



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 08:13 PM GMT

PDB ID : 2V10
Title : CRYSTAL STRUCTURE OF RENIN WITH INHIBITOR 9
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Deposited on : 2007-05-21
Resolution : 3.10 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

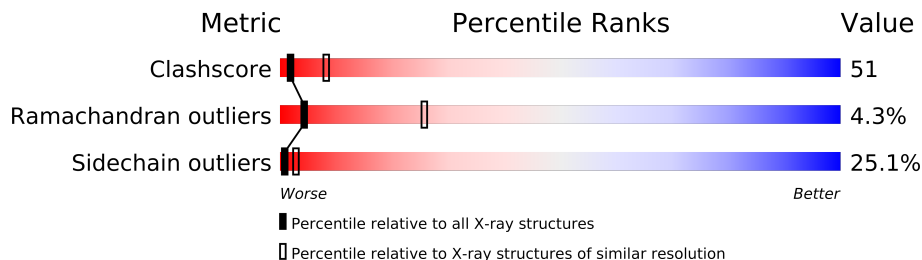
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
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 3.10 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	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	340	
1	O	340	

2 Entry composition i

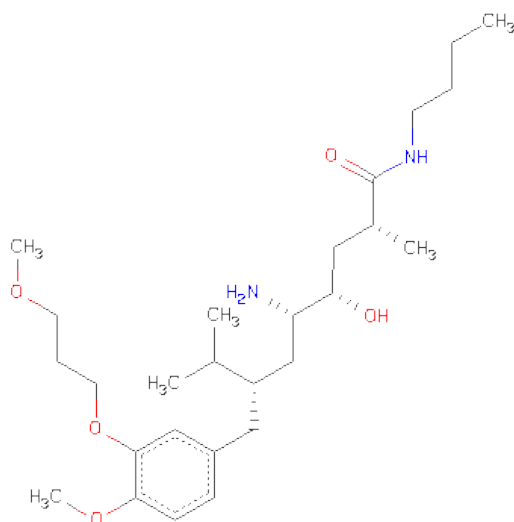
There are 2 unique types of molecules in this entry. The entry contains 5192 atoms, of which 0 are hydrogen and 0 are deuterium.

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 RENIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	334	Total	C	N	O	S	0	0	1
			2567	1639	416	498	14			
1	O	332	Total	C	N	O	S	0	0	1
			2557	1634	414	495	14			

- Molecule 2 is (2R,4S,5S,7S)-5-AMINO-N-BUTYL-4-HYDROXY-7-[4-METHOXY-3-(3-METHOXYPROPOXY)BENZYL]-2,8-DIMETHYLNONANAMIDE (three-letter code: C61) (formula: C₂₇H₄₈N₂O₅).



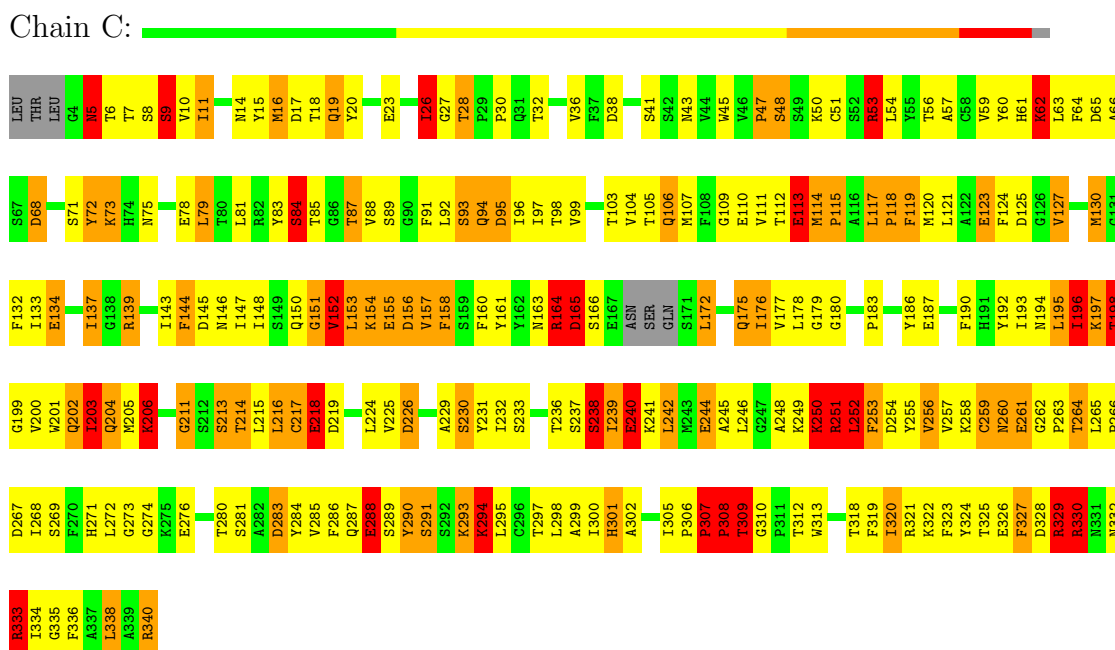
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			34	27	2	5		
2	O	1	Total	C	N	O	0	0
			34	27	2	5		

3 Residue-property plots

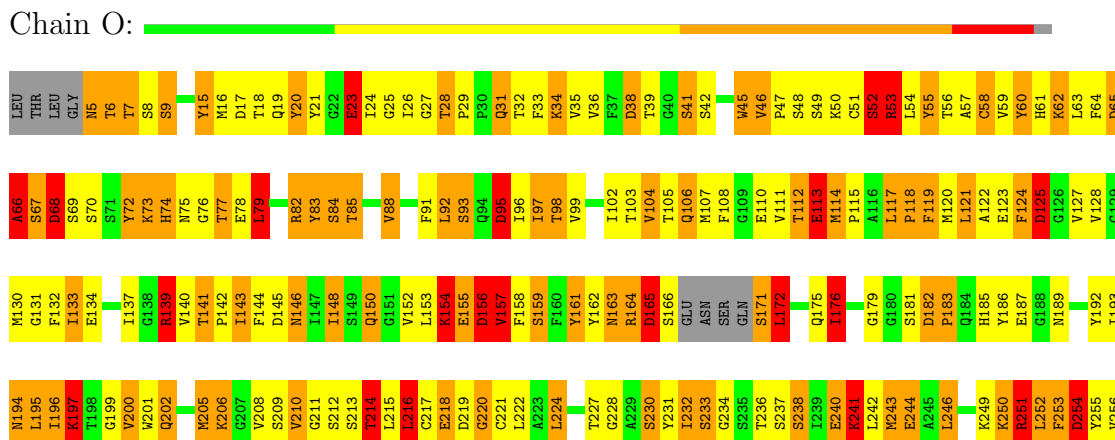
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

• Molecule 1: RENIN



• Molecule 1: RENIN



V257	T318
K258	F319
G259	I320
N260	R321
E261	K322
G262	F323
P263	Y324
L264	
L265	F327
P266	D328
D267	R329
L268	R330
S269	N331
F270	N332
H271	R333
L272	
G273	F336
G274	A337
K275	L338
E276	A339
Y277	R340
T278	
L279	
T280	
S281	
K282	
D283	
Y284	
V285	
F286	
Q287	
E288	
S289	
Y290	
S291	
S292	
K293	
V294	
L295	
G296	
T297	
L298	
A299	
I300	
H301	
A302	
N303	
D304	
I305	
P306	
P307	
P308	
T309	
G310	
P311	
T312	
N313	
A314	
A317	

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	143.00Å 143.00Å 143.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.10	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-3.10)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.210 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5192	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: C61

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	C	1.62	31/2626 (1.2%)	2.25	133/3560 (3.7%)
1	O	1.59	24/2616 (0.9%)	2.41	169/3547 (4.8%)
All	All	1.60	55/5242 (1.0%)	2.33	302/7107 (4.2%)

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	C	5	0
1	O	3	0
All	All	8	0

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	251	ARG	NE-CZ	11.26	1.47	1.33
1	C	244	GLU	CD-OE2	11.00	1.37	1.25
1	O	288	GLU	CD-OE2	10.50	1.37	1.25
1	O	78	GLU	CD-OE2	9.96	1.36	1.25
1	C	218	GLU	CD-OE2	9.77	1.36	1.25

The worst 5 of 302 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	330	ARG	NE-CZ-NH1	14.47	127.54	120.30
1	O	164	ARG	NE-CZ-NH1	13.08	126.84	120.30
1	C	15	TYR	CB-CG-CD2	12.78	128.66	121.00
1	C	15	TYR	CB-CG-CD1	-12.76	113.35	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	91	PHE	CB-CG-CD1	12.10	129.27	120.80

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	56	THR	CA
1	C	75	ASN	CA
1	C	203	ILE	CB
1	C	206	LYS	CA
1	C	259	CYS	CA

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	C	2567	0	2498	241	0
1	O	2557	0	2489	282	0
2	C	34	0	48	22	0
2	O	34	0	48	9	0
All	All	5192	0	5083	524	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 51.

The worst 5 of 524 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:260:ASN:HD22	1:C:261:GLU:N	1.41	1.16
1:C:216:LEU:HD12	1:C:238:SER:HB3	1.28	1.11
1:O:196:ILE:HG22	1:O:197:LYS:HG2	1.14	1.09
1:C:127:VAL:HG21	2:C:1341:C61:C19	1.83	1.09
1:C:96:ILE:HG22	1:C:105:THR:HG22	1.41	1.03

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	C	330/340 (97%)	288 (87%)	31 (9%)	11 (3%)	6	33
1	O	328/340 (96%)	281 (86%)	30 (9%)	17 (5%)	3	21
All	All	658/680 (97%)	569 (86%)	61 (9%)	28 (4%)	4	26

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	196	ILE
1	C	218	GLU
1	C	251	ARG
1	C	252	LEU
1	O	66	ALA

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	C	283/290 (98%)	222 (78%)	61 (22%)	1	6
1	O	282/290 (97%)	201 (71%)	81 (29%)	0	1
All	All	565/580 (97%)	423 (75%)	142 (25%)	1	3

5 of 142 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	9	SER
1	O	70	SER
1	O	288	GLU
1	O	23	GLU

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Mol	Chain	Res	Type
1	O	41	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	332	ASN
1	O	61	HIS
1	O	202	GLN
1	C	301	HIS
1	O	287	GLN

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 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
2	C61	C	1341	-	34,34,34	1.43	4 (11%)	43,43,43	1.87	11 (25%)
2	C61	O	1341	-	34,34,34	1.15	3 (8%)	43,43,43	2.18	10 (23%)

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	C61	C	1341	-	-	0/37/37/37	0/1/1/1
2	C61	O	1341	-	-	0/37/37/37	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1341	C61	O8-C12	4.22	1.43	1.37
2	C	1341	C61	C19-C18	-4.10	1.37	1.52
2	O	1341	C61	O8-C12	3.93	1.43	1.37
2	C	1341	C61	O7-C11	3.38	1.44	1.37
2	O	1341	C61	O7-C11	3.29	1.44	1.37

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	1341	C61	C9-O8-C12	8.60	130.30	117.59
2	C	1341	C61	C27-C26-C24	-5.62	106.81	114.11
2	O	1341	C61	C27-C26-C24	-5.18	107.38	114.11
2	O	1341	C61	C17-C21-C22	-4.75	109.09	115.42
2	C	1341	C61	C17-C21-C22	-4.32	109.66	115.42

There are no chirality outliers.

There are no torsion outliers.

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.