	B	500	RX0	O8-C7-C33	-4.14	114.34	120.81
2	A	500	RX0	O8-C7-N9	-3.41	117.41	121.66
2	A	500	RX0	C13-N9-C7	-3.00	113.59	123.73
2	B	500	RX0	C21-C19-C1	-2.75	113.69	118.78
2	A	500	RX0	C11-C10-C14	-2.62	107.46	110.97
2	B	500	RX0	O34-C30-C29	-2.56	102.27	110.74
2	A	500	RX0	O16-C15-C23	-2.54	103.29	108.98

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	RX0	C14-N9-C7	-2.52	113.95	123.19
2	A	500	RX0	C21-C19-C1	-2.51	114.13	118.78
2	B	500	RX0	C10-C11-C12	-2.42	108.00	112.37
2	A	500	RX0	C11-C12-C13	-2.19	104.30	108.67
2	B	500	RX0	C13-N9-C7	-2.17	116.39	123.73
2	B	500	RX0	C32-C33-C29	2.43	106.33	101.57
2	B	500	RX0	O8-C7-N9	2.58	124.89	121.66
5	B	600	NAG	C3-C4-C5	2.78	115.04	110.20
2	A	500	RX0	C33-C7-N9	2.95	121.84	119.06
5	B	600	NAG	C1-O5-C5	3.21	116.32	112.25
2	A	500	RX0	C14-N9-C13	3.38	119.57	112.76
2	A	500	RX0	C29-C30-C31	4.67	107.83	103.03
2	B	500	RX0	C29-C30-C31	4.84	108.00	103.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	RX0	2	0
2	B	500	RX0	2	0
5	B	600	NAG	3	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	337/340 (99%)	-0.43	2 (0%) 90 88	13, 27, 46, 60	0
1	B	333/340 (97%)	-0.31	0 100 100	15, 33, 56, 65	0
All	All	670/680 (98%)	-0.37	2 (0%) 94 93	13, 30, 54, 65	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	202	SER	3.9
1	A	203	THR	2.5

### 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
3	NAG	A	600	14/15	0.91	0.18	1.29	44,52,56,62	0
3	NAG	A	601	14/15	0.87	0.18	-	66,67,68,68	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(Å <sup>2</sup> )	Q<0.9
5	NAG	B	600	14/15	0.32	0.44	6.29	73,79,80,81	0
4	GOL	A	502	6/6	0.74	0.23	4.02	52,53,54,55	0
2	RX0	A	500	35/35	0.97	0.15	1.10	9,18,23,26	0
4	GOL	A	341	6/6	0.93	0.21	0.78	44,45,47,47	0
2	RX0	B	500	35/35	0.97	0.14	0.34	15,21,25,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.