Full wwPDB EM Model Validation Report ⓘ

May 27, 2020 – 04:47 pm BST

PDB ID	:	1AT9
Title	:	STRUCTURE OF BACTERIORHODOPSIN AT 3.0 ANGSTROM DETERMINED BY ELECTRON CRYSTALLOGRAPHY
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Deposited on	:	1997-08-20
Resolution	:	3.00 Å(reported)

This is a Full wwPDB EM Model Validation Report for a publicly released PDB/EMDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
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:

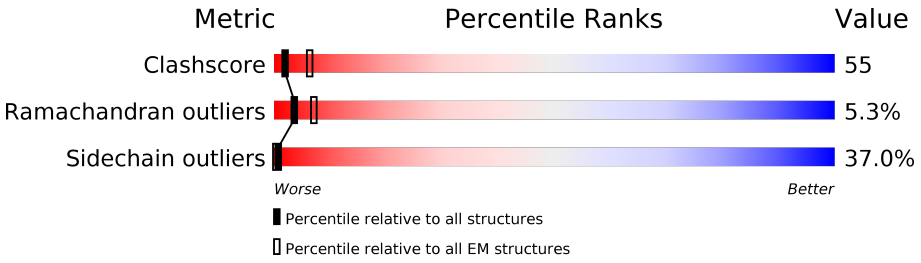
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON CRYSTALLOGRAPHY

The reported resolution of this entry is 3.00 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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%

Mol	Chain	Length	Quality of chain
1	A	248	21% 49% 21% • 7%

2 Entry composition

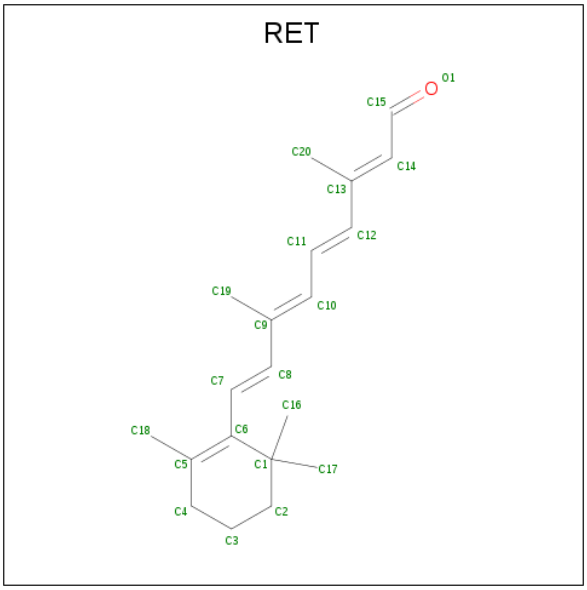
There are 2 unique types of molecules in this entry. The entry contains 1798 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 BACTERIORHODOPSIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	230	1778	1194	272	303	9	0	0

- Molecule 2 is RETINAL (three-letter code: RET) (formula: $C_{20}H_{28}O$).



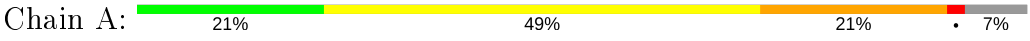
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
2	A	1	20	20	0

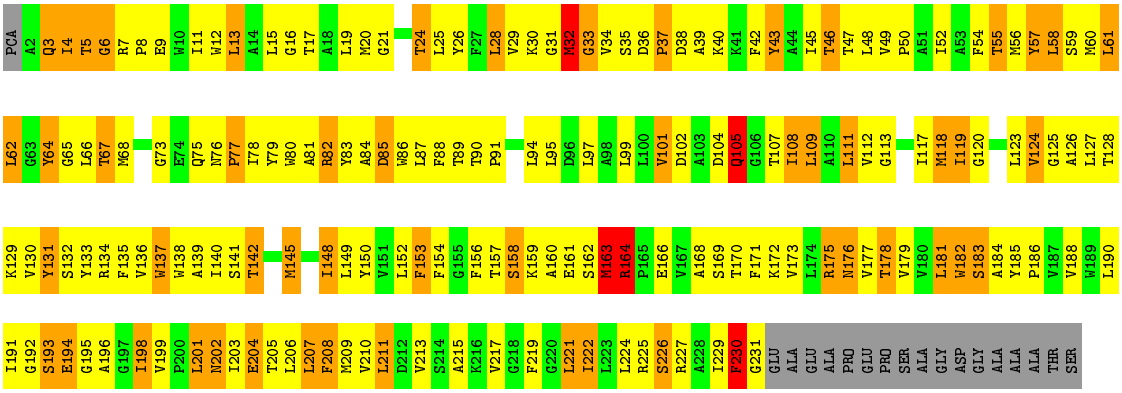
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: BACTERIORHODOPSIN

Chain A:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	CRYSTALLOGRAPHY	Depositor
Imposed symmetry	2D CRYSTAL, a=Not provided Å, b=Not provided Å, c=Not provided Å, γ=Not provided°, space group=Not provided	Depositor
Number of images used	Not provided	Depositor
Resolution determination method	DIFFRACTION PATTERN/LAYERLINES	Depositor
CTF correction method	Not provided	Depositor
Microscope	JEOL 4000, JEOL 3000SFF	Depositor
Voltage (kV)	400, 300	Depositor
Electron dose (e^-/Å^2)	10, 10	Depositor
Minimum defocus (nm)	Not provided, Not provided	Depositor
Maximum defocus (nm)	Not provided, Not provided	Depositor
Magnification	Not provided, Not provided	Depositor
Image detector	GENERIC GATAN (2k x 2k), KODAK SO-163 FILM	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.43	0/1826	0.65	2/2494 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	164	ARG	NE-CZ-NH2	7.62	124.11	120.30
1	A	163	MET	CG-SD-CE	6.82	111.12	100.20

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	1778	0	1837	201	0
2	A	20	0	27	4	0
All	All	1798	0	1864	201	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 55.

All (201) 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:A:4:ILE:HG23	1:A:61:LEU:HD11	1.50	0.93
1:A:35:SER:C	1:A:37:PRO:HD2	1.91	0.90
1:A:87:LEU:O	1:A:91:PRO:HD3	1.74	0.88
1:A:202:ASN:H	1:A:202:ASN:HD22	1.22	0.88
1:A:182:TRP:HA	1:A:185:TYR:HD2	1.39	0.86
1:A:94:LEU:HA	1:A:97:LEU:HD12	1.58	0.86
1:A:80:TRP:HA	1:A:83:TYR:HD2	1.40	0.85
1:A:80:TRP:HA	1:A:83:TYR:CD2	2.14	0.83
1:A:36:ASP:HB3	1:A:39:ALA:HB3	1.59	0.83
1:A:184:ALA:O	1:A:188:VAL:HG23	1.78	0.82
1:A:152:LEU:O	1:A:156:PHE:HB2	1.80	0.82
1:A:46:THR:O	1:A:50:PRO:HD3	1.80	0.81
1:A:87:LEU:O	1:A:91:PRO:CD	2.31	0.79
1:A:221:LEU:HD23	1:A:225:ARG:HG3	1.62	0.79
1:A:58:LEU:HD12	1:A:62:LEU:HD11	1.65	0.77
1:A:79:TYR:O	1:A:82:ARG:HG2	1.86	0.76
1:A:36:ASP:O	1:A:38:ASP:N	2.18	0.75
1:A:145:MET:O	1:A:148:ILE:HG23	1.88	0.74
1:A:131:TYR:HA	1:A:134:ARG:HD3	1.71	0.73
1:A:183:SER:O	1:A:186:PRO:HD2	1.87	0.73
1:A:34:VAL:C	1:A:36:ASP:H	1.92	0.72
1:A:182:TRP:HA	1:A:185:TYR:CD2	2.23	0.71
1:A:156:PHE:O	1:A:160:ALA:N	2.22	0.71
1:A:137:TRP:HA	1:A:140:ILE:HD12	1.72	0.71
1:A:36:ASP:O	1:A:39:ALA:N	2.23	0.71
1:A:46:THR:O	1:A:50:PRO:CD	2.40	0.70
1:A:207:LEU:O	1:A:211:LEU:HD22	1.92	0.70
1:A:37:PRO:HA	1:A:40:LYS:HB3	1.75	0.69
1:A:90:THR:OG1	1:A:91:PRO:HD3	1.93	0.69
1:A:163:MET:HB3	1:A:164:ARG:NH2	2.09	0.68
1:A:60:MET:HG3	1:A:81:ALA:HB3	1.75	0.68
1:A:36:ASP:N	1:A:37:PRO:HD2	2.08	0.68
1:A:19:LEU:HD13	1:A:213:VAL:HG21	1.76	0.67
1:A:178:THR:HG23	1:A:182:TRP:CE3	2.30	0.67
1:A:9:GLU:HA	1:A:12:TRP:HD1	1.60	0.67
1:A:149:LEU:HA	1:A:152:LEU:HD12	1.77	0.67
1:A:138:TRP:O	1:A:142:THR:HG22	1.94	0.66
1:A:185:TYR:HB2	1:A:186:PRO:HD3	1.76	0.66
1:A:108:ILE:HD13	1:A:109:LEU:N	2.10	0.66
1:A:163:MET:CB	1:A:164:ARG:HH21	2.08	0.66
1:A:37:PRO:HD3	1:A:40:LYS:HE3	1.78	0.66
1:A:105:GLN:O	1:A:108:ILE:HG23	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:LYS:HB3	1:A:43:TYR:OH	1.97	0.64
1:A:138:TRP:CZ2	1:A:190:LEU:HD22	2.33	0.63
1:A:168:ALA:O	1:A:172:LYS:HG3	1.98	0.63
1:A:138:TRP:CH2	1:A:190:LEU:HD22	2.33	0.63
1:A:26:TYR:CE1	1:A:30:LYS:HE3	2.34	0.63
1:A:202:ASN:N	1:A:202:ASN:HD22	1.96	0.62
1:A:88:PHE:O	1:A:91:PRO:HD2	1.99	0.62
1:A:175:ARG:O	1:A:179:VAL:HG23	2.00	0.62
1:A:222:ILE:O	1:A:226:SER:HB3	2.00	0.62
1:A:163:MET:HB2	1:A:164:ARG:HH21	1.65	0.61
1:A:182:TRP:O	1:A:186:PRO:HD3	2.00	0.61
1:A:82:ARG:HD3	1:A:86:TRP:CH2	2.36	0.61
1:A:26:TYR:HE1	1:A:30:LYS:HE3	1.64	0.61
1:A:128:THR:HG22	1:A:129:LYS:O	2.01	0.61
1:A:108:ILE:O	1:A:112:VAL:HG23	2.01	0.61
1:A:131:TYR:HA	1:A:134:ARG:HG3	1.82	0.61
1:A:49:VAL:HB	1:A:50:PRO:HD3	1.83	0.61
1:A:77:PRO:HD2	1:A:194:GLU:HG2	1.83	0.60
1:A:131:TYR:HA	1:A:134:ARG:CD	2.31	0.60
1:A:131:TYR:HA	1:A:134:ARG:CG	2.31	0.60
1:A:152:LEU:HA	1:A:156:PHE:CD2	2.37	0.60
1:A:21:GLY:O	1:A:24:THR:HG23	2.01	0.60
1:A:65:GLY:O	1:A:79:TYR:HA	2.02	0.60
1:A:84:ALA:O	1:A:87:LEU:HB3	2.01	0.60
1:A:20:MET:O	1:A:24:THR:HG22	2.01	0.60
1:A:118:MET:HG3	1:A:119:ILE:N	2.15	0.60
1:A:13:LEU:HD12	1:A:57:TYR:CE1	2.37	0.60
1:A:16:GLY:HA2	1:A:19:LEU:HD12	1.84	0.60
1:A:192:GLY:HA2	1:A:199:VAL:HB	1.84	0.59
1:A:9:GLU:HG2	1:A:201:LEU:HD22	1.83	0.59
1:A:5:THR:HG23	1:A:6:GLY:H	1.67	0.59
1:A:4:ILE:CG2	1:A:61:LEU:HD11	2.30	0.58
1:A:191:ILE:HD12	1:A:192:GLY:N	2.18	0.58
1:A:113:GLY:O	1:A:117:ILE:HG13	2.02	0.58
1:A:224:LEU:HA	1:A:229:ILE:HG12	1.86	0.58
1:A:65:GLY:HA2	1:A:81:ALA:HB2	1.86	0.58
1:A:25:LEU:O	1:A:28:LEU:HB2	2.04	0.57
1:A:82:ARG:HD3	1:A:86:TRP:CZ2	2.39	0.57
1:A:60:MET:SD	1:A:79:TYR:HD2	2.27	0.57
1:A:13:LEU:HD12	1:A:57:TYR:HE1	1.68	0.57
1:A:159:LYS:C	1:A:161:GLU:N	2.55	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:GLY:O	1:A:124:VAL:HG23	2.04	0.57
1:A:47:THR:O	1:A:50:PRO:HD2	2.04	0.56
1:A:159:LYS:C	1:A:161:GLU:H	2.09	0.56
1:A:34:VAL:HB	1:A:36:ASP:HB2	1.87	0.56
1:A:178:THR:HG23	1:A:182:TRP:HE3	1.70	0.56
1:A:182:TRP:O	1:A:186:PRO:CD	2.54	0.56
1:A:135:PHE:O	1:A:138:TRP:HB3	2.05	0.55
1:A:178:THR:HG1	1:A:182:TRP:HZ3	1.54	0.55
1:A:202:ASN:H	1:A:202:ASN:ND2	1.98	0.55
1:A:82:ARG:HB3	1:A:82:ARG:NH1	2.21	0.55
1:A:208:PHE:O	1:A:211:LEU:HB2	2.07	0.55
1:A:68:MET:HB3	1:A:75:GLN:NE2	2.22	0.54
1:A:203:ILE:HG22	1:A:207:LEU:HD11	1.89	0.54
1:A:20:MET:HE1	1:A:213:VAL:HA	1.89	0.54
1:A:45:ILE:O	1:A:49:VAL:HG23	2.08	0.54
1:A:36:ASP:OD1	1:A:231:GLY:HA3	2.07	0.54
1:A:178:THR:HG22	1:A:179:VAL:N	2.23	0.53
1:A:159:LYS:O	1:A:161:GLU:N	2.41	0.53
1:A:16:GLY:O	1:A:20:MET:HG2	2.08	0.53
1:A:20:MET:CE	1:A:213:VAL:HA	2.38	0.53
1:A:163:MET:CB	1:A:164:ARG:NH2	2.70	0.52
1:A:34:VAL:C	1:A:36:ASP:N	2.62	0.52
1:A:135:PHE:HD1	1:A:190:LEU:HD11	1.74	0.52
1:A:126:ALA:O	1:A:134:ARG:NH1	2.42	0.52
1:A:175:ARG:HG2	1:A:176:ASN:N	2.23	0.52
1:A:153:PHE:O	1:A:157:THR:HB	2.10	0.52
1:A:4:ILE:HG22	1:A:4:ILE:O	2.10	0.52
1:A:149:LEU:O	1:A:152:LEU:HB2	2.10	0.52
1:A:82:ARG:HB2	1:A:86:TRP:CE2	2.45	0.51
1:A:56:MET:HG3	1:A:85:ASP:HB2	1.90	0.51
1:A:5:THR:O	1:A:6:GLY:C	2.47	0.51
1:A:61:LEU:C	1:A:61:LEU:HD12	2.31	0.51
1:A:97:LEU:HD21	1:A:219:PHE:HE2	1.74	0.51
1:A:230:PHE:CD1	1:A:230:PHE:N	2.78	0.51
1:A:183:SER:C	1:A:186:PRO:HD2	2.31	0.51
1:A:60:MET:HA	1:A:64:TYR:O	2.11	0.50
1:A:170:THR:HG23	1:A:171:PHE:N	2.27	0.50
1:A:34:VAL:CG2	1:A:36:ASP:HB2	2.42	0.50
1:A:82:ARG:HH11	1:A:86:TRP:HZ2	1.59	0.49
1:A:215:ALA:O	1:A:219:PHE:HB3	2.12	0.49
1:A:65:GLY:CA	1:A:81:ALA:HB2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ILE:HG23	1:A:12:TRP:N	2.28	0.49
1:A:131:TYR:CD1	1:A:132:SER:N	2.81	0.49
1:A:181:LEU:O	1:A:184:ALA:HB3	2.14	0.48
1:A:34:VAL:HB	1:A:36:ASP:CB	2.43	0.48
1:A:219:PHE:CD1	1:A:219:PHE:C	2.87	0.48
1:A:138:TRP:CE2	1:A:190:LEU:HD13	2.48	0.48
1:A:202:ASN:N	1:A:202:ASN:ND2	2.59	0.48
1:A:193:SER:OG	1:A:194:GLU:N	2.46	0.48
1:A:52:ILE:O	1:A:55:THR:HG23	2.14	0.48
1:A:86:TRP:HB3	2:A:249(A):RET:H12	1.95	0.47
1:A:125:GLY:O	1:A:128:THR:HB	2.14	0.47
1:A:128:THR:O	1:A:129:LYS:HB2	2.14	0.47
1:A:36:ASP:N	1:A:37:PRO:CD	2.76	0.47
1:A:19:LEU:CD1	1:A:213:VAL:HG21	2.43	0.47
1:A:137:TRP:HA	1:A:140:ILE:CD1	2.44	0.46
1:A:39:ALA:O	1:A:42:PHE:N	2.49	0.46
1:A:85:ASP:O	1:A:89:THR:HG23	2.16	0.46
1:A:157:THR:HA	1:A:160:ALA:HB2	1.98	0.46
1:A:36:ASP:O	1:A:37:PRO:C	2.54	0.46
1:A:118:MET:CG	1:A:119:ILE:N	2.78	0.46
1:A:29:VAL:O	1:A:32:MET:HB2	2.16	0.45
1:A:82:ARG:CB	1:A:82:ARG:HH11	2.28	0.45
1:A:97:LEU:HD21	1:A:219:PHE:CE2	2.50	0.45
1:A:152:LEU:HD23	1:A:156:PHE:CD2	2.51	0.45
1:A:101:VAL:CG2	1:A:160:ALA:HA	2.47	0.45
1:A:5:THR:HG23	1:A:6:GLY:N	2.30	0.45
1:A:82:ARG:NH1	1:A:86:TRP:HZ2	2.14	0.45
1:A:82:ARG:HB2	1:A:86:TRP:CZ2	2.52	0.45
1:A:34:VAL:HB	1:A:36:ASP:CG	2.38	0.45
1:A:76:ASN:HB3	1:A:194:GLU:CG	2.47	0.45
1:A:185:TYR:CE2	2:A:249(A):RET:H11	2.52	0.44
1:A:94:LEU:HG	1:A:111:LEU:HD22	1.99	0.44
1:A:138:TRP:CD1	1:A:190:LEU:HD13	2.52	0.44
1:A:104:ASP:O	1:A:105:GLN:C	2.56	0.44
1:A:153:PHE:O	1:A:157:THR:CB	2.66	0.44
1:A:3:GLN:HE21	1:A:3:GLN:HA	1.82	0.44
1:A:5:THR:OG1	1:A:6:GLY:N	2.51	0.43
1:A:145:MET:CE	1:A:183:SER:HA	2.48	0.43
1:A:166:GLU:O	1:A:170:THR:HG22	2.18	0.43
1:A:58:LEU:O	1:A:61:LEU:HB3	2.18	0.43
1:A:131:TYR:O	1:A:134:ARG:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:SER:HB2	2:A:249(A):RET:H41	2.00	0.43
1:A:46:THR:O	1:A:50:PRO:HD2	2.18	0.43
1:A:48:LEU:HD23	1:A:48:LEU:HA	1.79	0.43
1:A:62:LEU:HD12	1:A:62:LEU:H	1.84	0.43
1:A:213:VAL:O	1:A:217:VAL:HG23	2.18	0.42
1:A:186:PRO:HG3	2:A:249(A):RET:H183	2.01	0.42
1:A:37:PRO:HA	1:A:40:LYS:CB	2.48	0.42
1:A:33:GLY:O	1:A:34:VAL:HG13	2.19	0.42
1:A:82:ARG:CB	1:A:82:ARG:NH1	2.82	0.42
1:A:206:LEU:O	1:A:210:VAL:HG23	2.19	0.42
1:A:34:VAL:CB	1:A:36:ASP:HB2	2.50	0.42
1:A:4:ILE:HD11	1:A:62:LEU:HD23	2.01	0.42
1:A:6:GLY:O	1:A:8:PRO:HD3	2.19	0.42
1:A:76:ASN:HB3	1:A:194:GLU:CB	2.49	0.42
1:A:67:THR:HG22	1:A:68:MET:H	1.83	0.42
1:A:7:ARG:HB3	1:A:9:GLU:OE1	2.19	0.42
1:A:173:VAL:O	1:A:177:VAL:HG23	2.20	0.42
1:A:26:TYR:HE2	1:A:225:ARG:HH21	1.67	0.41
1:A:152:LEU:HA	1:A:156:PHE:HD2	1.84	0.41
1:A:171:PHE:CE1	1:A:175:ARG:HD2	2.54	0.41
1:A:224:LEU:HD23	1:A:229:ILE:HD13	2.00	0.41
1:A:139:ALA:O	1:A:142:THR:HG23	2.20	0.41
1:A:135:PHE:CD1	1:A:190:LEU:HD11	2.56	0.41
1:A:204:GLU:HG3	1:A:205:THR:N	2.34	0.41
1:A:154:PHE:O	1:A:158:SER:HB2	2.19	0.41
1:A:88:PHE:C	1:A:91:PRO:HD2	2.41	0.41
1:A:171:PHE:C	1:A:171:PHE:CD1	2.95	0.41
1:A:31:GLY:O	1:A:32:MET:C	2.59	0.41
1:A:76:ASN:HB3	1:A:194:GLU:HG2	2.03	0.41
1:A:215:ALA:O	1:A:219:PHE:CB	2.69	0.40
1:A:25:LEU:HA	1:A:28:LEU:HD12	2.03	0.40
1:A:133:TYR:O	1:A:136:VAL:HB	2.21	0.40
1:A:161:GLU:OE2	1:A:162:SER:O	2.39	0.40
1:A:164:ARG:H	1:A:164:ARG:HG2	1.40	0.40
1:A:178:THR:HG23	1:A:182:TRP:CZ3	2.55	0.40
1:A:196:ALA:HB1	1:A:198:ILE:HD11	2.04	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 PDB entries followed by that with respect to all EM entries.

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	228/248 (92%)	177 (78%)	39 (17%)	12 (5%)	2 11

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	GLY
1	A	33	GLY
1	A	37	PRO
1	A	230	PHE
1	A	32	MET
1	A	73	GLY
1	A	195	GLY
1	A	102	ASP
1	A	105	GLN
1	A	77	PRO
1	A	130	VAL
1	A	4	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 PDB entries followed by that with respect to all EM entries.

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	184/193 (95%)	116 (63%)	68 (37%)	0 0

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	5	THR
1	A	13	LEU
1	A	15	LEU
1	A	17	THR
1	A	24	THR
1	A	28	LEU
1	A	32	MET
1	A	43	TYR
1	A	46	THR
1	A	54	PHE
1	A	55	THR
1	A	57	TYR
1	A	58	LEU
1	A	59	SER
1	A	61	LEU
1	A	62	LEU
1	A	64	TYR
1	A	66	LEU
1	A	67	THR
1	A	78	ILE
1	A	82	ARG
1	A	85	ASP
1	A	95	LEU
1	A	99	LEU
1	A	101	VAL
1	A	105	GLN
1	A	107	THR
1	A	108	ILE
1	A	109	LEU
1	A	111	LEU
1	A	118	MET
1	A	119	ILE
1	A	123	LEU
1	A	124	VAL
1	A	127	LEU
1	A	131	TYR
1	A	137	TRP
1	A	142	THR
1	A	145	MET
1	A	148	ILE
1	A	150	TYR
1	A	153	PHE

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Mol	Chain	Res	Type
1	A	158	SER
1	A	163	MET
1	A	164	ARG
1	A	169	SER
1	A	175	ARG
1	A	176	ASN
1	A	178	THR
1	A	181	LEU
1	A	182	TRP
1	A	183	SER
1	A	193	SER
1	A	194	GLU
1	A	198	ILE
1	A	201	LEU
1	A	202	ASN
1	A	204	GLU
1	A	207	LEU
1	A	208	PHE
1	A	209	MET
1	A	211	LEU
1	A	221	LEU
1	A	222	ILE
1	A	226	SER
1	A	227	ARG
1	A	230	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	75	GLN
1	A	176	ASN
1	A	202	ASN

5.3.3 RNA

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)

1 ligand is 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	RET	A	249(A)	1	20,20,21	0.92	1 (5%)	27,27,28	0.73	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
2	RET	A	249(A)	1	-	11/13/30/31	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	249(A)	RET	C1-C6	2.80	1.57	1.53

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	249(A)	RET	C1-C6-C7-C8
2	A	249(A)	RET	C11-C10-C9-C19
2	A	249(A)	RET	C12-C13-C14-C15
2	A	249(A)	RET	C20-C13-C14-C15
2	A	249(A)	RET	C7-C8-C9-C19
2	A	249(A)	RET	C7-C8-C9-C10
2	A	249(A)	RET	C11-C12-C13-C14
2	A	249(A)	RET	C9-C10-C11-C12
2	A	249(A)	RET	C11-C10-C9-C8
2	A	249(A)	RET	C11-C12-C13-C20
2	A	249(A)	RET	C5-C6-C7-C8

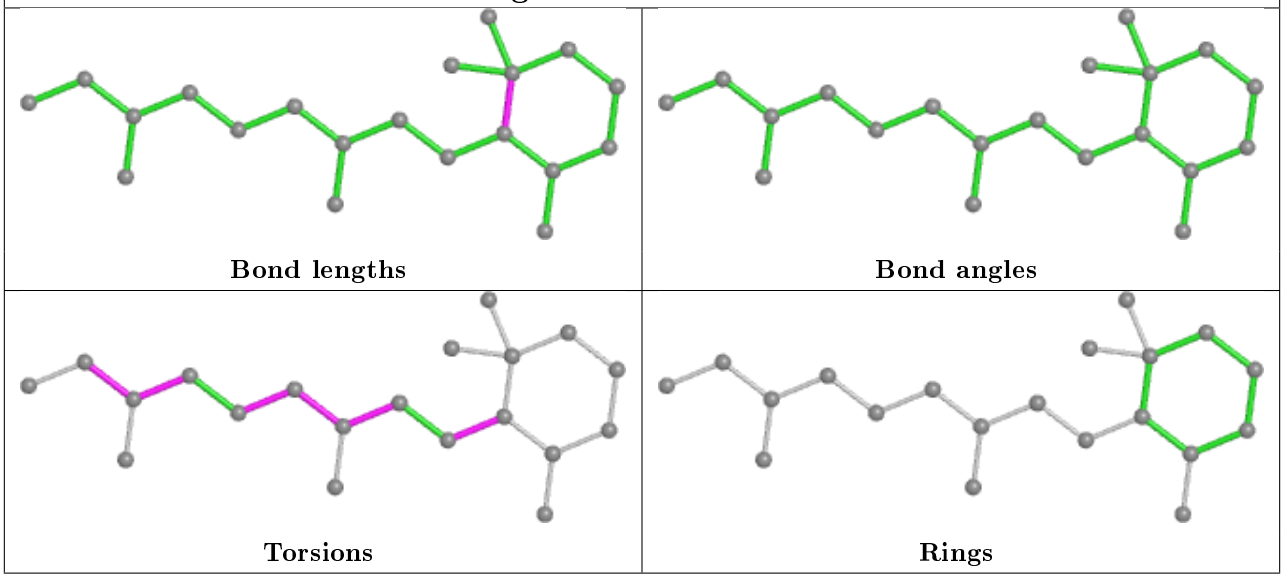
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	249(A)	RET	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand RET A 249A



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.