wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 05:50 AM GMT

PDB ID	:	2V16
Title	:	CRYSTAL STRUCTURE OF RENIN WITH INHIBITOR 3
Authors	:	Rahuel, J.; Rasetti, V.; Maibaum, J.; Rueger, H.; Goschke, R.; Cohen, N.C.; Stutz, S.; Cumin, F.; Fuhrer, W.; Wood, J.M.; Grutter, M.G.
Deposited on	:	2007-05-22
Resolution	:	2.80 Å(reported)

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

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

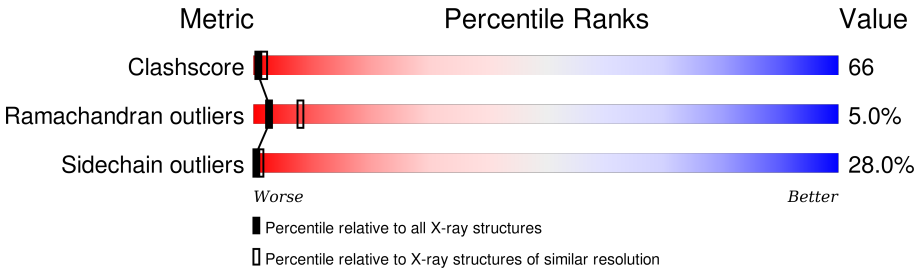
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	340	34% 46% 14%
1	O	340	24% 48% 22%

2 Entry composition

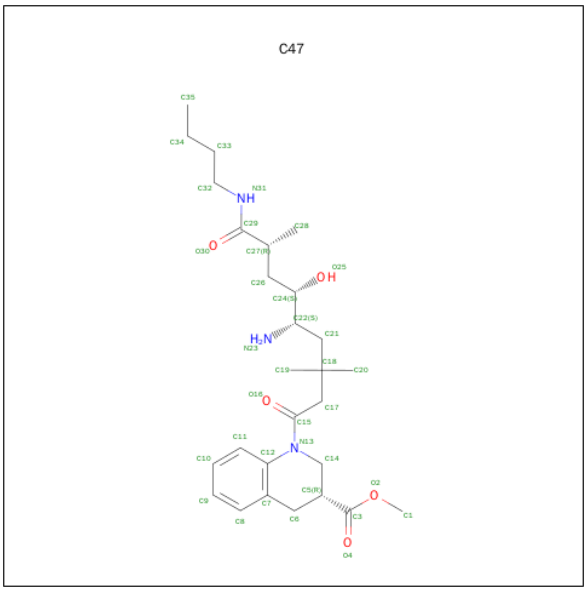
There are 3 unique types of molecules in this entry. The entry contains 5216 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	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 METHYL (3R)-1-[(5S,6S,8R)-5-AMINO-9-BUTYLAMINO-6-HYDROXY-3,3,8-TRIMETHYL-9-OXO-NONANOYL]-3,4-DIHYDRO-2H-QUINOLINE-3-CARBOXYLATE (three-letter code: C47) (formula: $C_{27}H_{43}N_3O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			35	27	3	5		
2	O	1	Total	C	N	O	0	0
			35	27	3	5		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	15	Total O 15 15	0	0
3	O	7	Total O 7 7	0	0

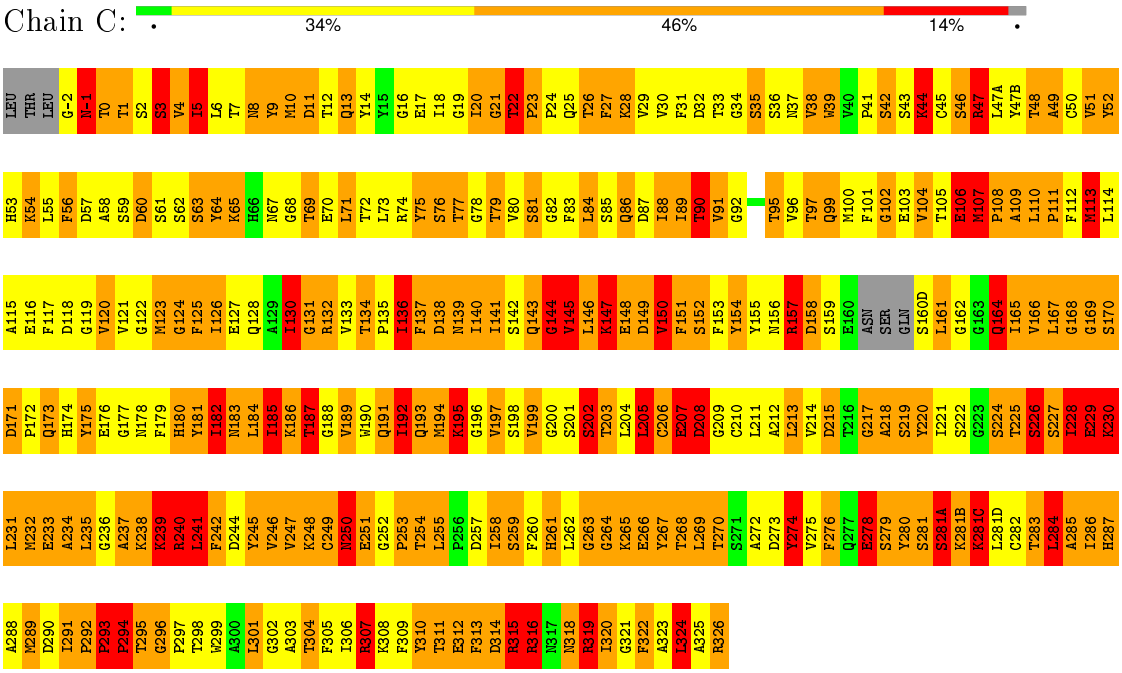
3 Residue-property plots (i)

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.

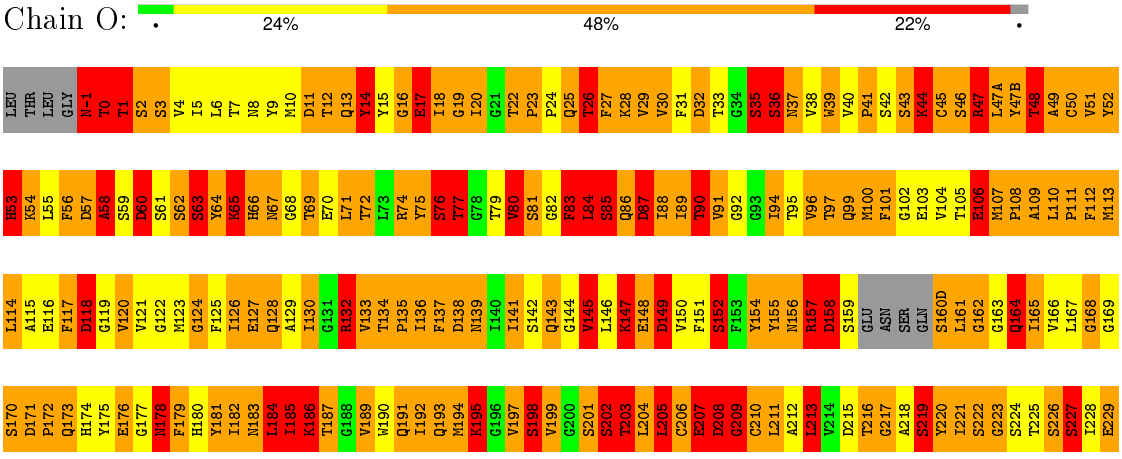
- Molecule 1: RENIN

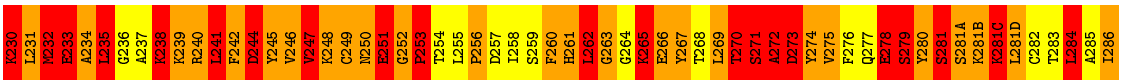
Chain C:



- Molecule 1: RENIN

Chain O:




K230
L231
M232
E233
A234
L235
G236
A237
K238
K239
R240
L241
F242
D244
Y245
V246
V247
K248
C249
N250
E251
G252
P253
T254
L255
P256
D257
I258
S259
F260
H261
L262
G263
G264
K265
E266
Y267
T268
L269
T270
S271
A272
D273
Y274
V275
F276
Q277
E278
S279
Y280
S281
S281A
K281B
K281C
L281D
C282
T283
L284
A285
I286


H287
A288
M289
D290
I291
P292
P293
P294
T295
G296
P297
T298
W299
A300
L301
G302
A303
T304
F305
I306
R307
K308
F309
Y310
T311
E312
F313
D314
R315
R316
N317
N318
R319
I320
G321
F322
A323
L324
A325
R326

4 Data and refinement statistics (i)

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	142.90Å 142.90Å 142.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.80)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.214 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5216	wwPDB-VP
Average B, all atoms (Å^2)	15.0	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: C47

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	4.39	458/2626 (17.4%)	3.84	531/3560 (14.9%)
1	O	4.37	424/2616 (16.2%)	4.21	596/3547 (16.8%)
All	All	4.38	882/5242 (16.8%)	4.03	1127/7107 (15.9%)

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	2	2
1	O	5	3
All	All	7	5

The worst 5 of 882 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	266	GLU	CD-OE2	33.99	1.63	1.25
1	O	207	GLU	CD-OE2	32.74	1.61	1.25
1	C	233	GLU	CD-OE1	31.09	1.59	1.25
1	O	316	ARG	CZ-NH1	30.09	1.72	1.33
1	C	266	GLU	CD-OE2	29.57	1.58	1.25

The worst 5 of 1127 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	316	ARG	NE-CZ-NH1	45.10	142.85	120.30
1	O	74	ARG	NE-CZ-NH2	42.22	141.41	120.30
1	O	157	ARG	NE-CZ-NH1	34.81	137.70	120.30
1	O	316	ARG	NE-CZ-NH2	-31.00	104.80	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	319	ARG	NE-CZ-NH1	28.55	134.58	120.30

5 of 7 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	182	ILE	CB
1	C	311	THR	CB
1	O	156	ASN	CA
1	O	183	ASN	CA
1	O	202	SER	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	154	TYR	Sidechain
1	C	220	TYR	Sidechain
1	O	157	ARG	Mainchain
1	O	272	ALA	Mainchain
1	O	310	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2567	0	2487	301	0
1	O	2557	0	2486	371	0
2	C	35	0	43	11	0
2	O	35	0	43	15	0
3	C	15	0	0	3	0
3	O	7	0	0	2	0
All	All	5216	0	5059	674	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 66.

The worst 5 of 674 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:C:186:LYS:CE	1:C:186:LYS:CD	1.75	1.64
1:C:186:LYS:CG	1:C:186:LYS:CD	1.76	1.61
1:O:204:LEU:CB	1:O:204:LEU:CG	1.79	1.60
1:C:281(C):LYS:CD	1:C:281(C):LYS:CE	1.76	1.59
1:O:173:GLN:CG	1:O:173:GLN:CB	1.76	1.59

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	330/340 (97%)	283 (86%)	34 (10%)	13 (4%)	4 12
1	O	328/340 (96%)	274 (84%)	34 (10%)	20 (6%)	2 5
All	All	658/680 (97%)	557 (85%)	68 (10%)	33 (5%)	3 8

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	185	ILE
1	C	207	GLU
1	C	234	ALA
1	C	235	LEU
1	C	240	ARG

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	283/290 (98%)	214 (76%)	69 (24%)	1 2
1	O	282/290 (97%)	193 (68%)	89 (32%)	0 1
All	All	565/580 (97%)	407 (72%)	158 (28%)	0 1

5 of 158 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	1	THR
1	O	62	SER
1	O	279	SER
1	O	3	SER
1	O	26	THR

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	O	99	GLN
1	O	139	ASN
1	O	191	GLN
1	C	318	ASN
1	O	193	GLN

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)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	C47	C	1327	-	36,36,36	3.12	20 (55%)	35,50,50	3.35	18 (51%)
2	C47	O	1327	-	36,36,36	3.92	20 (55%)	35,50,50	3.94	20 (57%)

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	C47	C	1327	-	-	0/37/49/49	0/2/2/2
2	C47	O	1327	-	-	0/37/49/49	0/2/2/2

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	1327	C47	C12-C7	-8.26	1.28	1.40
2	C	1327	C47	C17-C18	-5.91	1.45	1.54
2	O	1327	C47	C6-C7	-4.86	1.43	1.51
2	C	1327	C47	C21-C18	-4.70	1.44	1.55
2	O	1327	C47	C26-C27	-4.24	1.42	1.54

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1327	C47	O25-C24-C22	-8.91	96.28	109.49
2	C	1327	C47	C27-C26-C24	-6.87	105.71	114.24
2	O	1327	C47	C27-C26-C24	-6.09	106.67	114.24
2	O	1327	C47	C6-C7-C12	-6.05	111.98	120.07
2	O	1327	C47	C19-C18-C17	-5.29	98.98	109.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1327	C47	11	0
2	O	1327	C47	15	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

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.