



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:00 AM GMT

PDB ID : 3GW5
Title : Crystal structure of human renin complexed with a novel inhibitor
Authors : Wu, Z.; McKeever, B.M.
Deposited on : 2009-03-31
Resolution : 2.00 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
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

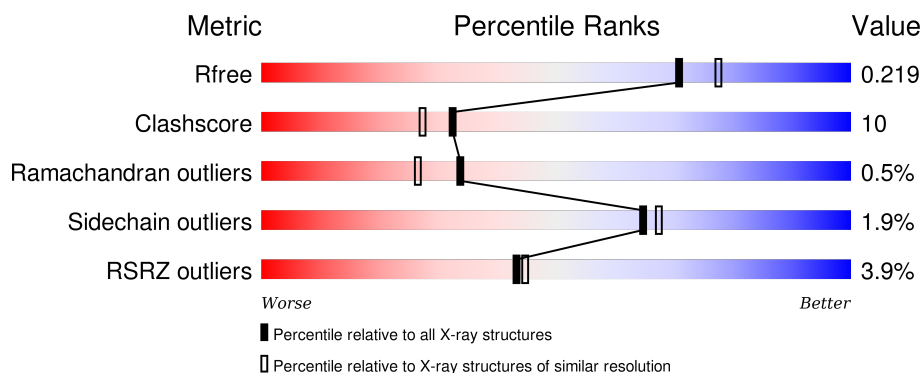
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


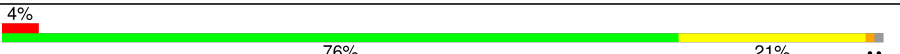
The reported resolution of this entry is 2.00 Å.

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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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 ≥ 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	337	 4% 77% 22% .
1	B	337	 4% 76% 21% ..

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	501	-	-	-	X
4	GOL	A	502	-	-	-	X
4	GOL	A	503	-	-	-	X
4	GOL	B	504	-	-	-	X

2 Entry composition [i](#)

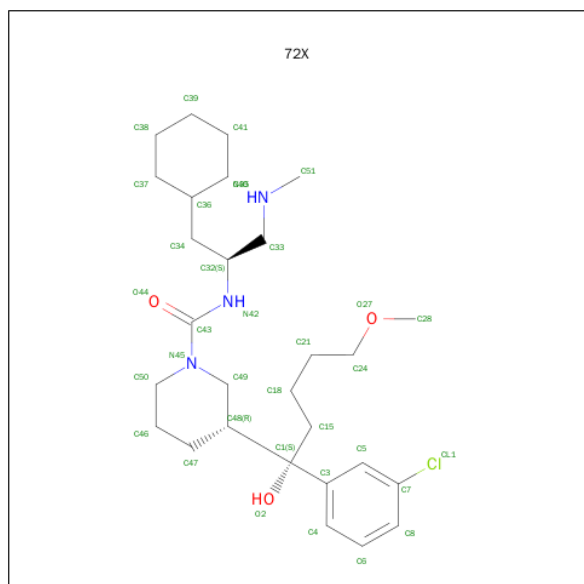
There are 7 unique types of molecules in this entry. The entry contains 5648 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			2595	1655	420	506	14			
1	B	332	Total	C	N	O	S	0	0	0
			2554	1633	411	496	14			

- Molecule 2 is (3R)-3-[(1S)-1-(3-CHLOROPHENYL)-1-HYDROXY-5-METHOXYPENTYL]-N-[(1S)-2-CYCLOHEXYL-1-[(METHYLAMINO)METHYL]ETHYL]PIPERIDINE-1-CARBOXAMIDE (three-letter code: 72X) (formula: C₂₈H₄₆ClN₃O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			35	28	1	3	3		
2	B	1	Total	C	Cl	N	O	0	0
			35	28	1	3	3		

- 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		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

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

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

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

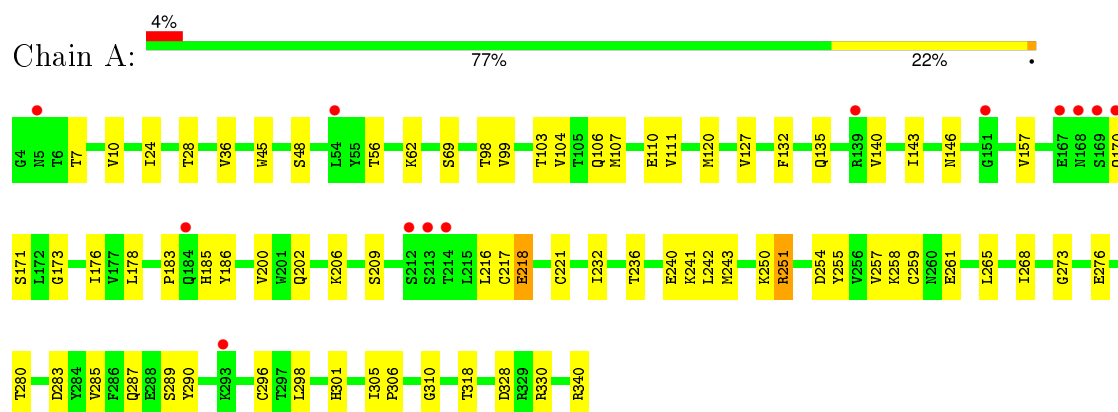
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	189	Total	O	0	0
			189	189		
7	B	167	Total	O	0	0
			167	167		

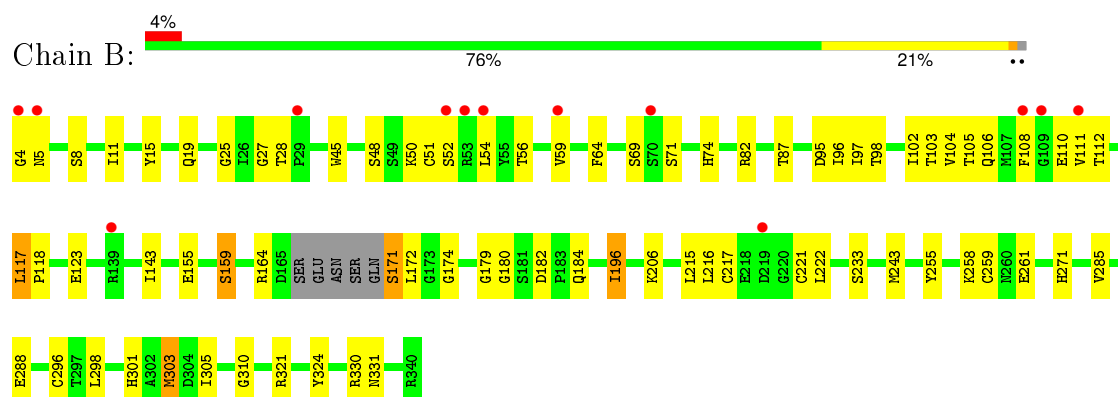
3 Residue-property plots

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, α , β , γ	54.20 Å 97.07 Å 149.55 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 19.99 – 2.00	Depositor EDS
% Data completeness (in resolution range)	83.5 (20.00-2.00) 83.7 (19.99-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.01 Å)	Xtriage
Refinement program	CNX	Depositor
R, R_{free}	0.210 , 0.256 0.217 , 0.219	Depositor DCC
R_{free} test set	2295 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 45324 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5648	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, NAG, 72X, 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	0.31	0/2655	0.50	0/3600
1	B	0.29	0/2613	0.50	0/3543
All	All	0.30	0/5268	0.50	0/7143

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	171	SER	Peptide

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	2595	0	2525	56	0
1	B	2554	0	2487	48	0
2	A	35	0	46	1	0
2	B	35	0	46	0	0
3	A	28	0	25	0	0
4	A	24	0	32	0	0
4	B	6	0	8	0	0
5	A	1	0	0	0	0
6	B	14	0	13	0	0
7	A	189	0	0	4	0
7	B	167	0	0	2	0
All	All	5648	0	5182	104	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 10.

All (104) 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:330:ARG:HH11	1:B:331:ASN:HD21	1.27	0.81
1:A:287:GLN:HG2	1:A:290:TYR:CE1	2.14	0.81
1:B:221:CYS:HB2	7:B:370:HOH:O	1.80	0.81
1:B:330:ARG:HH11	1:B:331:ASN:ND2	1.84	0.75
1:B:56:THR:O	1:B:59:VAL:HG22	1.89	0.73
1:B:48:SER:HB2	1:B:110:GLU:HB3	1.74	0.70
1:B:164:ARG:HG2	1:B:321:ARG:HD2	1.74	0.69
1:B:196:ILE:HD13	1:B:222:LEU:HD22	1.77	0.67
1:B:215:LEU:HG	1:B:216:LEU:HG	1.76	0.67
1:B:330:ARG:NH1	1:B:331:ASN:HD21	1.91	0.67
1:B:27:GLY:HA2	1:B:95:ASP:OD1	1.95	0.67
1:B:233:SER:OG	1:B:303:MET:HB3	1.93	0.67
1:A:206:LYS:HD2	1:A:206:LYS:N	2.11	0.66
1:A:10:VAL:HB	1:A:176:ILE:CG2	2.26	0.66
1:A:287:GLN:HG2	1:A:290:TYR:CZ	2.31	0.65
1:A:206:LYS:CD	1:A:206:LYS:N	2.61	0.64
1:B:285:VAL:HG22	1:B:298:LEU:CD2	2.28	0.63
1:B:82:ARG:HG2	1:B:87:THR:OG1	1.99	0.62
1:B:206:LYS:HB2	1:B:271:HIS:HD2	1.66	0.61
1:A:157:VAL:HG12	1:A:328:ASP:HA	1.82	0.60
1:B:258:LYS:HB2	1:B:261:GLU:HG3	1.85	0.59
1:B:15:TYR:HB3	1:B:19:GLN:HB2	1.84	0.58
1:B:96:ILE:HG23	1:B:103:THR:HG23	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:LYS:NZ	1:A:273:GLY:H	2.01	0.57
1:B:11:ILE:HD12	1:B:11:ILE:H	1.70	0.56
1:B:159:SER:HG	1:B:324:TYR:HE1	1.52	0.56
1:B:52:SER:OG	1:B:54:LEU:HB2	2.05	0.55
1:B:98:THR:HG22	1:B:103:THR:OG1	2.06	0.55
1:A:305:ILE:O	1:A:310:GLY:HA3	2.06	0.55
1:B:28:THR:O	1:B:69:SER:HA	2.07	0.55
1:A:24:ILE:HG22	1:A:99:VAL:HG22	1.89	0.54
1:A:45:TRP:NE1	1:A:127:VAL:HG13	2.23	0.54
1:B:217:CYS:HG	1:B:221:CYS:HG	0.67	0.54
1:A:48:SER:HB2	1:A:110:GLU:HB3	1.89	0.54
1:A:330:ARG:HH11	1:A:330:ARG:HG3	1.73	0.53
1:A:285:VAL:HG22	1:A:298:LEU:CD2	2.37	0.53
1:A:132:PHE:H	1:A:135:GLN:NE2	2.07	0.53
1:A:216:LEU:HD21	1:A:241:LYS:HB2	1.90	0.53
1:B:106:GLN:OE1	1:B:143:ILE:HA	2.08	0.53
1:A:259:CYS:HG	1:A:296:CYS:HG	0.58	0.53
1:A:217:CYS:HG	1:A:221:CYS:CB	2.20	0.51
1:B:196:ILE:CD1	1:B:222:LEU:HD22	2.39	0.51
1:A:104:VAL:HG21	1:A:146:ASN:HB3	1.92	0.51
1:A:185:HIS:HA	1:A:340:ARG:OXT	2.10	0.51
1:A:250:LYS:HD3	1:A:255:TYR:CZ	2.46	0.50
1:B:15:TYR:CG	1:B:123:GLU:HG3	2.46	0.50
1:A:10:VAL:HB	1:A:176:ILE:HG23	1.93	0.50
1:B:11:ILE:HG23	1:B:172:LEU:CD1	2.42	0.50
1:A:285:VAL:HG22	1:A:298:LEU:HD23	1.94	0.49
1:A:258:LYS:HB2	1:A:261:GLU:HG2	1.93	0.49
1:A:257:VAL:HG11	1:A:265:LEU:HD11	1.95	0.49
1:A:45:TRP:CE3	1:A:111:VAL:HG21	2.48	0.49
1:A:132:PHE:H	1:A:135:GLN:HE21	1.59	0.49
1:A:45:TRP:CE2	1:A:127:VAL:HG13	2.48	0.48
1:B:182:ASP:OD1	1:B:184:GLN:HB2	2.14	0.48
1:A:28:THR:O	1:A:69:SER:HA	2.14	0.48
1:B:171:SER:N	7:B:460:HOH:O	2.48	0.47
1:A:56:THR:HG22	1:A:120:MET:SD	2.54	0.47
1:A:217:CYS:SG	1:A:217:CYS:O	2.74	0.46
1:A:259:CYS:O	1:A:287:GLN:NE2	2.49	0.46
1:A:236:THR:O	1:A:240:GLU:HG3	2.16	0.46
1:B:96:ILE:CG2	1:B:103:THR:HG23	2.46	0.46
1:B:117:LEU:HD23	1:B:118:PRO:HA	1.98	0.46
1:B:305:ILE:O	1:B:310:GLY:HA3	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:ARG:NH1	1:A:330:ARG:HG3	2.31	0.45
1:A:287:GLN:CG	1:A:290:TYR:CE1	2.95	0.45
1:A:98:THR:HG22	1:A:103:THR:OG1	2.16	0.45
1:B:4:GLY:O	1:B:5:ASN:HB3	2.16	0.45
1:A:243:MET:HG3	1:A:255:TYR:CE1	2.52	0.45
1:B:159:SER:HB2	1:B:180:GLY:O	2.17	0.44
1:B:25:GLY:O	1:B:97:ILE:HA	2.18	0.44
1:A:259:CYS:HB3	1:A:289:SER:O	2.18	0.44
1:A:232:ILE:HG13	1:A:318:THR:HB	2.00	0.43
1:B:45:TRP:CE3	1:B:111:VAL:HG21	2.53	0.43
1:A:280:THR:O	1:A:283:ASP:HB2	2.18	0.43
1:B:259:CYS:CB	1:B:296:CYS:HG	2.26	0.43
1:A:106:GLN:OE1	1:A:143:ILE:HA	2.18	0.43
1:B:51:CYS:HB2	1:B:112:THR:HA	2.00	0.43
1:A:218:GLU:CD	1:A:218:GLU:N	2.71	0.43
1:A:183:PRO:HA	1:A:186:TYR:CE1	2.54	0.42
1:A:107:MET:HE1	7:A:403:HOH:O	2.18	0.42
1:A:36:VAL:HG21	2:A:400:72X:H21A	2.00	0.42
1:A:107:MET:HB3	1:A:140:VAL:HG13	2.01	0.42
1:B:243:MET:SD	1:B:298:LEU:HD12	2.59	0.42
1:B:27:GLY:HA2	1:B:95:ASP:CG	2.38	0.42
1:B:159:SER:OG	1:B:324:TYR:HE1	2.02	0.42
1:A:259:CYS:CB	1:A:296:CYS:HG	2.25	0.42
1:A:251:ARG:NH1	1:A:254:ASP:OD1	2.52	0.42
1:B:155:GLU:O	1:B:179:GLY:HA2	2.19	0.41
1:B:8:SER:HB2	1:B:102:ILE:HG13	2.02	0.41
1:A:305:ILE:HA	1:A:306:PRO:HD3	1.82	0.41
1:A:216:LEU:HD11	1:A:242:LEU:HB2	2.03	0.41
1:A:62:LYS:HG3	7:A:457:HOH:O	2.20	0.41
1:A:221:CYS:HB2	7:A:382:HOH:O	2.20	0.41
1:A:200:VAL:HG22	1:A:202:GLN:HB2	2.02	0.41
1:B:243:MET:HG3	1:B:255:TYR:CE1	2.56	0.41
1:A:173:GLY:HA2	7:A:490:HOH:O	2.20	0.41
1:A:218:GLU:CD	1:A:218:GLU:H	2.24	0.40
1:B:74:HIS:CD2	1:B:74:HIS:C	2.95	0.40
1:A:7:THR:HA	1:A:178:LEU:O	2.21	0.40
1:B:172:LEU:HD11	1:B:174:GLY:O	2.22	0.40
1:B:64:PHE:CE2	1:B:108:PHE:HZ	2.39	0.40
1:B:104:VAL:HG22	1:B:105:THR:N	2.37	0.40
1:A:209:SER:O	1:A:268:ILE:HA	2.21	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	335/337 (99%)	326 (97%)	7 (2%)	2 (1%)	30	22
1	B	328/337 (97%)	318 (97%)	9 (3%)	1 (0%)	46	41
All	All	663/674 (98%)	644 (97%)	16 (2%)	3 (0%)	34	26

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	170	GLN
1	A	171	SER
1	B	196	ILE

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	286/287 (100%)	282 (99%)	4 (1%)	74	77
1	B	281/287 (98%)	274 (98%)	7 (2%)	55	55
All	All	567/574 (99%)	556 (98%)	11 (2%)	65	67

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	218	GLU
1	A	251	ARG
1	A	276	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	301	HIS
1	B	50	LYS
1	B	71	SER
1	B	117	LEU
1	B	159	SER
1	B	288	GLU
1	B	301	HIS
1	B	303	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
1	A	135	GLN
1	A	150	GLN
1	A	194	ASN
1	A	202	GLN
1	A	331	ASN
1	B	74	HIS
1	B	94	GLN
1	B	150	GLN
1	B	175	GLN
1	B	271	HIS
1	B	331	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

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	0.54	0	15,19,21	0.69	0
3	NAG	A	601	3	14,14,15	0.53	0	15,19,21	0.79	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 (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	601	NAG	C2-N2-C7	-2.45	119.89	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

Of 9 ligands modelled in this entry, 1 is 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
2	72X	A	400	-	37,37,37	3.03	16 (43%)	38,49,49	1.85	6 (15%)
4	GOL	A	500	-	5,5,5	0.46	0	5,5,5	0.32	0
4	GOL	A	501	-	5,5,5	0.56	0	5,5,5	0.28	0
4	GOL	A	502	-	5,5,5	0.62	0	5,5,5	0.23	0
4	GOL	A	503	-	5,5,5	0.56	0	5,5,5	0.28	0
2	72X	B	400	-	37,37,37	3.10	16 (43%)	38,49,49	1.85	6 (15%)
4	GOL	B	504	-	5,5,5	0.52	0	5,5,5	0.28	0
6	NAG	B	600	1	14,14,15	0.51	0	15,19,21	0.81	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	72X	A	400	-	-	0/34/52/52	0/3/3/3
4	GOL	A	500	-	-	0/4/4/4	0/0/0/0
4	GOL	A	501	-	-	0/4/4/4	0/0/0/0
4	GOL	A	502	-	-	0/4/4/4	0/0/0/0
4	GOL	A	503	-	-	0/4/4/4	0/0/0/0
2	72X	B	400	-	-	0/34/52/52	0/3/3/3
4	GOL	B	504	-	-	0/4/4/4	0/0/0/0
6	NAG	B	600	1	-	0/6/23/26	0/1/1/1

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	72X	C7-CL1	-2.18	1.69	1.74
2	B	400	72X	C46-C50	2.09	1.58	1.51
2	B	400	72X	C41-C40	2.13	1.58	1.53
2	B	400	72X	C41-C39	2.17	1.60	1.51
2	A	400	72X	C41-C39	2.22	1.60	1.51
2	A	400	72X	C46-C50	2.23	1.59	1.51
2	A	400	72X	C43-N45	2.24	1.40	1.36
2	A	400	72X	C15-C1	2.29	1.58	1.54
2	B	400	72X	C43-N45	2.55	1.41	1.36
2	B	400	72X	C15-C1	2.99	1.59	1.54
2	B	400	72X	C40-C36	3.21	1.61	1.52
2	A	400	72X	C40-C36	3.62	1.62	1.52
2	A	400	72X	C5-C7	3.64	1.44	1.38
2	A	400	72X	C6-C8	3.68	1.46	1.38
2	B	400	72X	C5-C7	3.73	1.44	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	72X	C6-C4	3.86	1.46	1.38
2	A	400	72X	C6-C4	3.89	1.46	1.38
2	A	400	72X	C47-C48	3.94	1.63	1.53
2	B	400	72X	C47-C48	4.01	1.63	1.53
2	B	400	72X	C6-C8	4.21	1.47	1.38
2	B	400	72X	C1-C3	4.31	1.58	1.52
2	A	400	72X	C4-C3	4.44	1.46	1.39
2	A	400	72X	C1-C3	4.56	1.58	1.52
2	B	400	72X	C4-C3	4.62	1.46	1.39
2	A	400	72X	C8-C7	4.68	1.47	1.38
2	B	400	72X	C8-C7	4.87	1.47	1.38
2	B	400	72X	C49-N45	5.74	1.53	1.46
2	A	400	72X	C49-N45	5.87	1.53	1.46
2	B	400	72X	C49-C48	6.06	1.62	1.52
2	A	400	72X	C49-C48	6.18	1.63	1.52
2	A	400	72X	C5-C3	9.16	1.55	1.39
2	B	400	72X	C5-C3	9.73	1.56	1.39

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	72X	C5-C3-C1	-5.98	111.97	121.00
2	A	400	72X	C5-C3-C1	-5.67	112.44	121.00
2	A	400	72X	C46-C50-N45	-4.32	101.73	110.65
2	B	400	72X	C46-C50-N45	-3.95	102.51	110.65
2	A	400	72X	C47-C46-C50	-2.72	107.33	110.97
6	B	600	NAG	C2-N2-C7	-2.60	119.70	123.04
2	B	400	72X	C47-C46-C50	-2.28	107.92	110.97
2	B	400	72X	C18-C15-C1	2.84	119.95	114.71
2	A	400	72X	C18-C15-C1	3.06	120.35	114.71
2	B	400	72X	C32-N42-C43	3.41	128.59	122.13
2	A	400	72X	C32-N42-C43	3.65	129.04	122.13
2	A	400	72X	C4-C3-C1	4.96	127.99	121.06
2	B	400	72X	C4-C3-C1	5.02	128.07	121.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	72X	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

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, 95th 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 ²)	Q<0.9
1	A	337/337 (100%)	-0.07	13 (3%)	43	45	17, 30, 49, 66	0
1	B	332/337 (98%)	0.18	13 (3%)	43	45	21, 36, 61, 68	0
All	All	669/674 (99%)	0.05	26 (3%)	43	45	17, 33, 57, 68	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	169	SER	4.9
1	B	59	VAL	4.7
1	B	54	LEU	4.5
1	A	170	GLN	4.5
1	B	139	ARG	4.5
1	B	5	ASN	3.2
1	A	214	THR	2.9
1	B	53	ARG	2.8
1	A	212	SER	2.8
1	B	109	GLY	2.8
1	A	167	GLU	2.8
1	B	219	ASP	2.7
1	B	70	SER	2.6
1	A	54	LEU	2.5
1	A	293	LYS	2.4
1	B	4	GLY	2.4
1	A	168	ASN	2.3
1	B	111	VAL	2.3
1	A	139	ARG	2.1
1	B	52	SER	2.1
1	A	213	SER	2.1
1	A	5	ASN	2.1
1	A	184	GLN	2.1
1	A	151	GLY	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	108	PHE	2.0
1	B	29	PRO	2.0

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, 95th 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 ²)	Q<0.9
3	NAG	A	600	14/15	0.88	0.14	1.59	45,48,56,59	0
3	NAG	A	601	14/15	0.80	0.35	-	63,66,68,68	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, 95th 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 ²)	Q<0.9
4	GOL	A	502	6/6	0.80	0.26	8.34	49,54,56,58	0
4	GOL	A	503	6/6	0.84	0.21	3.47	45,47,49,50	0
4	GOL	A	501	6/6	0.79	0.22	3.20	57,59,60,60	0
4	GOL	B	504	6/6	0.85	0.14	2.72	64,64,64,65	0
4	GOL	A	500	6/6	0.80	0.24	1.31	53,54,55,58	0
2	72X	A	400	35/35	0.95	0.11	0.16	17,22,27,29	0
2	72X	B	400	35/35	0.95	0.11	0.07	28,32,35,38	0
5	CL	A	700	1/1	0.97	0.13	-	51,51,51,51	0
6	NAG	B	600	14/15	0.80	0.31	-	77,80,82,82	0

6.5 Other polymers [i](#)

There are no such residues in this entry.