



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 03:26 PM BST

PDB ID : 1LN6  
Title : STRUCTURE OF BOVINE RHODOPSIN (Metarhodopsin II)  
Authors : Choi, G.; Landin, J.; Galan, J.F.; Birge, R.R.; Albert, A.D.; Yeagle, P.L.  
Deposited on : 2002-05-03

This is a Full wwPDB NMR 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/NMRValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : rb-20027457  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027457

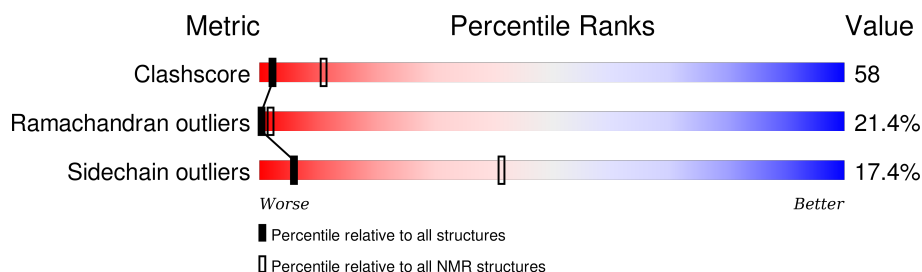
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	348	

## 2 Ensemble composition and analysis ⓘ

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

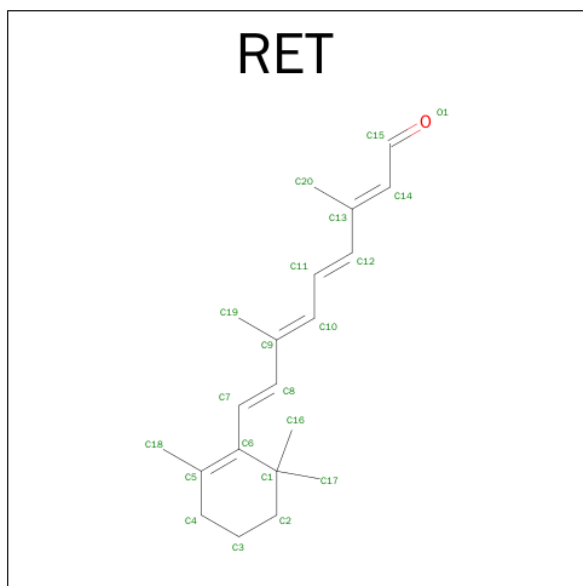
### 3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 4242 atoms, of which 1796 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called RHODOPSIN.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	309	4204	1607	1778	375	420	24	0

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



Mol	Chain	Residues	Atoms		
			Total	C	H
2	A	1	38	20	18



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *MULTI-DIMENSIONAL NMR, CD, SIMULATED ANNEALING WITH MMFF94 FORCE FIELD, MOLECULAR DYNAMICS WITH CHARMM FORCE FIELD*.

Of the 10 calculated structures, 1 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
SYBYL	refinement	6.6
SYBYL	structure solution	6.6

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality [i](#)

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

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 (average) 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	1.63	15/2511 (0.6%)	2.08	83/3421 (2.4%)
All	All	1.63	15/2511 (0.6%)	2.08	83/3421 (2.4%)

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	Planarity
1	A	6	19
All	All	6	19

All bond outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	324	GLY	N-CA	9.99	1.61	1.46
1	A	69	ARG	NE-CZ	7.75	1.43	1.33
1	A	90	GLY	CA-C	6.95	1.62	1.51
1	A	156	GLY	CA-C	6.41	1.62	1.51
1	A	182	GLY	CA-C	6.13	1.61	1.51
1	A	250	VAL	CB-CG1	6.09	1.65	1.52
1	A	341	GLU	CD-OE1	-5.96	1.19	1.25
1	A	249	GLU	CD-OE2	-5.93	1.19	1.25
1	A	268	TYR	CB-CG	5.81	1.60	1.51
1	A	329	GLY	CA-C	5.76	1.61	1.51
1	A	268	TYR	CE1-CZ	5.59	1.45	1.38
1	A	270	GLY	CA-C	5.54	1.60	1.51
1	A	181	GLU	CD-OE1	-5.51	1.19	1.25
1	A	206	TYR	CE1-CZ	5.14	1.45	1.38
1	A	174	GLY	CA-C	5.12	1.60	1.51

All angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	TYR	CB-CG-CD2	-13.19	113.08	121.00
1	A	69	ARG	NE-CZ-NH1	12.06	126.33	120.30
1	A	74	TYR	CB-CG-CD1	10.02	127.01	121.00
1	A	147	ARG	NE-CZ-NH2	-9.96	115.32	120.30
1	A	203	PHE	CB-CG-CD1	9.70	127.59	120.80
1	A	136	TYR	CB-CG-CD1	-9.66	115.20	121.00
1	A	43	TYR	CB-CG-CD1	9.25	126.55	121.00
1	A	306	TYR	CB-CG-CD1	8.99	126.39	121.00
1	A	105	PHE	CB-CG-CD2	8.37	126.66	120.80
1	A	331	ASP	CB-CG-OD2	8.30	125.78	118.30
1	A	45	PHE	CB-CG-CD2	-8.29	115.00	120.80
1	A	177	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	A	241	ALA	N-CA-CB	-7.73	99.28	110.10
1	A	282	ASP	CB-CG-OD2	7.44	125.00	118.30
1	A	317	MET	N-CA-CB	-7.19	97.65	110.60
1	A	208	PHE	CB-CG-CD1	-7.18	115.77	120.80
1	A	334	SER	CB-CA-C	7.15	123.69	110.10
1	A	281	SER	N-CA-CB	-7.07	99.89	110.50
1	A	193	THR	CB-CA-C	6.96	130.40	111.60
1	A	338	SER	N-CA-CB	-6.87	100.19	110.50
1	A	74	TYR	CB-CG-CD2	-6.86	116.88	121.00
1	A	127	SER	N-CA-CB	-6.78	100.33	110.50
1	A	250	VAL	CG1-CB-CG2	-6.78	100.06	110.90
1	A	56	PHE	N-CA-CB	-6.58	98.75	110.60
1	A	53	PRO	N-CA-CB	-6.53	95.42	102.60
1	A	69	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	A	88	PHE	CB-CG-CD2	6.45	125.31	120.80
1	A	69	ARG	CA-CB-CG	6.39	127.46	113.40
1	A	313	PHE	CB-CG-CD1	-6.36	116.35	120.80
1	A	212	PHE	CG-CD2-CE2	-6.36	113.81	120.80
1	A	159	PHE	CB-CG-CD1	-6.35	116.35	120.80
1	A	332	GLU	OE1-CD-OE2	-6.31	115.73	123.30
1	A	183	MET	CA-CB-CG	6.22	123.87	113.30
1	A	261	PHE	CB-CG-CD1	-6.21	116.45	120.80
1	A	177	ARG	NH1-CZ-NH2	-6.20	112.58	119.40
1	A	60	TYR	CG-CD1-CE1	-6.20	116.34	121.30
1	A	265	TRP	CB-CA-C	6.18	122.76	110.40
1	A	52	PHE	CG-CD2-CE2	-6.16	114.03	120.80
1	A	345	VAL	CB-CA-C	-6.14	99.73	111.40
1	A	230	VAL	CA-CB-CG2	6.10	120.05	110.90
1	A	136	TYR	N-CA-CB	-6.08	99.65	110.60
1	A	136	TYR	CG-CD2-CE2	-5.87	116.60	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	PHE	CB-CG-CD2	5.79	124.85	120.80
1	A	177	ARG	NE-CZ-NH2	5.78	123.19	120.30
1	A	212	PHE	CB-CG-CD2	-5.70	116.81	120.80
1	A	124	ALA	CB-CA-C	5.69	118.63	110.10
1	A	265	TRP	CD2-CE3-CZ3	5.67	126.17	118.80
1	A	40	LEU	O-C-N	5.66	131.75	122.70
1	A	105	PHE	CB-CG-CD1	-5.65	116.85	120.80
1	A	214	ILE	CA-CB-CG1	5.62	121.68	111.00
1	A	252	ARG	NE-CZ-NH1	-5.57	117.52	120.30
1	A	243	THR	CA-C-N	-5.53	105.04	117.20
1	A	273	PHE	CB-CG-CD1	-5.52	116.94	120.80
1	A	228	PHE	CZ-CE2-CD2	5.50	126.69	120.10
1	A	135	ARG	NE-CZ-NH2	5.49	123.05	120.30
1	A	247	GLU	CB-CA-C	5.49	121.37	110.40
1	A	60	TYR	CD1-CE1-CZ	5.48	124.73	119.80
1	A	129	VAL	CA-CB-CG2	-5.47	102.69	110.90
1	A	72	LEU	O-C-N	5.40	131.34	122.70
1	A	313	PHE	CB-CA-C	5.38	121.16	110.40
1	A	175	TRP	CH2-CZ2-CE2	5.34	122.74	117.40
1	A	72	LEU	CB-CA-C	-5.32	100.09	110.20
1	A	45	PHE	CG-CD1-CE1	-5.28	114.99	120.80
1	A	139	VAL	N-CA-C	-5.27	96.78	111.00
1	A	116	PHE	CB-CG-CD2	-5.26	117.11	120.80
1	A	41	ALA	CB-CA-C	5.25	117.98	110.10
1	A	301	TYR	CB-CG-CD2	-5.23	117.86	121.00
1	A	223	TYR	CB-CG-CD1	5.23	124.14	121.00
1	A	287	PHE	CB-CG-CD1	5.23	124.46	120.80
1	A	49	MET	CA-C-N	-5.22	105.72	117.20
1	A	219	ILE	C-N-CA	5.21	134.72	121.70
1	A	118	THR	CA-CB-OG1	5.19	119.89	109.00
1	A	295	ALA	C-N-CA	-5.19	108.73	121.70
1	A	265	TRP	CH2-CZ2-CE2	5.17	122.57	117.40
1	A	183	MET	C-N-CA	-5.16	108.81	121.70
1	A	115	PHE	CB-CG-CD2	-5.11	117.23	120.80
1	A	72	LEU	CB-CG-CD1	-5.10	102.33	111.00
1	A	141	LYS	N-CA-CB	5.08	119.74	110.60
1	A	178	TYR	CB-CG-CD1	-5.08	117.95	121.00
1	A	136	TYR	CB-CG-CD2	5.05	124.03	121.00
1	A	235	ALA	C-N-CA	5.03	134.28	121.70
1	A	274	TYR	CG-CD2-CE2	-5.03	117.28	121.30
1	A	146	PHE	O-C-N	5.02	130.73	122.70

All chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms
1	A	110	CYS	CA
1	A	140	CYS	CA
1	A	187	CYS	CA
1	A	198	THR	CB
1	A	242	THR	CB
1	A	319	THR	CB

All planar outliers are listed below.

Mol	Chain	Res	Type	Group
1	A	187	CYS	Peptide
1	A	253	MET	Peptide
1	A	246	ALA	Peptide
1	A	135	ARG	Sidechain,Peptide
1	A	313	PHE	Peptide
1	A	306	TYR	Sidechain
1	A	147	ARG	Peptide
1	A	341	GLU	Peptide
1	A	163	MET	Peptide
1	A	52	PHE	Sidechain
1	A	285	PRO	Peptide
1	A	60	TYR	Sidechain
1	A	78	ASN	Peptide
1	A	311	LYS	Peptide
1	A	346	ALA	Peptide
1	A	107	PRO	Peptide
1	A	329	GLY	Peptide
1	A	203	PHE	Peptide

## 6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	2426	1778	2397	282
2	A	20	18	15	25
All	All	2446	1796	2412	282

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 58.

All clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:207:MET:HG3	2:A:400:RET:C3	1.53	1.32
1:A:102:TYR:CB	1:A:103:PHE:HB2	1.50	1.32
1:A:207:MET:HB3	2:A:400:RET:C4	1.49	1.30
1:A:102:TYR:HB2	1:A:103:PHE:CB	1.48	1.38
1:A:207:MET:CB	2:A:400:RET:C4	1.47	1.89
1:A:207:MET:CG	2:A:400:RET:H31	1.41	1.43
1:A:135:ARG:O	1:A:136:TYR:CD2	1.35	1.76
1:A:334:SER:O	1:A:335:THR:CG2	1.33	1.75
1:A:43:TYR:OH	1:A:296:LYS:HG2	1.29	1.10
1:A:110:CYS:CB	1:A:187:CYS:SG	1.29	2.18
1:A:247:GLU:O	1:A:250:VAL:CG2	1.28	1.81
1:A:195:HIS:HB3	1:A:198:THR:OG1	1.26	1.27
1:A:102:TYR:N	1:A:103:PHE:HB3	1.26	1.43
1:A:132:ALA:O	1:A:136:TYR:HB3	1.26	1.14
1:A:103:PHE:CZ	1:A:105:PHE:O	1.24	1.90
1:A:179:ILE:HD11	1:A:191:TYR:CD2	1.24	1.66
1:A:43:TYR:OH	1:A:296:LYS:CG	1.22	1.87
1:A:131:LEU:O	1:A:136:TYR:CD2	1.19	1.95
1:A:61:VAL:O	1:A:318:VAL:HG11	1.17	1.40
1:A:207:MET:CB	2:A:400:RET:H41	1.16	1.58
1:A:43:TYR:CZ	1:A:296:LYS:HG2	1.15	1.75
1:A:131:LEU:CD2	1:A:136:TYR:CE2	1.14	2.30
1:A:334:SER:O	1:A:335:THR:HG23	1.14	0.92
1:A:43:TYR:CE2	1:A:296:LYS:CD	1.13	2.32
1:A:131:LEU:O	1:A:136:TYR:CE2	1.11	2.03
1:A:345:VAL:O	1:A:345:VAL:HG23	1.10	1.43
1:A:195:HIS:CB	1:A:198:THR:OG1	1.10	1.98
1:A:207:MET:CG	2:A:400:RET:C3	1.10	2.16
1:A:43:TYR:CE2	1:A:296:LYS:HD2	1.09	1.82
1:A:43:TYR:CZ	1:A:296:LYS:CD	1.08	2.35
1:A:179:ILE:HD11	1:A:191:TYR:CE2	1.08	1.84
1:A:182:GLY:HA2	1:A:187:CYS:HB3	1.08	1.22
1:A:191:TYR:CD2	1:A:191:TYR:O	1.07	2.06
1:A:131:LEU:HD23	1:A:136:TYR:CE2	1.07	1.85
1:A:110:CYS:SG	1:A:187:CYS:CB	1.07	2.41
1:A:94:THR:HA	1:A:98:SER:HB3	1.06	1.26
1:A:43:TYR:CZ	1:A:296:LYS:CG	1.06	2.37
1:A:207:MET:CB	2:A:400:RET:H42	1.05	1.61
1:A:102:TYR:CB	1:A:103:PHE:CB	1.04	2.13
1:A:72:LEU:HB3	1:A:310:ASN:CB	1.04	1.81
1:A:241:ALA:O	1:A:242:THR:CG2	1.04	2.06
1:A:132:ALA:O	1:A:136:TYR:CB	1.04	2.06

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:137:VAL:HG23	1:A:140:CYS:HB2	1.03	1.21
1:A:247:GLU:O	1:A:250:VAL:HG22	1.02	1.41
1:A:52:PHE:CD1	1:A:56:PHE:CD1	1.00	2.48
1:A:61:VAL:C	1:A:318:VAL:HG11	1.00	1.66
1:A:131:LEU:CD2	1:A:136:TYR:HE2	1.00	1.67
1:A:94:THR:CA	1:A:98:SER:HB3	0.99	1.86
1:A:131:LEU:HD23	1:A:136:TYR:HE2	0.99	1.12
1:A:72:LEU:CB	1:A:310:ASN:CB	0.99	2.40
1:A:182:GLY:HA2	1:A:187:CYS:CB	0.99	1.85
1:A:207:MET:CG	2:A:400:RET:C4	0.98	2.39
1:A:103:PHE:HA	1:A:104:VAL:HG23	0.98	1.31
1:A:247:GLU:O	1:A:250:VAL:HG23	0.98	1.55
1:A:135:ARG:HD2	1:A:257:MET:SD	0.97	1.99
1:A:179:ILE:CD1	1:A:191:TYR:CD2	0.97	2.46
1:A:334:SER:C	1:A:335:THR:HG23	0.96	1.80
1:A:207:MET:HB2	2:A:400:RET:H42	0.96	1.32
1:A:102:TYR:N	1:A:103:PHE:CB	0.96	2.27
1:A:97:THR:O	1:A:98:SER:HB2	0.96	1.60
1:A:103:PHE:HA	1:A:104:VAL:CG2	0.95	1.89
1:A:103:PHE:CE2	1:A:105:PHE:O	0.95	2.14
1:A:52:PHE:CG	1:A:56:PHE:CE1	0.95	2.51
1:A:72:LEU:HB3	1:A:310:ASN:HB3	0.94	1.37
1:A:135:ARG:O	1:A:136:TYR:CG	0.93	2.04
1:A:186:SER:O	1:A:187:CYS:SG	0.92	2.27
1:A:313:PHE:HE2	1:A:342:THR:HG23	0.92	1.23
1:A:313:PHE:HE2	1:A:342:THR:CG2	0.91	1.77
1:A:131:LEU:HG	1:A:136:TYR:CZ	0.90	2.01
1:A:135:ARG:O	1:A:136:TYR:CE2	0.90	2.23
1:A:241:ALA:O	1:A:242:THR:HG23	0.89	1.66
1:A:240:SER:OG	1:A:251:THR:HA	0.89	1.66
1:A:110:CYS:HG	1:A:187:CYS:CB	0.89	1.78
1:A:185:CYS:SG	1:A:189:ILE:O	0.89	2.30
1:A:103:PHE:HZ	1:A:105:PHE:O	0.89	1.46
1:A:94:THR:HA	1:A:98:SER:CB	0.88	1.96
1:A:241:ALA:C	1:A:242:THR:HG23	0.88	1.88
1:A:345:VAL:CG2	1:A:345:VAL:O	0.87	2.20
1:A:102:TYR:H	1:A:103:PHE:HB3	0.86	1.27
1:A:137:VAL:HG23	1:A:140:CYS:CB	0.86	2.00
1:A:337:VAL:HG12	1:A:338:SER:H	0.86	1.31
1:A:135:ARG:HG2	1:A:257:MET:HE1	0.85	1.47
1:A:195:HIS:CG	1:A:198:THR:OG1	0.85	2.29
1:A:182:GLY:CA	1:A:187:CYS:HB3	0.85	2.00

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:72:LEU:CD2	1:A:308:MET:O	0.84	2.24
1:A:317:MET:O	1:A:318:VAL:HG23	0.84	1.72
1:A:332:GLU:O	1:A:333:ALA:CB	0.84	2.26
1:A:61:VAL:O	1:A:318:VAL:CG1	0.84	2.26
1:A:103:PHE:CA	1:A:104:VAL:HG23	0.83	2.02
1:A:94:THR:CA	1:A:98:SER:CB	0.83	2.55
1:A:43:TYR:HH	1:A:296:LYS:HG2	0.83	1.31
1:A:132:ALA:HA	1:A:136:TYR:HD2	0.83	1.32
1:A:313:PHE:CE2	1:A:342:THR:HG23	0.83	2.08
1:A:97:THR:CG2	1:A:105:PHE:CD1	0.82	2.63
1:A:313:PHE:CE2	1:A:342:THR:CG2	0.82	2.62
1:A:43:TYR:CE2	1:A:296:LYS:HD3	0.82	2.08
1:A:102:TYR:CA	1:A:103:PHE:CB	0.82	2.58
1:A:207:MET:HB3	2:A:400:RET:H41	0.81	0.82
1:A:131:LEU:O	1:A:136:TYR:CG	0.81	2.33
1:A:110:CYS:HB3	1:A:187:CYS:SG	0.81	2.13
1:A:131:LEU:CG	1:A:136:TYR:CZ	0.80	2.64
1:A:131:LEU:CD2	1:A:136:TYR:CZ	0.80	2.64
1:A:72:LEU:CB	1:A:310:ASN:HB2	0.80	2.04
1:A:132:ALA:HA	1:A:136:TYR:CD2	0.79	2.12
1:A:317:MET:HG3	1:A:318:VAL:HG23	0.79	1.52
1:A:240:SER:HB2	1:A:250:VAL:C	0.79	1.96
1:A:182:GLY:CA	1:A:187:CYS:CB	0.79	2.59
1:A:104:VAL:O	1:A:105:PHE:HB3	0.78	1.77
1:A:131:LEU:CG	1:A:136:TYR:OH	0.78	2.32
1:A:137:VAL:HA	1:A:140:CYS:SG	0.77	2.19
1:A:191:TYR:O	1:A:191:TYR:HD2	0.77	1.62
1:A:241:ALA:O	1:A:242:THR:HG22	0.77	1.79
1:A:72:LEU:HB2	1:A:310:ASN:HB2	0.77	1.57
1:A:332:GLU:O	1:A:333:ALA:HB2	0.77	1.79
1:A:94:THR:N	1:A:98:SER:CB	0.76	2.42
1:A:265:TRP:CE3	2:A:400:RET:H181	0.76	2.16
1:A:72:LEU:CB	1:A:310:ASN:HB3	0.75	2.08
1:A:169:ALA:HB2	1:A:207:MET:SD	0.75	2.22
1:A:135:ARG:CD	1:A:257:MET:SD	0.75	2.75
1:A:207:MET:CB	2:A:400:RET:C3	0.75	2.57
1:A:336:THR:O	1:A:337:VAL:HB	0.74	1.81
1:A:265:TRP:CE3	2:A:400:RET:C19	0.73	2.70
1:A:131:LEU:HD21	1:A:136:TYR:OH	0.73	1.82
1:A:105:PHE:CE2	1:A:111:ASN:OD1	0.73	2.42
1:A:52:PHE:CD1	1:A:56:PHE:CE1	0.73	2.75
1:A:317:MET:O	1:A:318:VAL:CG2	0.73	2.37

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:207:MET:CG	2:A:400:RET:H41	0.73	2.07
1:A:337:VAL:HG12	1:A:338:SER:N	0.72	1.99
1:A:313:PHE:HZ	1:A:342:THR:HA	0.72	1.44
1:A:247:GLU:C	1:A:250:VAL:HG22	0.72	2.04
1:A:247:GLU:C	1:A:250:VAL:CG2	0.72	2.57
1:A:134:GLU:H	1:A:136:TYR:CB	0.72	1.97
1:A:105:PHE:HE2	1:A:111:ASN:OD1	0.71	1.68
1:A:135:ARG:CG	1:A:257:MET:HE1	0.71	2.16
1:A:43:TYR:HE2	1:A:296:LYS:HD2	0.71	1.40
1:A:131:LEU:CD2	1:A:136:TYR:OH	0.70	2.40
1:A:296:LYS:O	1:A:296:LYS:HG3	0.69	1.88
1:A:337:VAL:CG1	1:A:338:SER:H	0.68	1.97
1:A:317:MET:C	1:A:318:VAL:HG23	0.68	2.07
1:A:131:LEU:HD21	1:A:136:TYR:CE2	0.68	2.18
1:A:132:ALA:CA	1:A:136:TYR:CD2	0.67	2.77
1:A:113:GLU:O	1:A:117:ALA:HB3	0.66	1.90
1:A:131:LEU:O	1:A:136:TYR:CZ	0.66	2.48
1:A:43:TYR:CZ	1:A:296:LYS:HD3	0.66	2.20
1:A:265:TRP:CD2	2:A:400:RET:H181	0.65	2.26
1:A:102:TYR:CA	1:A:103:PHE:HB3	0.65	2.19
1:A:336:THR:O	1:A:337:VAL:CB	0.65	2.44
1:A:135:ARG:HG2	1:A:220:PHE:CE2	0.64	2.28
1:A:209:VAL:HG13	1:A:211:HIS:H	0.63	1.53
1:A:195:HIS:CB	1:A:198:THR:HG1	0.62	2.06
1:A:265:TRP:CE2	2:A:400:RET:C18	0.62	2.80
1:A:317:MET:O	1:A:318:VAL:CB	0.62	2.47
1:A:104:VAL:O	1:A:105:PHE:CB	0.62	2.47
1:A:97:THR:O	1:A:98:SER:CB	0.62	2.44
1:A:131:LEU:CG	1:A:136:TYR:CE2	0.61	2.83
1:A:179:ILE:CD1	1:A:191:TYR:CE2	0.61	2.73
1:A:191:TYR:CG	1:A:191:TYR:O	0.61	2.49
1:A:139:VAL:O	1:A:140:CYS:HB2	0.61	1.94
1:A:343:SER:OG	1:A:343:SER:O	0.61	2.09
1:A:240:SER:HB2	1:A:251:THR:N	0.61	2.10
1:A:313:PHE:CZ	1:A:342:THR:HA	0.61	2.28
1:A:179:ILE:HD11	1:A:191:TYR:CG	0.60	2.28
1:A:137:VAL:CG2	1:A:140:CYS:HB2	0.60	2.14
1:A:120:GLY:HA3	2:A:400:RET:C11	0.59	2.27
1:A:72:LEU:HB2	1:A:310:ASN:CB	0.59	2.20
1:A:190:ASP:O	1:A:191:TYR:CB	0.59	2.51
1:A:190:ASP:O	1:A:191:TYR:HB3	0.59	1.98
1:A:51:GLY:O	1:A:56:PHE:CG	0.59	2.54

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:247:GLU:CA	1:A:250:VAL:CG2	0.58	2.81
1:A:296:LYS:CG	1:A:296:LYS:O	0.58	2.52
1:A:313:PHE:CE2	1:A:342:THR:HG22	0.58	2.33
1:A:179:ILE:HG12	1:A:191:TYR:HB3	0.58	1.74
1:A:134:GLU:H	1:A:136:TYR:HB2	0.58	1.58
1:A:265:TRP:HE3	2:A:400:RET:H193	0.58	1.58
1:A:181:GLU:O	1:A:185:CYS:HB3	0.57	1.99
1:A:97:THR:HG22	1:A:105:PHE:CD1	0.57	2.33
1:A:265:TRP:CE3	2:A:400:RET:H193	0.57	2.33
1:A:131:LEU:HD21	1:A:136:TYR:CZ	0.57	2.28
1:A:135:ARG:CG	1:A:257:MET:SD	0.56	2.92
1:A:137:VAL:CA	1:A:140:CYS:SG	0.56	2.92
1:A:337:VAL:CG1	1:A:338:SER:N	0.56	2.64
1:A:240:SER:OG	1:A:251:THR:CA	0.56	2.50
1:A:134:GLU:N	1:A:136:TYR:HB2	0.56	2.16
1:A:344:GLN:C	1:A:345:VAL:HG22	0.56	2.20
1:A:337:VAL:HG12	1:A:338:SER:OG	0.55	2.00
1:A:239:GLU:O	1:A:240:SER:HB3	0.55	2.01
1:A:330:ASP:HB3	1:A:343:SER:HB3	0.55	1.79
1:A:131:LEU:C	1:A:136:TYR:CD2	0.54	2.80
1:A:165:LEU:C	1:A:167:CYS:H	0.54	2.06
1:A:131:LEU:CD1	1:A:136:TYR:OH	0.54	2.56
1:A:135:ARG:CG	1:A:257:MET:CE	0.54	2.86
1:A:265:TRP:CE3	2:A:400:RET:C18	0.53	2.87
1:A:131:LEU:C	1:A:136:TYR:CE2	0.53	2.80
1:A:61:VAL:O	1:A:318:VAL:HG21	0.53	2.03
1:A:131:LEU:HD11	1:A:136:TYR:OH	0.53	2.03
1:A:103:PHE:C	1:A:104:VAL:HG23	0.52	2.25
1:A:66:LYS:NZ	1:A:77:LEU:O	0.52	2.41
1:A:336:THR:C	1:A:337:VAL:HG23	0.52	2.24
1:A:66:LYS:NZ	1:A:80:ALA:O	0.51	2.42
1:A:207:MET:HB2	2:A:400:RET:C4	0.51	2.01
1:A:101:GLY:C	1:A:103:PHE:HB3	0.51	2.19
1:A:266:LEU:C	1:A:266:LEU:HD23	0.51	2.26
1:A:102:TYR:H	1:A:103:PHE:CB	0.50	2.06
1:A:265:TRP:CD2	2:A:400:RET:C18	0.50	2.95
1:A:72:LEU:HD11	1:A:250:VAL:CG1	0.50	2.37
1:A:179:ILE:HG12	1:A:191:TYR:CB	0.49	2.37
1:A:52:PHE:CG	1:A:56:PHE:CD1	0.49	2.85
1:A:317:MET:C	1:A:318:VAL:CG2	0.49	2.78
1:A:185:CYS:SG	1:A:189:ILE:C	0.49	2.90
1:A:167:CYS:O	1:A:171:PRO:CD	0.48	2.61

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:94:THR:N	1:A:98:SER:HB3	0.48	2.10
1:A:103:PHE:CA	1:A:104:VAL:CG2	0.48	2.63
1:A:315:ASN:O	1:A:316:CYS:CB	0.47	2.61
1:A:102:TYR:HB2	1:A:103:PHE:HB2	0.47	0.53
1:A:186:SER:O	1:A:187:CYS:CB	0.47	2.62
1:A:135:ARG:NH1	1:A:261:PHE:CE2	0.47	2.83
1:A:131:LEU:O	1:A:136:TYR:CD1	0.47	2.67
1:A:231:LYS:NZ	1:A:232:GLU:OE2	0.47	2.48
1:A:118:THR:HA	2:A:400:RET:H173	0.47	1.87
1:A:208:PHE:CB	1:A:269:ALA:HB3	0.46	2.40
1:A:134:GLU:O	1:A:136:TYR:CB	0.46	2.61
1:A:334:SER:C	1:A:335:THR:CG2	0.46	2.49
1:A:182:GLY:O	1:A:187:CYS:SG	0.46	2.73
1:A:149:GLY:O	1:A:151:ASN:ND2	0.45	2.49
1:A:141:LYS:CG	1:A:225:GLN:HB2	0.45	2.41
1:A:131:LEU:HG	1:A:136:TYR:OH	0.45	2.00
1:A:296:LYS:CB	1:A:296:LYS:NZ	0.44	2.80
1:A:72:LEU:CD1	1:A:250:VAL:HG11	0.44	2.43
1:A:317:MET:HG3	1:A:318:VAL:CG2	0.44	2.36
1:A:134:GLU:N	1:A:136:TYR:CG	0.44	2.86
1:A:134:GLU:O	1:A:136:TYR:HB2	0.44	2.12
1:A:55:ASN:O	1:A:59:LEU:N	0.43	2.51
1:A:135:ARG:HG3	1:A:257:MET:SD	0.43	2.52
1:A:179:ILE:CG1	1:A:191:TYR:CG	0.43	3.01
1:A:239:GLU:O	1:A:240:SER:CB	0.43	2.67
1:A:182:GLY:HA2	1:A:187:CYS:HB2	0.43	1.79
1:A:185:CYS:SG	1:A:185:CYS:O	0.43	2.77
1:A:207:MET:HG3	2:A:400:RET:H31	0.42	0.50
1:A:165:LEU:C	1:A:167:CYS:N	0.42	2.72
1:A:138:VAL:HG23	1:A:245:LYS:HE3	0.42	1.92
1:A:296:LYS:HB2	1:A:296:LYS:NZ	0.42	2.29
1:A:43:TYR:OH	1:A:296:LYS:CB	0.42	2.62
1:A:72:LEU:HD11	1:A:250:VAL:HG11	0.42	1.90
1:A:265:TRP:CE2	2:A:400:RET:H182	0.42	2.49
1:A:43:TYR:CZ	1:A:296:LYS:HD2	0.42	2.19
1:A:240:SER:CB	1:A:250:VAL:C	0.42	2.80
1:A:312:GLN:O	1:A:313:PHE:CB	0.42	2.67
1:A:330:ASP:N	1:A:342:THR:HG21	0.42	2.29
1:A:179:ILE:CD1	1:A:191:TYR:CG	0.42	3.00
1:A:72:LEU:HD23	1:A:308:MET:O	0.41	1.91
1:A:288:MET:O	1:A:289:THR:O	0.41	2.39
1:A:135:ARG:NE	1:A:261:PHE:CD2	0.41	2.89

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:181:GLU:O	1:A:185:CYS:CB	0.41	2.67
1:A:99:LEU:HG	1:A:288:MET:SD	0.41	2.56
1:A:79:LEU:O	1:A:81:VAL:N	0.41	2.54
1:A:121:GLY:O	1:A:122:GLU:C	0.41	2.59
1:A:167:CYS:O	1:A:171:PRO:HD2	0.41	2.16
1:A:135:ARG:HG2	1:A:257:MET:CE	0.41	2.33
1:A:135:ARG:CG	1:A:220:PHE:CE2	0.41	3.02
1:A:312:GLN:O	1:A:313:PHE:HB3	0.41	2.16
1:A:315:ASN:O	1:A:316:CYS:HB2	0.40	2.16
1:A:94:THR:CA	1:A:98:SER:OG	0.40	2.66
1:A:67:LYS:NZ	1:A:318:VAL:HG21	0.40	2.31
1:A:44:MET:SD	1:A:44:MET:C	0.40	3.00

## 6.3 Torsion angles ⓘ

### 6.3.1 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 NMR 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	309/348 (89%)	163 (53%)	80 (26%)	66 (21%)	0	2
All	All	309/348 (89%)	163 (53%)	80 (26%)	66 (21%)	0	2

All 66 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	103	PHE
1	A	122	GLU
1	A	150	GLU
1	A	309[A]	MET
1	A	316	CYS
1	A	107	PRO
1	A	308	MET
1	A	193	THR
1	A	289	THR
1	A	264	CYS
1	A	191	TYR

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Mol	Chain	Res	Type
1	A	278	HIS
1	A	50	LEU
1	A	335	THR
1	A	139	VAL
1	A	98	SER
1	A	135	ARG
1	A	159	PHE
1	A	313	PHE
1	A	134	GLU
1	A	319	THR
1	A	140	CYS
1	A	237	GLN
1	A	166	ALA
1	A	203	PHE
1	A	209	VAL
1	A	345	VAL
1	A	41	ALA
1	A	94	THR
1	A	242	THR
1	A	105	PHE
1	A	95	LEU
1	A	255	ILE
1	A	234	ALA
1	A	240	SER
1	A	171	PRO
1	A	110	CYS
1	A	309[B]	MET
1	A	323	CYS
1	A	279	GLN
1	A	337	VAL
1	A	282	ASP
1	A	115	PHE
1	A	66	LYS
1	A	230	VAL
1	A	167	CYS
1	A	64	GLN
1	A	99	LEU
1	A	222	CYS
1	A	318	VAL
1	A	201	GLU
1	A	324	GLY
1	A	247	GLU

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Mol	Chain	Res	Type
1	A	83	ASP
1	A	113	GLU
1	A	80	ALA
1	A	248	LYS
1	A	228	PHE
1	A	136	TYR
1	A	72	LEU
1	A	153	ALA
1	A	152	HIS
1	A	326	ASN
1	A	302	ASN
1	A	333	ALA
1	A	104	VAL

### 6.3.2 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 NMR 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	264/296 (89%)	218 (83%)	46 (17%)	6	41
All	All	264/296 (89%)	218 (83%)	46 (17%)	6	41

All 46 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	268	TYR
1	A	151	ASN
1	A	203	PHE
1	A	122	GLU
1	A	100	HIS
1	A	336	THR
1	A	223	TYR
1	A	179	ILE
1	A	309[B]	MET
1	A	239	GLU
1	A	178	TYR
1	A	99	LEU

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Mol	Chain	Res	Type
1	A	249	GLU
1	A	181	GLU
1	A	134	GLU
1	A	43	TYR
1	A	197	GLU
1	A	78	ASN
1	A	309[A]	MET
1	A	141	LYS
1	A	340[B]	THR
1	A	176	SER
1	A	111	ASN
1	A	58	THR
1	A	154	ILE
1	A	279	GLN
1	A	194	PRO
1	A	55	ASN
1	A	262	LEU
1	A	160	THR
1	A	69	ARG
1	A	296	LYS
1	A	186	SER
1	A	238	GLN
1	A	77	LEU
1	A	332	GLU
1	A	161	TRP
1	A	212	PHE
1	A	247	GLU
1	A	340[A]	THR
1	A	206	TYR
1	A	136	TYR
1	A	72	LEU
1	A	314	ARG
1	A	73	ASN
1	A	343	SER

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.5 Carbohydrates

There are no carbohydrates in this entry.

## 6.6 Ligand geometry

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds 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 is the number of standard deviations the observed value is removed from the expected value. A bond length with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	RET	A	400	-	19,20,21	2.15	0 (0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of 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 angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	RET	A	400	-	27,27,28	12.01	16 (59%)

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	400	-	-	0,13,30,31	0,1,1,1

There are no bond-length outliers.

All angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	RET	C11-C10-C9	28.30	168.36	127.22
2	A	400	RET	C7-C8-C9	27.78	168.18	126.21
2	A	400	RET	C8-C9-C10	23.96	157.58	118.95
2	A	400	RET	C19-C9-C10	15.62	100.17	122.89
2	A	400	RET	C8-C7-C6	14.59	169.61	127.24
2	A	400	RET	C11-C12-C13	14.36	168.44	126.34
2	A	400	RET	C10-C11-C12	13.70	165.40	123.11
2	A	400	RET	C12-C13-C14	12.08	159.47	118.92
2	A	400	RET	C7-C6-C5	11.58	148.23	121.36
2	A	400	RET	C1-C6-C5	9.89	109.26	122.50
2	A	400	RET	C19-C9-C8	9.70	102.23	118.08
2	A	400	RET	C4-C5-C6	9.64	133.33	122.73
2	A	400	RET	C20-C13-C12	9.08	103.25	118.08
2	A	400	RET	C20-C13-C14	8.99	97.29	123.71
2	A	400	RET	C18-C5-C6	7.20	116.95	124.62
2	A	400	RET	C15-C14-C13	6.96	164.29	128.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided