



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 02:14 PM UTC

PDB ID : 1LN6 / pdb_00001ln6
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

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<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

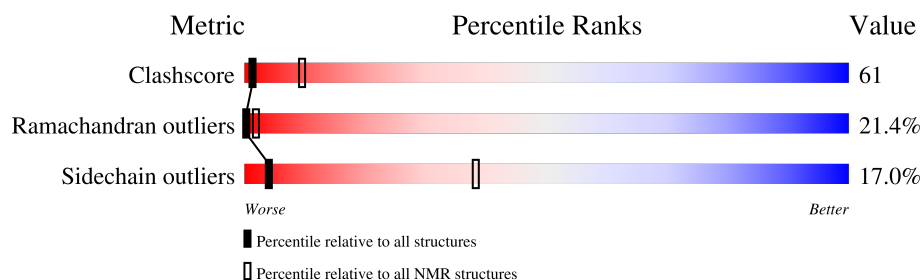
1 Overall quality at a glance

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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 ≥ 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	22% 35% 25% 7% 11%

2 Ensemble composition and analysis ⓘ

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

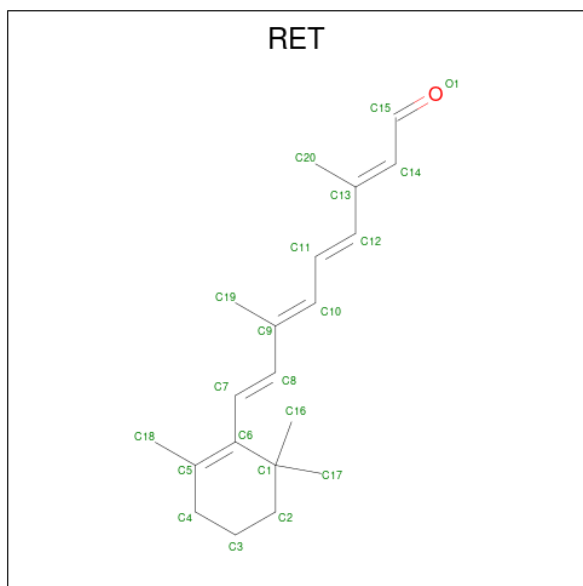
3 Entry composition [i](#)

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 (CCD ID: RET) (formula: $C_{20}H_{28}O$).

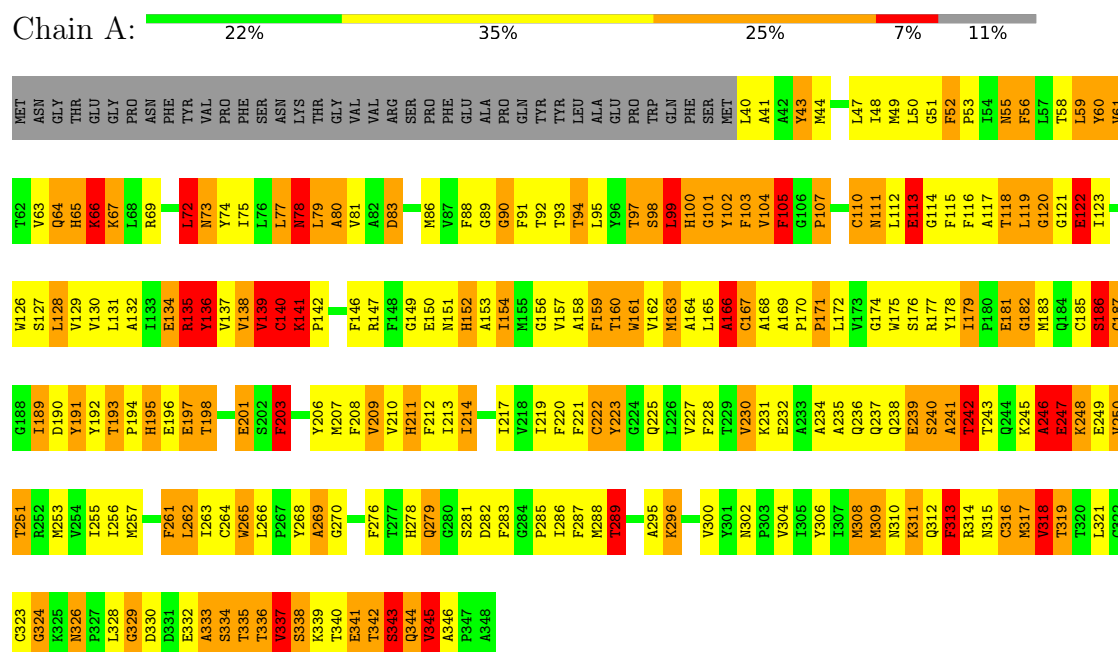


Mol	Chain	Residues	Atoms		
			Total	C	H
2	A	1	38	20	18

4 Residue-property plots

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: RHODOPSIN



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.

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	2.13	74/2511 (2.9%)	2.35	122/3421 (3.6%)
All	All	2.13	74/2511 (2.9%)	2.35	122/3421 (3.6%)

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	10.81	1.61	1.45
1	A	69	ARG	NE-CZ	9.16	1.43	1.33
1	A	67	LYS	C-N	8.77	1.45	1.33
1	A	227	VAL	CA-C	8.56	1.63	1.52
1	A	49	MET	CA-CB	8.08	1.63	1.52
1	A	90	GLY	CA-C	7.87	1.62	1.51
1	A	201	GLU	CA-C	7.81	1.63	1.52
1	A	172	LEU	N-CA	7.56	1.55	1.46
1	A	262	LEU	N-CA	7.56	1.55	1.46
1	A	192	TYR	CA-C	7.35	1.57	1.53
1	A	243	THR	C-N	7.32	1.44	1.33
1	A	100	HIS	CG-CD2	7.13	1.43	1.35
1	A	219	ILE	CA-C	-7.05	1.44	1.52
1	A	136	TYR	C-N	7.04	1.43	1.33
1	A	182	GLY	CA-C	6.94	1.61	1.51
1	A	329	GLY	CA-C	6.75	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	166	ALA	N-CA	6.75	1.54	1.46
1	A	300	VAL	N-CA	-6.65	1.38	1.46
1	A	53	PRO	C-N	6.62	1.42	1.33
1	A	198	THR	CA-C	6.58	1.61	1.52
1	A	63	VAL	N-CA	6.54	1.54	1.46
1	A	217	ILE	CA-C	6.51	1.60	1.52
1	A	174	GLY	CA-C	6.50	1.60	1.51
1	A	211	HIS	CG-CD2	6.38	1.42	1.35
1	A	83	ASP	C-N	6.36	1.41	1.33
1	A	270	GLY	CA-C	6.30	1.60	1.51
1	A	193	THR	CB-OG1	-6.25	1.33	1.43
1	A	186	SER	CA-C	6.20	1.61	1.52
1	A	100	HIS	CG-ND1	-6.17	1.31	1.38
1	A	142	PRO	CA-C	6.11	1.59	1.52
1	A	100	HIS	CA-C	6.11	1.59	1.52
1	A	269	ALA	N-CA	6.08	1.53	1.46
1	A	47	LEU	CA-C	6.06	1.60	1.52
1	A	212	PHE	CA-C	6.05	1.60	1.52
1	A	162	VAL	CA-C	6.03	1.60	1.52
1	A	195	HIS	CE1-NE2	5.93	1.38	1.32
1	A	338	SER	C-N	5.93	1.42	1.33
1	A	152	HIS	CG-CD2	5.88	1.42	1.35
1	A	328	LEU	CA-C	5.81	1.59	1.52
1	A	138	VAL	CA-C	5.75	1.60	1.52
1	A	152	HIS	CD2-NE2	-5.74	1.31	1.37
1	A	156	GLY	CA-C	5.59	1.62	1.52
1	A	61	VAL	CA-C	5.58	1.59	1.52
1	A	243	THR	CA-C	5.58	1.59	1.52
1	A	227	VAL	C-N	5.57	1.41	1.33
1	A	313	PHE	CA-C	5.53	1.60	1.52
1	A	140	CYS	CA-C	5.52	1.60	1.52
1	A	154	ILE	CA-CB	5.49	1.60	1.54
1	A	66	LYS	N-CA	-5.44	1.39	1.46
1	A	69	ARG	CA-C	5.44	1.60	1.52
1	A	161	TRP	N-CA	5.42	1.53	1.46
1	A	74	TYR	CA-C	5.41	1.60	1.52
1	A	300	VAL	C-N	5.38	1.40	1.33
1	A	67	LYS	CA-CB	5.38	1.62	1.53
1	A	128	LEU	N-CA	5.38	1.53	1.46
1	A	183	MET	CA-C	5.36	1.59	1.52
1	A	343	SER	N-CA	-5.33	1.40	1.46
1	A	114	GLY	CA-C	5.31	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	113	GLU	C-O	-5.30	1.17	1.24
1	A	341	GLU	C-N	5.25	1.40	1.33
1	A	321	LEU	N-CA	5.21	1.52	1.45
1	A	119	LEU	N-CA	-5.19	1.40	1.46
1	A	69	ARG	CZ-NH2	-5.17	1.26	1.33
1	A	214	ILE	C-N	5.17	1.38	1.33
1	A	246	ALA	CA-C	5.15	1.59	1.52
1	A	56	PHE	CA-C	5.11	1.59	1.52
1	A	276	PHE	CA-C	5.10	1.59	1.52
1	A	222	CYS	N-CA	-5.08	1.39	1.46
1	A	242	THR	CA-C	5.05	1.59	1.52
1	A	287	PHE	CA-C	5.04	1.58	1.53
1	A	135	ARG	CA-CB	5.04	1.61	1.53
1	A	175	TRP	CZ2-CH2	5.01	1.46	1.37
1	A	158	ALA	N-CA	-5.01	1.40	1.46
1	A	289	THR	CA-C	5.01	1.59	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	ASN	CA-CB-CG	10.98	123.58	112.60
1	A	193	THR	CB-CA-C	10.27	130.40	110.17
1	A	59	LEU	N-CA-C	-9.79	100.61	111.28
1	A	192	TYR	O-C-N	9.10	128.30	121.47
1	A	295	ALA	CA-C-N	-8.69	108.73	122.73
1	A	295	ALA	C-N-CA	-8.69	108.73	122.73
1	A	261	PHE	CA-CB-CG	8.66	122.46	113.80
1	A	211	HIS	ND1-CE1-NE2	8.54	116.94	108.40
1	A	279	GLN	OE1-CD-NE2	-8.43	114.17	122.60
1	A	170	PRO	CB-CA-C	8.23	120.96	110.92
1	A	146	PHE	O-C-N	8.13	130.73	122.12
1	A	78	ASN	OD1-CG-ND2	-7.83	114.77	122.60
1	A	116	PHE	CA-CB-CG	-7.77	106.03	113.80
1	A	295	ALA	N-CA-C	-7.66	102.94	111.82
1	A	219	ILE	CA-C-O	-7.59	112.29	121.54
1	A	183	MET	CA-C-N	-7.57	108.81	120.31
1	A	183	MET	C-N-CA	-7.57	108.81	120.31
1	A	265	TRP	CB-CA-C	7.57	122.76	110.88
1	A	130	VAL	CA-C-N	7.56	134.11	122.24
1	A	130	VAL	C-N-CA	7.56	134.11	122.24
1	A	317	MET	N-CA-CB	-7.51	97.65	109.51
1	A	250	VAL	CA-C-N	-7.34	109.86	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	VAL	C-N-CA	-7.34	109.86	120.29
1	A	219	ILE	CA-C-N	7.23	134.72	121.70
1	A	219	ILE	C-N-CA	7.23	134.72	121.70
1	A	338	SER	N-CA-CB	-7.12	100.19	110.45
1	A	241	ALA	N-CA-CB	-7.10	99.28	110.22
1	A	174	GLY	O-C-N	7.09	130.01	122.28
1	A	345	VAL	CB-CA-C	-7.05	99.73	111.29
1	A	217	ILE	CB-CA-C	6.96	121.13	112.02
1	A	56	PHE	N-CA-CB	-6.95	98.75	110.49
1	A	118	THR	CA-CB-OG1	6.86	119.89	109.60
1	A	129	VAL	N-CA-C	-6.83	102.51	111.05
1	A	146	PHE	CA-C-O	-6.74	113.41	120.55
1	A	69	ARG	CA-CB-CG	6.68	127.46	114.10
1	A	235	ALA	CA-C-N	6.67	134.28	121.54
1	A	235	ALA	C-N-CA	6.67	134.28	121.54
1	A	197	GLU	O-C-N	6.64	129.95	122.11
1	A	214	ILE	CA-CB-CG1	6.64	121.68	110.40
1	A	221	PHE	O-C-N	6.63	129.15	122.12
1	A	203	PHE	CA-CB-CG	6.61	120.41	113.80
1	A	287	PHE	CA-CB-CG	6.59	120.39	113.80
1	A	72	LEU	O-C-N	6.58	131.34	122.59
1	A	53	PRO	N-CA-CB	-6.53	95.42	102.60
1	A	189	ILE	CA-C-N	6.51	133.41	121.70
1	A	189	ILE	C-N-CA	6.51	133.41	121.70
1	A	93	THR	CA-CB-OG1	6.48	119.32	109.60
1	A	128	LEU	N-CA-C	6.47	120.89	113.19
1	A	243	THR	CA-C-O	6.42	128.87	120.21
1	A	136	TYR	N-CA-CB	-6.41	99.65	110.49
1	A	112	LEU	O-C-N	6.30	128.84	122.03
1	A	112	LEU	N-CA-C	-6.30	104.03	111.03
1	A	281	SER	N-CA-CB	-6.27	99.89	109.92
1	A	175	TRP	N-CA-C	-6.26	104.51	111.71
1	A	91	PHE	CA-C-N	6.18	129.41	120.38
1	A	91	PHE	C-N-CA	6.18	129.41	120.38
1	A	256	ILE	O-C-N	6.16	128.12	121.90
1	A	283	PHE	N-CA-CB	6.08	119.48	110.49
1	A	263	ILE	CA-C-N	6.07	133.13	121.54
1	A	263	ILE	C-N-CA	6.07	133.13	121.54
1	A	139	VAL	N-CA-C	-6.04	96.78	109.34
1	A	127	SER	N-CA-CB	-6.01	100.33	110.49
1	A	102	TYR	CA-C-N	5.97	132.45	121.70
1	A	102	TYR	C-N-CA	5.97	132.45	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	265	TRP	CD2-CE3-CZ3	5.83	126.17	118.60
1	A	65	HIS	ND1-CE1-NE2	5.82	114.22	108.40
1	A	211	HIS	ND1-CG-CD2	5.77	111.87	106.10
1	A	120	GLY	CA-C-N	5.72	132.61	121.41
1	A	120	GLY	C-N-CA	5.72	132.61	121.41
1	A	72	LEU	N-CA-CB	-5.71	100.83	110.49
1	A	337	VAL	N-CA-CB	-5.70	101.83	111.23
1	A	101	GLY	CA-C-N	5.69	131.94	121.70
1	A	101	GLY	C-N-CA	5.69	131.94	121.70
1	A	230	VAL	CA-CB-CG2	5.67	120.05	110.40
1	A	210	VAL	N-CA-CB	-5.62	104.07	112.67
1	A	48	ILE	N-CA-CB	-5.61	105.83	112.39
1	A	163	MET	CB-CA-C	5.60	120.09	110.79
1	A	279	GLN	O-C-N	5.58	130.01	122.59
1	A	344	GLN	N-CA-C	-5.57	100.97	109.65
1	A	49	MET	N-CA-CB	5.56	119.00	110.60
1	A	123	ILE	N-CA-C	5.56	118.00	111.05
1	A	247	GLU	CB-CA-C	5.50	121.37	110.42
1	A	157	VAL	O-C-N	5.50	127.49	121.83
1	A	236	GLN	CB-CG-CD	5.49	121.94	112.60
1	A	100	HIS	N-CA-C	-5.48	100.74	109.23
1	A	40	LEU	O-C-N	5.47	131.75	123.00
1	A	213	ILE	CA-C-O	5.42	124.95	119.20
1	A	313	PHE	CB-CA-C	5.40	121.16	110.42
1	A	86	MET	CA-C-O	5.37	126.25	120.55
1	A	159	PHE	CA-C-N	5.30	127.82	120.29
1	A	159	PHE	C-N-CA	5.30	127.82	120.29
1	A	88	PHE	CA-CB-CG	5.28	119.08	113.80
1	A	334	SER	O-C-N	5.28	127.98	121.33
1	A	304	VAL	O-C-N	5.27	129.16	122.57
1	A	141	LYS	N-CA-CB	5.26	119.74	110.37
1	A	213	ILE	N-CA-C	-5.24	106.77	113.22
1	A	160	THR	OG1-CB-CG2	-5.23	98.83	109.30
1	A	196	GLU	CA-C-O	5.23	125.81	119.49
1	A	263	ILE	N-CA-C	-5.22	100.93	108.71
1	A	72	LEU	CB-CA-C	-5.19	100.09	110.42
1	A	177	ARG	NH1-CZ-NH2	-5.17	112.58	119.30
1	A	172	LEU	CA-C-O	5.15	125.88	120.42
1	A	43	TYR	CB-CG-CD2	-5.14	113.08	120.80
1	A	105	PHE	N-CA-C	-5.14	99.86	110.80
1	A	83	ASP	CA-C-N	5.13	127.47	120.54
1	A	83	ASP	C-N-CA	5.13	127.47	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	318	VAL	CA-C-N	5.13	131.34	121.54
1	A	318	VAL	C-N-CA	5.13	131.34	121.54
1	A	97	THR	CB-CA-C	5.13	118.14	111.42
1	A	178	TYR	CA-C-N	5.13	130.93	121.70
1	A	178	TYR	C-N-CA	5.13	130.93	121.70
1	A	60	TYR	O-C-N	5.12	127.98	122.15
1	A	92	THR	CA-CB-OG1	-5.11	101.94	109.60
1	A	342	THR	CA-C-N	5.08	129.72	122.21
1	A	342	THR	C-N-CA	5.08	129.72	122.21
1	A	219	ILE	N-CA-C	-5.04	102.59	109.55
1	A	195	HIS	ND1-CE1-NE2	5.04	113.44	108.40
1	A	319	THR	CA-CB-CG2	5.04	119.07	110.50
1	A	164	ALA	O-C-N	5.04	129.08	122.68
1	A	326	ASN	OD1-CG-ND2	5.03	127.63	122.60
1	A	141	LYS	CA-CB-CG	5.03	124.16	114.10
1	A	223	TYR	N-CA-C	-5.01	107.17	113.28

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	52	PHE	Sidechain
1	A	60	TYR	Sidechain
1	A	78	ASN	Peptide
1	A	107	PRO	Peptide
1	A	135	ARG	Sidechain,Peptide
1	A	147	ARG	Peptide
1	A	163	MET	Peptide
1	A	187	CYS	Peptide
1	A	203	PHE	Peptide
1	A	246	ALA	Peptide
1	A	253	MET	Peptide
1	A	285	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	A	306	TYR	Sidechain
1	A	311	LYS	Peptide
1	A	313	PHE	Peptide
1	A	329	GLY	Peptide
1	A	341	GLU	Peptide
1	A	346	ALA	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	294
2	A	20	18	15	25
All	All	2446	1796	2412	294

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 61.

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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
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:HG23	1:A:345:VAL:O	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:43:TYR:CZ	1:A:296:LYS:CG	1.06	2.37
1:A:94:THR:HA	1:A:98:SER:HB3	1.06	1.26
1:A:61:VAL:C	1:A:318:VAL:HG11	1.05	1.66
1:A:207:MET:CB	2:A:400:RET:H42	1.05	1.61
1:A:72:LEU:HB3	1:A:310:ASN:CB	1.04	1.81
1:A:102:TYR:CB	1:A:103:PHE:CB	1.04	2.13
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
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:334:SER:C	1:A:335:THR:HG23	1.01	1.80
1:A:52:PHE:CD1	1:A:56:PHE:CD1	1.00	2.48
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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
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: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:241:ALA:C	1:A:242:THR:HG23	0.92	1.88
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:345:VAL:O	1:A:345:VAL:CG2	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: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
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:240:SER:HB2	1:A:250:VAL:C	0.84	1.96
1:A:94:THR:CA	1:A:98:SER:CB	0.83	2.55
1:A:103:PHE:CA	1:A:104:VAL:HG23	0.83	2.02
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:135:ARG:HG2	1:A:257:MET:HE1	0.82	1.49
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:110:CYS:HB3	1:A:187:CYS:SG	0.81	2.13
1:A:131:LEU:O	1:A:136:TYR:CG	0.81	2.33
1:A:207:MET:HB3	2:A:400:RET:H41	0.81	0.82
1:A:131:LEU:CG	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:131:LEU:CD2	1:A:136:TYR:CZ	0.80	2.64

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:103:PHE:CE2	1:A:105:PHE:O	0.80	2.14
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: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:247:GLU:C	1:A:250:VAL:HG22	0.77	2.04
1:A:247:GLU:C	1:A:250:VAL:CG2	0.77	2.57
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:43:TYR:HH	1:A:296:LYS:HG2	0.76	0.94
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:52:PHE:CD1	1:A:56:PHE:CE1	0.73	2.75
1:A:105:PHE:CE2	1:A:111:ASN:OD1	0.73	2.42
1:A:317:MET:O	1:A:318:VAL:CG2	0.73	2.37
1:A:207:MET:CG	2:A:400:RET:H41	0.73	2.07
1:A:317:MET:C	1:A:318:VAL:HG23	0.72	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: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:43:TYR:HE2	1:A:296:LYS:HD2	0.71	1.40
1:A:135:ARG:CG	1:A:257:MET:HE1	0.70	2.16
1:A:131:LEU:CD2	1:A:136:TYR:OH	0.70	2.40
1:A:135:ARG:O	1:A:136:TYR:CG	0.70	2.04
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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:43:TYR:CZ	1:A:296:LYS:HD3	0.66	2.20
1:A:102:TYR:CA	1:A:103:PHE:HB3	0.65	2.19
1:A:265:TRP:CD2	2:A:400:RET:H181	0.65	2.26
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:101:GLY:C	1:A:103:PHE:HB3	0.63	2.19
1:A:209:VAL:HG13	1:A:211:HIS:H	0.63	1.53
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:139:VAL:O	1:A:140:CYS:HB2	0.61	1.94
1:A:179:ILE:CD1	1:A:191:TYR:CE2	0.61	2.73
1:A:191:TYR:O	1:A:191:TYR:CG	0.61	2.49
1:A:343:SER:O	1:A:343:SER:OG	0.61	2.09
1:A:195:HIS:CB	1:A:198:THR:HG1	0.61	2.08
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:344:GLN:C	1:A:345:VAL:HG22	0.60	2.20
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:43:TYR:HH	1:A:296:LYS:CG	0.59	1.86
1:A:72:LEU:HB2	1:A:310:ASN:CB	0.59	2.20
1:A:120:GLY:HA3	2:A:400:RET:C11	0.59	2.27
1:A:165:LEU:C	1:A:167:CYS:H	0.59	2.06
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
1:A:131:LEU:C	1:A:136:TYR:CD2	0.59	2.80
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:131:LEU:C	1:A:136:TYR:CE2	0.58	2.80
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:131:LEU:HD21	1:A:136:TYR:CZ	0.57	2.28
1:A:265:TRP:CE3	2:A:400:RET:H193	0.57	2.33
1:A:103:PHE:C	1:A:104:VAL:HG23	0.57	2.25

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:135:ARG:CG	1:A:257:MET:SD	0.56	2.92
1:A:336:THR:C	1:A:337:VAL:HG23	0.56	2.24
1:A:61:VAL:C	1:A:318:VAL:CG1	0.56	2.60
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:266:LEU:HD23	1:A:266:LEU:C	0.56	2.26
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: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:185:CYS:SG	1:A:189:ILE:C	0.53	2.90
1:A:265:TRP:CE3	2:A:400:RET:C18	0.53	2.87
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:66:LYS:NZ	1:A:77:LEU:O	0.52	2.41
1:A:317:MET:C	1:A:318:VAL:CG2	0.52	2.78
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:334:SER:C	1:A:335:THR:CG2	0.51	2.49
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:240:SER:CB	1:A:250:VAL:C	0.49	2.80
1:A:167:CYS:O	1:A:171:PRO:CD	0.48	2.61
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:165:LEU:C	1:A:167:CYS:N	0.47	2.72
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:182:GLY:O	1:A:187:CYS:SG	0.46	2.73

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:121:GLY:O	1:A:122:GLU:C	0.46	2.59
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:134:GLU:C	1:A:134:GLU:CD	0.45	2.84
1:A:44:MET:C	1:A:44:MET:SD	0.45	3.00
1:A:131:LEU:HG	1:A:136:TYR:OH	0.45	2.00
1:A:72:LEU:CD1	1:A:250:VAL:HG11	0.44	2.43
1:A:296:LYS:NZ	1:A:296:LYS:CB	0.44	2.80
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:55:ASN:O	1:A:56:PHE:C	0.44	2.60
1:A:89:GLY:O	1:A:90:GLY:C	0.44	2.60
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:344:GLN:C	1:A:345:VAL:CG2	0.43	2.91
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:138:VAL:HG23	1:A:245:LYS:HE3	0.42	1.92
1:A:43:TYR:OH	1:A:296:LYS:CB	0.42	2.62
1:A:296:LYS:NZ	1:A:296:LYS:HB2	0.42	2.29
1:A:64:GLN:O	1:A:65:HIS:C	0.42	2.63
1:A:72:LEU:HD11	1:A:250:VAL:HG11	0.42	1.90
1:A:126:TRP:C	1:A:128:LEU:H	0.42	2.23
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:126:TRP:C	1:A:128:LEU:N	0.42	2.78
1:A:134:GLU:O	1:A:136:TYR:HB2	0.42	2.12
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:168:ALA:HB3	1:A:207:MET:HE1	0.42	1.92
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:166:ALA:C	1:A:168:ALA:H	0.41	2.23
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
1:A:79:LEU:O	1:A:81:VAL:N	0.41	2.54
1:A:99:LEU:HG	1:A:288:MET:SD	0.41	2.56
1:A:181:GLU:O	1:A:185:CYS:CB	0.41	2.67
1:A:166:ALA:C	1:A:168:ALA:N	0.41	2.79

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
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

6.3 Torsion angles [i](#)

6.3.1 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 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	41	ALA
1	A	50	LEU
1	A	64	GLN
1	A	66	LYS
1	A	72	LEU
1	A	80	ALA
1	A	83	ASP
1	A	94	THR
1	A	95	LEU
1	A	98	SER
1	A	99	LEU
1	A	103	PHE
1	A	104	VAL
1	A	105	PHE
1	A	107	PRO
1	A	110	CYS

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Mol	Chain	Res	Type
1	A	113	GLU
1	A	115	PHE
1	A	122	GLU
1	A	134	GLU
1	A	135	ARG
1	A	136	TYR
1	A	139	VAL
1	A	140	CYS
1	A	150	GLU
1	A	152	HIS
1	A	153	ALA
1	A	159	PHE
1	A	166	ALA
1	A	167	CYS
1	A	171	PRO
1	A	191	TYR
1	A	193	THR
1	A	201	GLU
1	A	203	PHE
1	A	209	VAL
1	A	222	CYS
1	A	228	PHE
1	A	230	VAL
1	A	234	ALA
1	A	237	GLN
1	A	240	SER
1	A	242	THR
1	A	247	GLU
1	A	248	LYS
1	A	255	ILE
1	A	264	CYS
1	A	278	HIS
1	A	279	GLN
1	A	282	ASP
1	A	289	THR
1	A	302	ASN
1	A	308	MET
1	A	309[A]	MET
1	A	309[B]	MET
1	A	313	PHE
1	A	316	CYS
1	A	318	VAL

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Mol	Chain	Res	Type
1	A	319	THR
1	A	323	CYS
1	A	324	GLY
1	A	326	ASN
1	A	333	ALA
1	A	335	THR
1	A	337	VAL
1	A	345	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%)	219 (83%)	45 (17%)	4	38
All	All	264/296 (89%)	219 (83%)	45 (17%)	4	38

All 45 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	55	ASN
1	A	58	THR
1	A	72	LEU
1	A	73	ASN
1	A	75	ILE
1	A	77	LEU
1	A	78	ASN
1	A	79	LEU
1	A	99	LEU
1	A	100	HIS
1	A	111	ASN
1	A	119	LEU
1	A	122	GLU
1	A	136	TYR
1	A	141	LYS
1	A	154	ILE
1	A	160	THR

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Mol	Chain	Res	Type
1	A	161	TRP
1	A	176	SER
1	A	179	ILE
1	A	181	GLU
1	A	186	SER
1	A	194	PRO
1	A	197	GLU
1	A	206	TYR
1	A	214	ILE
1	A	223	TYR
1	A	238	GLN
1	A	239	GLU
1	A	247	GLU
1	A	248	LYS
1	A	249	GLU
1	A	251	THR
1	A	262	LEU
1	A	268	TYR
1	A	286	ILE
1	A	296	LYS
1	A	309[A]	MET
1	A	309[B]	MET
1	A	314	ARG
1	A	336	THR
1	A	339	LYS
1	A	340[A]	THR
1	A	340[B]	THR
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 oligosaccharides 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	-	20,20,21	2.19	5 (25%)

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	12.39	21 (77%)

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	RET	C12-C13	5.07	1.35	1.46
2	A	400	RET	C8-C9	5.06	1.35	1.46
2	A	400	RET	C15-C14	3.95	1.34	1.49
2	A	400	RET	C7-C6	2.75	1.35	1.45
2	A	400	RET	C11-C10	2.71	1.34	1.43

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

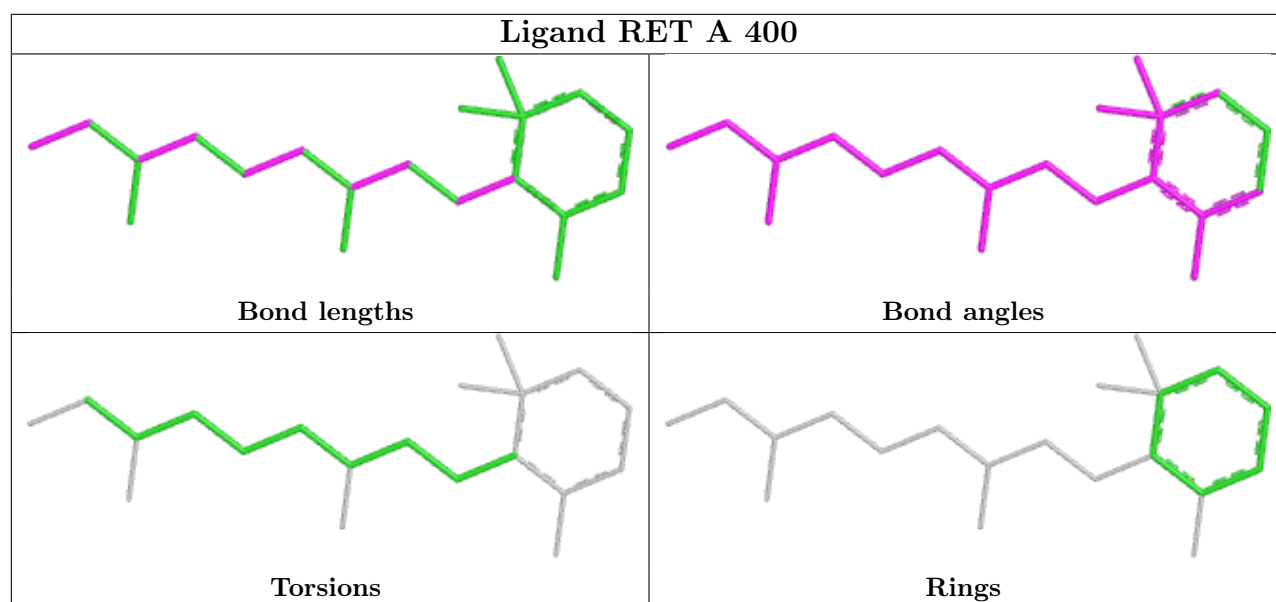
Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	RET	C11-C10-C9	29.30	168.36	127.28
2	A	400	RET	C7-C8-C9	28.36	168.18	126.23
2	A	400	RET	C8-C9-C10	24.52	157.58	119.01
2	A	400	RET	C8-C7-C6	15.95	169.61	127.00
2	A	400	RET	C12-C13-C14	15.39	159.47	118.55
2	A	400	RET	C11-C12-C13	15.35	168.44	126.36
2	A	400	RET	C10-C11-C12	14.56	165.40	123.20
2	A	400	RET	C19-C9-C10	13.98	100.17	122.82
2	A	400	RET	C7-C6-C5	11.58	148.23	121.56
2	A	400	RET	C19-C9-C8	10.38	102.23	118.09
2	A	400	RET	C1-C6-C5	9.79	109.26	122.64
2	A	400	RET	C20-C13-C12	9.72	103.25	118.09
2	A	400	RET	C20-C13-C14	9.55	97.29	123.63
2	A	400	RET	C4-C5-C6	7.86	133.33	122.70
2	A	400	RET	C18-C5-C6	6.90	116.95	124.48
2	A	400	RET	C15-C14-C13	6.82	164.29	127.72
2	A	400	RET	C1-C6-C7	4.95	102.24	115.65
2	A	400	RET	C17-C1-C6	3.77	116.16	110.24
2	A	400	RET	C2-C1-C6	3.56	115.61	110.44
2	A	400	RET	C16-C1-C6	2.17	106.85	110.24
2	A	400	RET	C18-C5-C4	2.03	109.27	113.60

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 than 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.



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