



Full wwPDB NMR Structure Validation Report ⓘ

Mar 10, 2026 – 09:46 AM UTC

PDB ID : 1JFP / pdb_00001jfp
Title : Structure of bovine rhodopsin (dark adapted)
Authors : Yeagle, P.L.; Choi, G.; Albert, A.D.
Deposited on : 2001-06-21

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<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

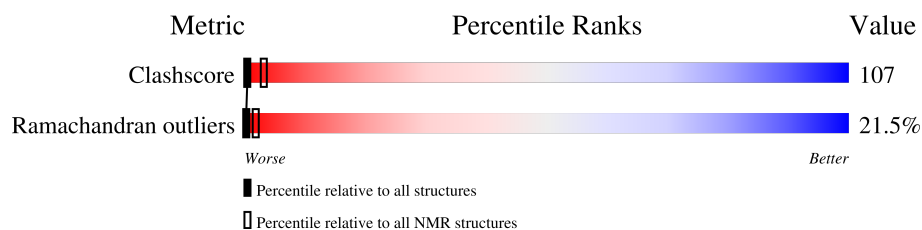
1 Overall quality at a glance

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

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	

2 Ensemble composition and analysis ⓘ

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

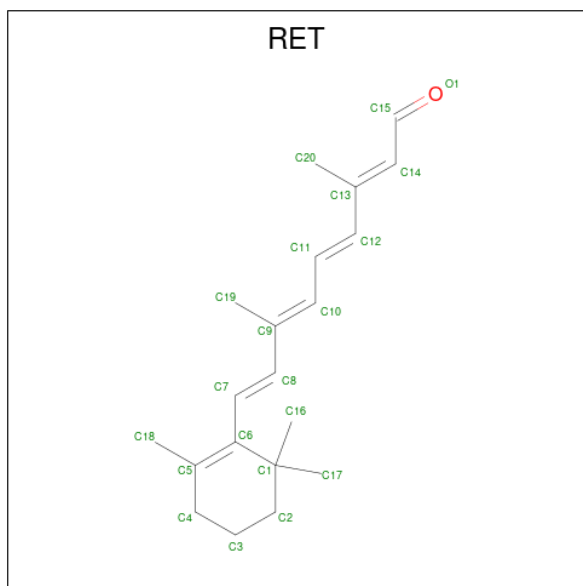
3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 4890 atoms, of which 2444 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	4842	1607	2416	375	420	24	0

- Molecule 2 is RETINAL (CCD ID: RET) (formula: $C_{20}H_{28}O$).

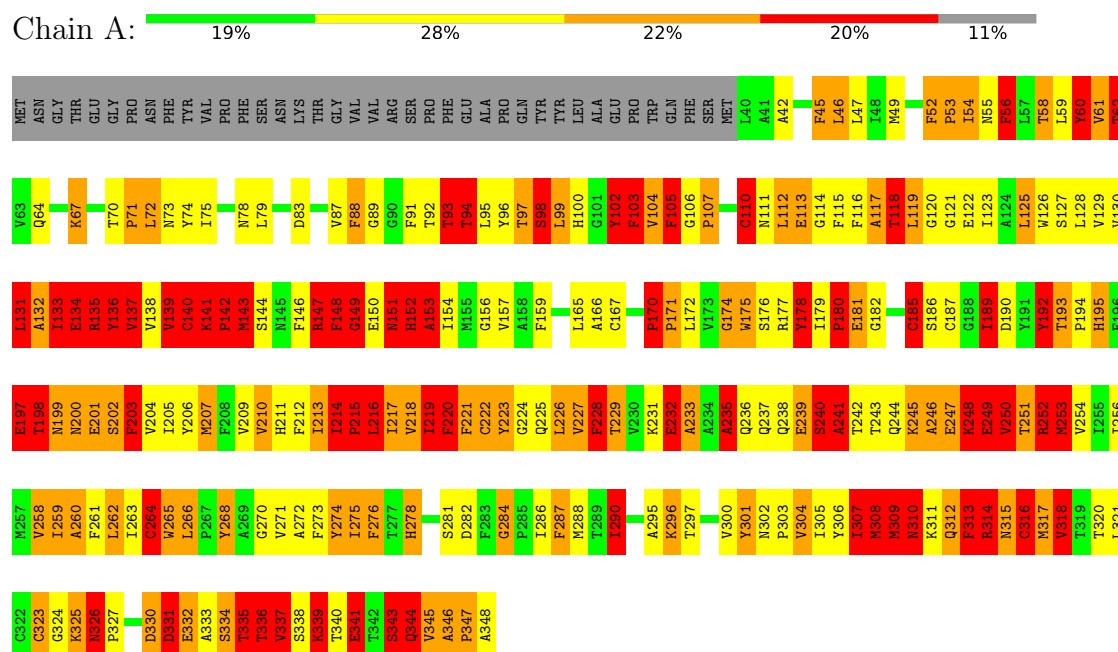


Mol	Chain	Residues	Atoms		
			Total	C	H
2	A	1	48	20	28

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: ?.

Of the 3 calculated structures, 1 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
SYBYL	refinement	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	2.00	55/2496 (2.2%)	2.71	220/3401 (6.5%)
All	All	2.00	55/2496 (2.2%)	2.71	220/3401 (6.5%)

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	117
All	All	6	117

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	296	LYS	C-N	27.92	1.68	1.33
1	A	310	ASN	N-CA	15.45	1.66	1.46
1	A	246	ALA	CA-C	12.88	1.66	1.53
1	A	253	MET	CA-CB	11.96	1.73	1.53
1	A	339	LYS	N-CA	10.32	1.59	1.46
1	A	331	ASP	N-CA	10.15	1.60	1.46
1	A	313	PHE	CA-CB	9.74	1.78	1.54
1	A	307	ILE	N-CA	9.37	1.64	1.46
1	A	344	GLN	N-CA	9.32	1.59	1.46
1	A	314	ARG	N-CA	8.95	1.57	1.46
1	A	345	VAL	CA-CB	8.62	1.66	1.54
1	A	113	GLU	C-N	8.10	1.44	1.34
1	A	205	ILE	CA-C	7.97	1.62	1.52
1	A	213	ILE	C-N	7.86	1.42	1.33
1	A	274	TYR	C-N	7.80	1.41	1.33
1	A	210	VAL	CA-C	7.73	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	332	GLU	C-N	7.65	1.40	1.33
1	A	217	ILE	CA-C	7.65	1.63	1.52
1	A	341	GLU	N-CA	7.55	1.55	1.46
1	A	330	ASP	C-N	7.52	1.39	1.33
1	A	248	LYS	N-CA	7.27	1.55	1.46
1	A	311	LYS	N-CA	7.00	1.55	1.45
1	A	135	ARG	CA-C	6.71	1.61	1.52
1	A	340	THR	N-CA	6.61	1.54	1.46
1	A	140	CYS	CA-C	6.59	1.61	1.52
1	A	314	ARG	CA-CB	6.55	1.64	1.53
1	A	330	ASP	CA-CB	6.33	1.64	1.53
1	A	330	ASP	N-CA	6.25	1.54	1.46
1	A	135	ARG	C-N	6.23	1.42	1.33
1	A	259	ILE	CA-C	6.18	1.60	1.52
1	A	309	MET	C-N	6.16	1.42	1.33
1	A	178	TYR	C-N	5.90	1.40	1.33
1	A	215	PRO	N-CA	-5.89	1.39	1.47
1	A	207	MET	C-N	5.77	1.41	1.33
1	A	210	VAL	C-N	5.71	1.41	1.33
1	A	304	VAL	C-N	5.60	1.39	1.33
1	A	137	VAL	C-N	5.54	1.40	1.33
1	A	334	SER	CA-C	5.51	1.60	1.52
1	A	214	ILE	N-CA	-5.46	1.39	1.46
1	A	309	MET	CA-CB	5.42	1.62	1.53
1	A	336	THR	N-CA	5.41	1.53	1.46
1	A	241	ALA	C-N	5.37	1.41	1.33
1	A	228	PHE	C-N	5.33	1.41	1.33
1	A	303	PRO	N-CA	-5.31	1.41	1.47
1	A	218	VAL	CA-C	5.30	1.59	1.52
1	A	309	MET	N-CA	5.23	1.52	1.46
1	A	344	GLN	CA-CB	5.16	1.61	1.53
1	A	229	THR	C-N	5.12	1.39	1.34
1	A	140	CYS	C-N	5.07	1.40	1.33
1	A	317	MET	N-CA	5.06	1.52	1.46
1	A	222	CYS	C-N	5.03	1.40	1.33
1	A	59	LEU	C-N	5.02	1.40	1.33
1	A	126	TRP	C-N	5.01	1.40	1.33
1	A	94	THR	C-N	5.00	1.40	1.33
1	A	341	GLU	CA-CB	5.00	1.61	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	142	PRO	CB-CA-C	19.27	143.35	111.56
1	A	246	ALA	N-CA-CB	-17.97	90.22	110.35
1	A	246	ALA	N-CA-C	15.16	131.08	109.71
1	A	309	MET	CB-CA-C	-14.82	80.93	110.42
1	A	330	ASP	CA-CB-CG	-14.30	98.30	112.60
1	A	113	GLU	O-C-N	-13.65	104.43	122.59
1	A	198	THR	CB-CA-C	-13.46	86.07	110.70
1	A	140	CYS	CB-CA-C	-12.68	85.18	110.42
1	A	138	VAL	N-CA-C	12.46	122.59	112.12
1	A	246	ALA	CB-CA-C	-12.16	94.07	112.07
1	A	133	ILE	CB-CA-C	11.65	130.39	111.29
1	A	45	PHE	CA-CB-CG	11.61	125.41	113.80
1	A	126	TRP	CD2-CE3-CZ3	-11.25	103.97	118.60
1	A	126	TRP	CE3-CZ3-CH2	-10.27	107.75	121.10
1	A	215	PRO	CA-N-CD	-9.89	98.15	112.00
1	A	313	PHE	N-CA-C	-9.82	97.30	113.50
1	A	170	PRO	CB-CA-C	9.76	122.83	110.92
1	A	215	PRO	N-CA-CB	-9.62	93.15	103.25
1	A	143	MET	N-CA-CB	-9.26	98.04	111.84
1	A	310	ASN	CA-CB-CG	-9.26	103.34	112.60
1	A	218	VAL	CA-C-N	9.15	138.17	121.70
1	A	218	VAL	C-N-CA	9.15	138.17	121.70
1	A	215	PRO	CA-C-N	9.14	139.00	121.54
1	A	215	PRO	C-N-CA	9.14	139.00	121.54
1	A	128	LEU	N-CA-C	9.12	124.72	113.50
1	A	249	GLU	CB-CA-C	9.11	128.05	109.55
1	A	274	TYR	CA-C-N	-9.10	111.80	122.63
1	A	274	TYR	C-N-CA	-9.10	111.80	122.63
1	A	247	GLU	CA-C-N	9.07	138.87	121.54
1	A	247	GLU	C-N-CA	9.07	138.87	121.54
1	A	137	VAL	CA-C-N	-9.06	113.26	122.77
1	A	137	VAL	C-N-CA	-9.06	113.26	122.77
1	A	308	MET	N-CA-C	-8.95	103.47	114.75
1	A	152	HIS	CA-CB-CG	8.94	122.74	113.80
1	A	180	PRO	CA-N-CD	-8.93	99.00	111.50
1	A	214	ILE	CA-C-N	-8.80	108.84	119.84
1	A	214	ILE	C-N-CA	-8.80	108.84	119.84
1	A	153	ALA	CA-C-N	-8.78	109.72	120.70
1	A	153	ALA	C-N-CA	-8.78	109.72	120.70
1	A	147	ARG	CA-C-N	-8.69	108.74	122.73
1	A	147	ARG	C-N-CA	-8.69	108.74	122.73
1	A	78	ASN	N-CA-C	-8.60	100.14	111.24
1	A	134	GLU	CB-CG-CD	8.59	127.20	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	THR	N-CA-C	8.54	122.19	111.69
1	A	312	GLN	CA-C-N	8.47	133.21	120.17
1	A	312	GLN	C-N-CA	8.47	133.21	120.17
1	A	248	LYS	CA-C-O	8.43	132.57	120.51
1	A	143	MET	N-CA-C	-8.39	100.14	111.54
1	A	276	PHE	CB-CA-C	8.31	123.88	111.17
1	A	142	PRO	N-CA-CB	-8.29	94.55	103.25
1	A	131	LEU	N-CA-C	8.21	122.26	111.75
1	A	232	GLU	CB-CA-C	8.10	124.52	111.24
1	A	222	CYS	CB-CA-C	8.08	125.35	111.45
1	A	142	PRO	CA-N-CD	-8.04	100.75	112.00
1	A	229	THR	N-CA-CB	7.97	122.79	111.15
1	A	217	ILE	N-CA-C	7.95	123.55	112.50
1	A	296	LYS	O-C-N	7.95	131.42	121.64
1	A	197	GLU	CA-C-O	7.95	127.44	119.97
1	A	61	VAL	CB-CA-C	7.93	124.29	111.29
1	A	245	LYS	CA-C-N	7.90	133.03	122.06
1	A	245	LYS	C-N-CA	7.90	133.03	122.06
1	A	142	PRO	CA-C-N	7.89	133.36	122.07
1	A	142	PRO	C-N-CA	7.89	133.36	122.07
1	A	54	ILE	CB-CA-C	7.88	121.26	112.19
1	A	134	GLU	CA-C-O	7.88	130.64	121.34
1	A	137	VAL	CB-CA-C	7.85	124.16	111.29
1	A	193	THR	N-CA-C	7.76	126.95	109.81
1	A	216	LEU	N-CA-C	7.74	127.28	110.80
1	A	330	ASP	CA-C-N	-7.71	110.81	122.23
1	A	330	ASP	C-N-CA	-7.71	110.81	122.23
1	A	314	ARG	O-C-N	-7.54	112.57	122.59
1	A	98	SER	N-CA-CB	-7.49	97.83	110.49
1	A	60	TYR	N-CA-C	-7.48	103.13	111.28
1	A	175	TRP	CD2-CE2-CZ2	-7.48	114.92	122.40
1	A	249	GLU	N-CA-C	-7.46	103.98	113.23
1	A	305	ILE	CB-CA-C	-7.37	102.83	110.93
1	A	306	TYR	O-C-N	-7.35	112.34	122.19
1	A	115	PHE	CA-C-O	7.29	130.94	120.51
1	A	315	ASN	CB-CA-C	-7.26	97.23	109.65
1	A	199	ASN	N-CA-CB	7.25	121.07	110.26
1	A	232	GLU	N-CA-CB	7.25	120.49	111.79
1	A	126	TRP	CG-CD2-CE3	-7.20	126.70	133.90
1	A	148	PHE	CA-CB-CG	7.19	120.99	113.80
1	A	223	TYR	CA-CB-CG	7.18	126.83	113.90
1	A	341	GLU	N-CA-C	-7.18	95.50	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	TYR	N-CA-C	-7.13	95.62	110.80
1	A	139	VAL	N-CA-CB	-7.05	99.60	111.23
1	A	126	TRP	CB-CA-C	-7.03	99.79	110.90
1	A	248	LYS	N-CA-CB	7.01	122.35	110.49
1	A	310	ASN	N-CA-CB	6.94	122.23	110.49
1	A	315	ASN	OD1-CG-ND2	-6.93	115.67	122.60
1	A	278	HIS	CA-C-O	6.90	124.84	119.18
1	A	253	MET	N-CA-CB	6.83	122.04	110.49
1	A	315	ASN	CB-CG-ND2	6.81	126.62	116.40
1	A	175	TRP	NE1-CE2-CD2	-6.81	98.54	107.40
1	A	135	ARG	N-CA-CB	-6.80	99.00	110.49
1	A	151	ASN	CA-C-O	6.80	130.23	120.51
1	A	331	ASP	N-CA-CB	-6.68	98.90	110.86
1	A	140	CYS	N-CA-CB	-6.68	99.21	110.49
1	A	337	VAL	CB-CA-C	-6.67	100.36	111.29
1	A	266	LEU	CB-CA-C	6.64	123.25	110.17
1	A	192	TYR	CA-C-N	-6.64	105.61	121.80
1	A	192	TYR	C-N-CA	-6.64	105.61	121.80
1	A	175	TRP	CE2-CD2-CG	-6.62	99.25	107.20
1	A	178	TYR	CG-CD1-CE1	-6.62	111.27	121.20
1	A	110	CYS	CA-C-N	6.62	133.62	121.70
1	A	110	CYS	C-N-CA	6.62	133.62	121.70
1	A	171	PRO	CA-N-CD	-6.62	102.73	112.00
1	A	310	ASN	CA-C-N	-6.58	111.90	122.24
1	A	310	ASN	C-N-CA	-6.58	111.90	122.24
1	A	125	LEU	N-CA-C	-6.53	104.08	111.07
1	A	250	VAL	N-CA-CB	-6.51	100.48	111.23
1	A	113	GLU	CA-C-N	-6.51	109.40	120.79
1	A	113	GLU	C-N-CA	-6.51	109.40	120.79
1	A	136	TYR	N-CA-C	-6.51	96.94	110.80
1	A	231	LYS	CA-C-N	6.49	131.46	121.53
1	A	231	LYS	C-N-CA	6.49	131.46	121.53
1	A	148	PHE	CB-CA-C	6.46	121.61	110.94
1	A	159	PHE	CA-CB-CG	6.37	120.17	113.80
1	A	56	PHE	CA-CB-CG	6.37	120.17	113.80
1	A	312	GLN	CB-CA-C	6.36	122.48	111.86
1	A	136	TYR	CA-CB-CG	6.35	125.34	113.90
1	A	345	VAL	CB-CA-C	-6.33	102.01	112.26
1	A	331	ASP	O-C-N	-6.29	111.67	122.11
1	A	195	HIS	CB-CA-C	-6.28	102.90	110.94
1	A	62	THR	CA-CB-CG2	6.23	121.08	110.50
1	A	215	PRO	CB-CA-C	6.20	121.79	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	TYR	CB-CG-CD1	-6.19	111.52	120.80
1	A	304	VAL	CB-CA-C	6.17	121.40	111.29
1	A	88	PHE	O-C-N	-6.15	115.45	122.09
1	A	200	ASN	CA-CB-CG	6.14	118.74	112.60
1	A	203	PHE	CA-CB-CG	-6.11	107.69	113.80
1	A	220	PHE	CA-C-N	-6.09	113.35	122.24
1	A	220	PHE	C-N-CA	-6.09	113.35	122.24
1	A	337	VAL	O-C-N	-6.08	114.98	122.57
1	A	137	VAL	CA-C-O	6.05	128.34	120.78
1	A	235	ALA	CA-C-N	-6.04	113.04	123.25
1	A	235	ALA	C-N-CA	-6.04	113.04	123.25
1	A	248	LYS	CB-CA-C	-6.03	98.42	110.42
1	A	313	PHE	CG-CD1-CE1	-6.01	110.48	120.70
1	A	139	VAL	CB-CA-C	-6.01	101.44	111.29
1	A	54	ILE	CA-C-N	6.00	133.22	123.37
1	A	54	ILE	C-N-CA	6.00	133.22	123.37
1	A	140	CYS	O-C-N	-6.00	114.61	122.59
1	A	275	ILE	N-CA-C	5.98	117.35	111.67
1	A	221	PHE	CA-CB-CG	5.98	119.78	113.80
1	A	318	VAL	CB-CA-C	-5.94	101.55	111.29
1	A	332	GLU	N-CA-CB	5.91	120.55	110.50
1	A	306	TYR	CA-C-N	5.90	132.32	121.70
1	A	306	TYR	C-N-CA	5.90	132.32	121.70
1	A	258	VAL	N-CA-C	5.89	121.60	109.34
1	A	274	TYR	N-CA-C	-5.88	103.49	111.55
1	A	343	SER	N-CA-C	-5.86	97.03	107.28
1	A	250	VAL	CA-CB-CG2	5.80	120.26	110.40
1	A	254	VAL	CB-CA-C	5.79	116.43	110.70
1	A	110	CYS	O-C-N	-5.78	114.91	122.59
1	A	171	PRO	N-CA-C	5.76	124.34	112.47
1	A	185	CYS	N-CA-CB	-5.73	101.66	110.20
1	A	273	PHE	CA-CB-CG	5.73	119.53	113.80
1	A	302	ASN	CA-C-N	-5.73	114.99	120.83
1	A	302	ASN	C-N-CA	-5.73	114.99	120.83
1	A	341	GLU	O-C-N	-5.73	114.97	122.59
1	A	239	GLU	CB-CA-C	5.72	120.83	111.74
1	A	87	VAL	CA-C-O	5.71	124.12	118.98
1	A	235	ALA	N-CA-CB	5.71	120.15	110.49
1	A	71	PRO	CA-N-CD	-5.70	104.02	112.00
1	A	314	ARG	N-CA-C	-5.70	98.66	110.80
1	A	308	MET	N-CA-CB	5.68	119.44	111.15
1	A	151	ASN	CA-CB-CG	5.67	118.27	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	TRP	CG-CD2-CE3	-5.63	128.27	133.90
1	A	177	ARG	N-CA-C	-5.61	105.31	111.82
1	A	151	ASN	O-C-N	-5.60	115.14	122.59
1	A	192	TYR	CA-C-O	5.58	127.35	120.15
1	A	225	GLN	N-CA-CB	5.58	118.66	110.57
1	A	165	LEU	N-CA-C	-5.58	106.31	113.23
1	A	60	TYR	CB-CA-C	-5.56	101.56	110.79
1	A	174	GLY	N-CA-C	-5.56	100.01	113.18
1	A	112	LEU	N-CA-C	-5.55	104.92	110.97
1	A	185	CYS	CB-CA-C	-5.53	100.57	110.70
1	A	218	VAL	O-C-N	-5.52	115.21	121.94
1	A	300	VAL	CA-C-O	5.50	127.66	120.78
1	A	326	ASN	CA-CB-CG	-5.49	107.11	112.60
1	A	233	ALA	N-CA-C	5.49	118.78	112.97
1	A	248	LYS	N-CA-C	-5.48	99.14	110.80
1	A	217	ILE	CA-C-N	5.45	127.53	120.88
1	A	217	ILE	C-N-CA	5.45	127.53	120.88
1	A	122	GLU	CA-C-O	5.45	126.52	120.63
1	A	97	THR	N-CA-C	-5.45	99.20	110.80
1	A	241	ALA	N-CA-C	-5.41	99.28	110.80
1	A	290	ILE	N-CA-CB	5.40	118.77	111.21
1	A	247	GLU	O-C-N	5.37	129.61	123.48
1	A	253	MET	CA-CB-CG	-5.37	103.37	114.10
1	A	251	THR	CA-C-O	5.36	126.12	119.79
1	A	201	GLU	CA-C-O	5.34	126.12	119.12
1	A	126	TRP	CZ3-CH2-CZ2	-5.32	114.59	121.50
1	A	312	GLN	N-CA-C	-5.30	97.52	108.18
1	A	232	GLU	N-CA-C	-5.30	104.15	110.41
1	A	141	LYS	CB-CA-C	-5.30	100.03	110.10
1	A	118	THR	N-CA-C	-5.29	99.52	110.80
1	A	221	PHE	N-CA-CB	5.29	116.44	110.35
1	A	117	ALA	CA-C-O	5.29	124.76	118.79
1	A	241	ALA	CA-C-N	-5.28	111.46	121.54
1	A	241	ALA	C-N-CA	-5.28	111.46	121.54
1	A	282	ASP	CA-CB-CG	5.24	117.84	112.60
1	A	251	THR	CA-CB-OG1	-5.20	101.79	109.60
1	A	198	THR	N-CA-CB	-5.19	102.47	110.20
1	A	340	THR	N-CA-C	-5.18	106.19	112.88
1	A	249	GLU	N-CA-CB	-5.18	102.36	110.44
1	A	189	ILE	CA-CB-CG1	5.17	119.19	110.40
1	A	134	GLU	N-CA-CB	5.13	119.03	111.43
1	A	45	PHE	N-CA-CB	5.13	119.16	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	THR	N-CA-C	5.11	118.55	111.71
1	A	59	LEU	CA-C-N	-5.09	113.46	120.28
1	A	59	LEU	C-N-CA	-5.09	113.46	120.28
1	A	73	ASN	N-CA-C	5.09	118.58	111.56
1	A	264	CYS	CB-CA-C	-5.08	101.26	110.56
1	A	46	LEU	N-CA-C	5.05	116.87	111.36
1	A	252	ARG	CA-C-N	5.05	131.18	121.54
1	A	252	ARG	C-N-CA	5.05	131.18	121.54
1	A	246	ALA	O-C-N	-5.01	116.26	122.83

All chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms
1	A	110	CYS	CA
1	A	140	CYS	CA
1	A	191	TYR	CA
1	A	242	THR	CA
1	A	335	THR	CB,CA

All planar outliers are listed below.

Mol	Chain	Res	Type	Group
1	A	42	ALA	Peptide
1	A	45	PHE	Peptide
1	A	46	LEU	Peptide
1	A	47	LEU	Peptide
1	A	49	MET	Peptide
1	A	52	PHE	Peptide
1	A	53	PRO	Peptide
1	A	54	ILE	Peptide
1	A	60	TYR	Peptide
1	A	61	VAL	Peptide
1	A	62	THR	Peptide
1	A	67	LYS	Peptide
1	A	72	LEU	Peptide
1	A	79	LEU	Peptide
1	A	83	ASP	Peptide
1	A	88	PHE	Peptide
1	A	91	PHE	Peptide
1	A	93	THR	Peptide
1	A	94	THR	Peptide
1	A	97	THR	Peptide

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Mol	Chain	Res	Type	Group
1	A	98	SER	Peptide
1	A	99	LEU	Peptide
1	A	100	HIS	Peptide
1	A	102	TYR	Peptide
1	A	103	PHE	Peptide
1	A	105	PHE	Peptide
1	A	107	PRO	Peptide
1	A	117	ALA	Peptide
1	A	131	LEU	Peptide
1	A	132	ALA	Peptide
1	A	133	ILE	Peptide
1	A	134	GLU	Peptide
1	A	135	ARG	Peptide
1	A	136	TYR	Sidechain
1	A	137	VAL	Peptide
1	A	140	CYS	Peptide
1	A	141	LYS	Peptide
1	A	143	MET	Peptide
1	A	146	PHE	Peptide
1	A	147	ARG	Peptide
1	A	148	PHE	Peptide
1	A	149	GLY	Peptide
1	A	151	ASN	Peptide
1	A	153	ALA	Peptide
1	A	166	ALA	Peptide
1	A	167	CYS	Peptide
1	A	170	PRO	Peptide
1	A	176	SER	Peptide
1	A	178	TYR	Sidechain
1	A	185	CYS	Peptide
1	A	186	SER	Peptide
1	A	187	CYS	Peptide
1	A	189	ILE	Peptide
1	A	190	ASP	Peptide
1	A	192	TYR	Peptide
1	A	194	PRO	Peptide
1	A	197	GLU	Peptide
1	A	198	THR	Peptide,Mainchain
1	A	202	SER	Peptide
1	A	203	PHE	Sidechain
1	A	204	VAL	Peptide
1	A	207	MET	Peptide

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Mol	Chain	Res	Type	Group
1	A	210	VAL	Peptide
1	A	211	HIS	Sidechain
1	A	215	PRO	Peptide
1	A	219	ILE	Peptide
1	A	220	PHE	Peptide
1	A	221	PHE	Peptide
1	A	222	CYS	Peptide
1	A	223	TYR	Peptide
1	A	224	GLY	Peptide
1	A	226	LEU	Peptide
1	A	227	VAL	Peptide
1	A	228	PHE	Peptide
1	A	232	GLU	Peptide
1	A	233	ALA	Peptide
1	A	235	ALA	Peptide
1	A	238	GLN	Peptide
1	A	240	SER	Peptide
1	A	241	ALA	Peptide
1	A	249	GLU	Peptide
1	A	252	ARG	Peptide
1	A	253	MET	Peptide
1	A	258	VAL	Peptide,Mainchain
1	A	260	ALA	Peptide
1	A	262	LEU	Peptide
1	A	264	CYS	Peptide
1	A	265	TRP	Peptide
1	A	268	TYR	Sidechain
1	A	274	TYR	Peptide
1	A	276	PHE	Peptide
1	A	278	HIS	Peptide
1	A	281	SER	Peptide
1	A	284	GLY	Peptide
1	A	286	ILE	Peptide
1	A	287	PHE	Peptide
1	A	290	ILE	Mainchain
1	A	301	TYR	Sidechain
1	A	308	MET	Peptide
1	A	309	MET	Peptide
1	A	310	ASN	Peptide
1	A	312	GLN	Peptide
1	A	313	PHE	Sidechain
1	A	314	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	A	316	CYS	Peptide
1	A	320	THR	Peptide
1	A	323	CYS	Peptide
1	A	326	ASN	Peptide
1	A	327	PRO	Peptide
1	A	331	ASP	Peptide
1	A	341	GLU	Peptide
1	A	343	SER	Peptide
1	A	344	GLN	Peptide
1	A	346	ALA	Peptide
1	A	347	PRO	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	2416	2402	523
2	A	20	28	24	26
All	All	2446	2444	2426	523

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 107.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:317:MET:CB	1:A:343:SER:HB2	1.63	1.11
1:A:313:PHE:CA	1:A:313:PHE:CB	1.60	1.78
1:A:317:MET:CB	1:A:343:SER:CB	1.60	1.79
1:A:140:CYS:HB3	1:A:141:LYS:CA	1.55	1.11
1:A:249:GLU:HB3	1:A:313:PHE:CE2	1.51	1.37
1:A:296:LYS:C	1:A:297:THR:N	1.51	1.68
1:A:135:ARG:NH1	1:A:139:VAL:HG21	1.50	1.20
1:A:309:MET:O	1:A:313:PHE:CE1	1.49	1.64
1:A:105:PHE:CD2	1:A:107:PRO:HD3	1.49	1.43
1:A:246:ALA:HB1	1:A:310:ASN:CA	1.47	1.37
1:A:248:LYS:N	1:A:250:VAL:CG2	1.44	1.80
1:A:55:ASN:O	1:A:56:PHE:CD1	1.42	1.72

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:140:CYS:SG	1:A:142:PRO:HD2	1.41	1.56
1:A:339:LYS:CG	1:A:345:VAL:HA	1.39	1.34
1:A:295:ALA:O	1:A:296:LYS:CE	1.39	1.70
1:A:317:MET:HB2	1:A:343:SER:CB	1.38	1.33
1:A:248:LYS:N	1:A:250:VAL:HG22	1.38	1.24
1:A:125:LEU:CD2	2:A:400:RET:H22	1.35	1.28
1:A:98:SER:HB3	1:A:102:TYR:OH	1.34	1.13
1:A:140:CYS:CB	1:A:141:LYS:HA	1.33	1.43
1:A:135:ARG:NH1	1:A:139:VAL:CG2	1.33	1.92
1:A:125:LEU:CD2	2:A:400:RET:C2	1.31	1.94
1:A:93:THR:CA	1:A:102:TYR:OH	1.30	1.78
1:A:295:ALA:O	1:A:296:LYS:HE3	1.30	1.08
1:A:133:ILE:HG12	1:A:136:TYR:CE1	1.29	1.62
1:A:72:LEU:CD2	1:A:134:GLU:OE2	1.29	1.80
1:A:333:ALA:CB	1:A:343:SER:OG	1.28	1.81
1:A:246:ALA:HB2	1:A:310:ASN:O	1.28	1.17
1:A:125:LEU:HD21	2:A:400:RET:C17	1.27	1.37
1:A:135:ARG:N	1:A:136:TYR:CG	1.27	1.68
1:A:240:SER:O	1:A:250:VAL:HG21	1.26	1.10
1:A:249:GLU:CB	1:A:313:PHE:CE2	1.26	2.19
1:A:133:ILE:CG1	1:A:136:TYR:CZ	1.26	2.09
1:A:333:ALA:HB3	1:A:343:SER:OG	1.26	1.18
1:A:246:ALA:HB2	1:A:310:ASN:C	1.25	1.57
1:A:105:PHE:CD2	1:A:107:PRO:CD	1.25	2.18
1:A:318:VAL:CB	1:A:331:ASP:HB2	1.25	1.57
1:A:246:ALA:CB	1:A:310:ASN:CA	1.24	2.15
1:A:248:LYS:CA	1:A:250:VAL:HG22	1.24	1.61
1:A:133:ILE:HG12	1:A:136:TYR:CZ	1.24	1.19
1:A:331:ASP:OD1	1:A:332:GLU:HB2	1.23	1.30
1:A:103:PHE:HB2	1:A:104:VAL:O	1.23	1.04
1:A:249:GLU:HB3	1:A:313:PHE:CD2	1.23	1.68
1:A:317:MET:O	1:A:318:VAL:HG22	1.21	1.33
1:A:318:VAL:CG1	1:A:331:ASP:HB3	1.21	1.65
1:A:98:SER:CB	1:A:102:TYR:CZ	1.21	1.95
1:A:136:TYR:CZ	1:A:253:MET:HE3	1.21	1.70
1:A:249:GLU:CB	1:A:313:PHE:HE2	1.21	1.47
1:A:72:LEU:HD22	1:A:134:GLU:OE2	1.21	1.02
1:A:248:LYS:H	1:A:250:VAL:CG2	1.21	1.40
1:A:134:GLU:CA	1:A:136:TYR:HB2	1.20	1.66
1:A:317:MET:SD	1:A:348:ALA:HB1	1.20	1.76
1:A:248:LYS:C	1:A:250:VAL:HG22	1.19	1.58
1:A:94:THR:HA	1:A:98:SER:CB	1.19	1.66

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:125:LEU:HD22	2:A:400:RET:C2	1.18	1.60
1:A:98:SER:HB3	1:A:102:TYR:CZ	1.17	1.16
1:A:135:ARG:HH12	1:A:139:VAL:CG2	1.17	1.48
1:A:318:VAL:CB	1:A:331:ASP:CB	1.17	2.23
1:A:136:TYR:OH	1:A:253:MET:HE3	1.17	1.38
1:A:316:CYS:O	1:A:343:SER:CB	1.17	1.92
1:A:339:LYS:CG	1:A:345:VAL:CA	1.17	2.22
1:A:246:ALA:C	1:A:313:PHE:HE1	1.16	1.48
1:A:309:MET:O	1:A:313:PHE:CD1	1.16	1.99
1:A:309:MET:C	1:A:313:PHE:HB3	1.15	1.64
1:A:181:GLU:HG3	1:A:185:CYS:SG	1.15	1.81
1:A:246:ALA:CB	1:A:310:ASN:C	1.14	2.19
1:A:316:CYS:O	1:A:343:SER:OG	1.14	1.65
1:A:317:MET:C	1:A:318:VAL:HG22	1.14	1.66
1:A:103:PHE:CB	1:A:104:VAL:O	1.14	1.95
1:A:125:LEU:CD2	2:A:400:RET:H172	1.13	1.72
1:A:140:CYS:CB	1:A:141:LYS:CA	1.13	2.08
1:A:198:THR:HG21	1:A:199:ASN:OD1	1.13	1.40
1:A:198:THR:CG2	1:A:199:ASN:CG	1.10	2.23
1:A:151:ASN:CG	1:A:152:HIS:C	1.10	2.17
1:A:307:ILE:C	1:A:309:MET:HG2	1.10	1.48
1:A:125:LEU:CD2	2:A:400:RET:C17	1.09	2.28
1:A:247:GLU:N	1:A:313:PHE:CE1	1.09	2.21
1:A:295:ALA:C	1:A:296:LYS:HE3	1.09	1.72
1:A:331:ASP:CG	1:A:332:GLU:HB2	1.09	1.72
1:A:317:MET:O	1:A:318:VAL:CG2	1.08	2.01
1:A:246:ALA:C	1:A:313:PHE:CE1	1.08	2.31
1:A:249:GLU:CA	1:A:313:PHE:HE2	1.07	1.63
1:A:104:VAL:O	1:A:105:PHE:CG	1.07	2.08
1:A:318:VAL:CG1	1:A:331:ASP:CB	1.07	2.32
1:A:104:VAL:O	1:A:105:PHE:CD2	1.06	2.08
1:A:248:LYS:CA	1:A:250:VAL:CG2	1.06	2.28
1:A:336:THR:O	1:A:337:VAL:HB	1.06	1.37
1:A:181:GLU:CD	1:A:185:CYS:HB3	1.06	1.74
1:A:318:VAL:HG11	1:A:331:ASP:CB	1.05	1.82
1:A:318:VAL:HG11	1:A:331:ASP:HB3	1.05	1.10
1:A:93:THR:HA	1:A:102:TYR:OH	1.05	0.82
1:A:103:PHE:HB2	1:A:104:VAL:C	1.05	1.77
1:A:98:SER:CB	1:A:102:TYR:OH	1.04	1.94
1:A:318:VAL:HB	1:A:331:ASP:CB	1.04	1.82
1:A:246:ALA:CB	1:A:310:ASN:HA	1.03	1.78
1:A:309:MET:O	1:A:313:PHE:CG	1.03	2.11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:94:THR:CA	1:A:98:SER:HB2	1.03	1.82
1:A:125:LEU:HD21	2:A:400:RET:H172	1.03	1.05
1:A:240:SER:O	1:A:250:VAL:CG2	1.02	2.07
1:A:236:GLN:CG	1:A:240:SER:HB2	1.02	1.82
1:A:198:THR:CG2	1:A:199:ASN:OD1	1.01	2.07
1:A:317:MET:SD	1:A:343:SER:HA	1.01	1.94
1:A:140:CYS:SG	1:A:142:PRO:CD	1.01	2.48
1:A:316:CYS:O	1:A:343:SER:HB2	1.01	1.56
1:A:317:MET:HB3	1:A:343:SER:CB	1.01	1.56
1:A:134:GLU:HA	1:A:136:TYR:HB2	1.00	1.10
1:A:181:GLU:CG	1:A:185:CYS:SG	1.00	2.48
1:A:339:LYS:HG2	1:A:345:VAL:CA	1.00	1.80
1:A:95:LEU:N	1:A:98:SER:OG	1.00	1.94
1:A:140:CYS:HB3	1:A:141:LYS:CB	1.00	1.85
1:A:248:LYS:C	1:A:250:VAL:CG2	1.00	2.34
1:A:105:PHE:HB2	1:A:106:GLY:C	0.99	1.81
1:A:105:PHE:HB2	1:A:107:PRO:CD	0.99	1.86
1:A:318:VAL:HB	1:A:331:ASP:HB2	0.99	1.04
1:A:317:MET:HB3	1:A:343:SER:HB3	0.99	1.26
1:A:246:ALA:CB	1:A:310:ASN:O	0.99	2.06
1:A:94:THR:HA	1:A:98:SER:HB2	0.98	1.01
1:A:136:TYR:CE1	1:A:253:MET:CE	0.98	2.45
1:A:55:ASN:C	1:A:56:PHE:CD1	0.98	2.41
1:A:134:GLU:CA	1:A:136:TYR:CB	0.98	2.42
1:A:105:PHE:HB2	1:A:107:PRO:N	0.97	1.73
1:A:105:PHE:CG	1:A:107:PRO:HD3	0.96	1.94
1:A:309:MET:O	1:A:313:PHE:HB3	0.95	1.61
1:A:136:TYR:CZ	1:A:253:MET:CE	0.95	2.50
1:A:103:PHE:CG	1:A:105:PHE:CE2	0.95	2.39
1:A:55:ASN:O	1:A:56:PHE:HD1	0.94	1.15
1:A:198:THR:HG21	1:A:199:ASN:CG	0.94	1.82
1:A:317:MET:O	1:A:318:VAL:HG13	0.94	1.63
1:A:250:VAL:H	1:A:313:PHE:HZ	0.94	0.94
1:A:125:LEU:HD13	2:A:400:RET:H32	0.93	1.40
1:A:308:MET:N	1:A:309:MET:HG2	0.93	1.76
1:A:309:MET:O	1:A:313:PHE:CB	0.93	2.16
1:A:104:VAL:HG12	1:A:105:PHE:N	0.93	1.79
1:A:139:VAL:HG12	1:A:139:VAL:O	0.92	1.62
1:A:53:PRO:HG3	1:A:56:PHE:CE1	0.92	1.99
1:A:198:THR:HG23	1:A:199:ASN:N	0.92	1.78
1:A:331:ASP:HB3	1:A:332:GLU:HB3	0.92	1.38
1:A:53:PRO:CG	1:A:56:PHE:CE1	0.91	2.49

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:105:PHE:HD2	1:A:107:PRO:CD	0.91	1.60
1:A:317:MET:CB	1:A:343:SER:CA	0.91	2.47
1:A:135:ARG:N	1:A:136:TYR:CB	0.91	2.32
1:A:134:GLU:HA	1:A:136:TYR:CB	0.90	1.94
1:A:248:LYS:N	1:A:250:VAL:HG21	0.90	1.80
1:A:198:THR:HG23	1:A:199:ASN:CG	0.90	1.92
1:A:317:MET:C	1:A:318:VAL:CG2	0.90	2.40
1:A:331:ASP:CG	1:A:332:GLU:CB	0.89	2.44
1:A:105:PHE:CB	1:A:107:PRO:CD	0.89	2.51
1:A:133:ILE:O	1:A:136:TYR:HB3	0.89	1.22
1:A:144:SER:H	1:A:149:GLY:H	0.88	1.05
1:A:309:MET:CB	1:A:310:ASN:HB2	0.88	1.99
1:A:317:MET:O	1:A:318:VAL:CG1	0.88	2.21
1:A:93:THR:HA	1:A:102:TYR:HH	0.88	1.24
1:A:236:GLN:OE1	1:A:240:SER:HB3	0.88	1.68
1:A:317:MET:SD	1:A:348:ALA:CB	0.88	2.61
1:A:103:PHE:HD1	1:A:104:VAL:H	0.87	1.08
1:A:246:ALA:O	1:A:313:PHE:HE1	0.87	1.53
1:A:72:LEU:CD1	1:A:131:LEU:HD11	0.87	2.00
1:A:250:VAL:HG13	1:A:313:PHE:CZ	0.86	2.05
1:A:135:ARG:N	1:A:136:TYR:CD2	0.86	2.44
1:A:140:CYS:HB2	1:A:141:LYS:HG3	0.86	1.45
1:A:339:LYS:HG2	1:A:345:VAL:HA	0.86	0.87
1:A:98:SER:OG	1:A:102:TYR:HE1	0.86	1.23
1:A:151:ASN:ND2	1:A:152:HIS:O	0.86	2.09
1:A:309:MET:HB3	1:A:310:ASN:CA	0.85	1.99
1:A:140:CYS:CB	1:A:141:LYS:CB	0.85	2.52
1:A:195:HIS:O	1:A:198:THR:HG22	0.84	1.71
1:A:135:ARG:HH11	1:A:139:VAL:HG21	0.84	1.18
1:A:249:GLU:CA	1:A:313:PHE:CE2	0.84	2.55
1:A:318:VAL:HG23	1:A:330:ASP:N	0.84	1.66
1:A:309:MET:CB	1:A:310:ASN:CA	0.84	2.56
1:A:331:ASP:CB	1:A:332:GLU:CB	0.83	2.55
1:A:317:MET:O	1:A:318:VAL:CB	0.83	2.25
1:A:105:PHE:CD2	1:A:107:PRO:CG	0.83	2.62
1:A:246:ALA:O	1:A:313:PHE:CE1	0.83	2.31
1:A:103:PHE:CD1	1:A:104:VAL:N	0.83	2.47
1:A:307:ILE:C	1:A:309:MET:CG	0.83	2.40
1:A:250:VAL:O	1:A:253:MET:CB	0.82	2.27
1:A:134:GLU:HA	1:A:137:VAL:H	0.82	1.32
1:A:249:GLU:N	1:A:313:PHE:CE2	0.82	2.47
1:A:133:ILE:CG1	1:A:136:TYR:CE1	0.82	2.50

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:309:MET:CB	1:A:310:ASN:CB	0.82	2.57
1:A:151:ASN:CG	1:A:152:HIS:O	0.82	2.21
1:A:317:MET:HB2	1:A:343:SER:CA	0.82	2.04
1:A:317:MET:SD	1:A:343:SER:CA	0.82	2.67
1:A:295:ALA:HB1	2:A:400:RET:H201	0.82	1.50
1:A:105:PHE:CG	1:A:107:PRO:CD	0.81	2.60
1:A:113:GLU:OE1	2:A:400:RET:H12	0.81	1.73
1:A:246:ALA:HB1	1:A:310:ASN:HA	0.81	0.83
1:A:316:CYS:O	1:A:317:MET:HB2	0.81	1.74
1:A:105:PHE:CG	1:A:107:PRO:CG	0.81	2.64
1:A:331:ASP:HB3	1:A:332:GLU:CB	0.80	2.06
1:A:93:THR:HA	1:A:98:SER:HB3	0.80	1.53
1:A:181:GLU:CD	1:A:185:CYS:CB	0.80	2.55
1:A:133:ILE:HG12	1:A:136:TYR:OH	0.80	1.75
1:A:265:TRP:CZ3	1:A:268:TYR:HB3	0.80	2.12
1:A:309:MET:CA	1:A:313:PHE:HB3	0.80	2.06
1:A:105:PHE:CG	1:A:107:PRO:HG3	0.80	2.12
1:A:93:THR:C	1:A:98:SER:HB2	0.79	2.02
1:A:339:LYS:HG3	1:A:345:VAL:HA	0.79	1.48
1:A:250:VAL:N	1:A:313:PHE:CZ	0.79	2.50
1:A:195:HIS:O	1:A:198:THR:CG2	0.78	2.30
1:A:236:GLN:HG3	1:A:240:SER:HB2	0.78	1.52
1:A:308:MET:N	1:A:309:MET:CG	0.78	2.46
1:A:317:MET:CB	1:A:343:SER:HA	0.78	2.09
1:A:133:ILE:O	1:A:136:TYR:CB	0.78	2.16
1:A:144:SER:N	1:A:149:GLY:H	0.77	1.77
1:A:98:SER:HG	1:A:102:TYR:HE1	0.77	0.78
1:A:96:TYR:N	1:A:98:SER:OG	0.77	2.17
1:A:103:PHE:CD1	1:A:105:PHE:CE2	0.77	2.73
1:A:198:THR:CG2	1:A:199:ASN:ND2	0.77	2.47
1:A:198:THR:CG2	1:A:199:ASN:N	0.76	2.42
1:A:103:PHE:CA	1:A:104:VAL:HB	0.76	2.11
1:A:104:VAL:CG1	1:A:105:PHE:N	0.76	2.49
1:A:141:LYS:C	1:A:143:MET:H	0.76	1.82
1:A:250:VAL:O	1:A:253:MET:CA	0.76	2.34
1:A:98:SER:OG	1:A:102:TYR:CE1	0.75	2.01
1:A:307:ILE:HG13	1:A:309:MET:HE2	0.75	1.58
1:A:125:LEU:HD13	2:A:400:RET:C3	0.75	2.10
1:A:331:ASP:CB	1:A:332:GLU:HB3	0.75	2.10
1:A:336:THR:O	1:A:337:VAL:CB	0.75	2.27
1:A:317:MET:CA	1:A:343:SER:HB2	0.74	2.11
1:A:309:MET:O	1:A:313:PHE:CZ	0.74	2.39

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:249:GLU:CB	1:A:313:PHE:CD2	0.74	2.61
1:A:72:LEU:HD13	1:A:131:LEU:HD11	0.74	1.57
1:A:313:PHE:CD1	1:A:313:PHE:O	0.74	2.40
1:A:309:MET:HB2	1:A:310:ASN:CB	0.74	2.12
1:A:105:PHE:CB	1:A:107:PRO:HG3	0.73	2.14
1:A:236:GLN:OE1	1:A:240:SER:CB	0.73	2.37
1:A:333:ALA:HB1	1:A:343:SER:OG	0.73	1.79
1:A:247:GLU:CA	1:A:313:PHE:CE1	0.73	2.71
1:A:247:GLU:HA	1:A:313:PHE:CZ	0.73	2.17
1:A:295:ALA:O	1:A:296:LYS:NZ	0.72	2.23
1:A:307:ILE:CG1	1:A:309:MET:HE2	0.72	2.13
1:A:250:VAL:N	1:A:313:PHE:HZ	0.72	1.78
1:A:104:VAL:HG12	1:A:105:PHE:H	0.72	1.41
1:A:317:MET:SD	1:A:344:GLN:N	0.71	2.64
1:A:236:GLN:CD	1:A:240:SER:HB2	0.71	2.11
1:A:250:VAL:O	1:A:253:MET:HB2	0.71	1.85
1:A:313:PHE:HB2	1:A:323:CYS:O	0.71	1.85
1:A:139:VAL:O	1:A:139:VAL:CG1	0.71	2.37
1:A:333:ALA:HB3	1:A:343:SER:CB	0.71	2.16
1:A:105:PHE:CB	1:A:107:PRO:HD3	0.71	2.10
1:A:105:PHE:CB	1:A:107:PRO:CG	0.70	2.70
1:A:181:GLU:HG3	1:A:185:CYS:CB	0.70	2.15
1:A:212:PHE:CD1	2:A:400:RET:C3	0.70	2.75
1:A:136:TYR:CE1	1:A:253:MET:SD	0.70	2.84
1:A:313:PHE:CB	1:A:313:PHE:C	0.70	2.64
1:A:246:ALA:N	1:A:314:ARG:HH21	0.69	1.85
1:A:212:PHE:CD1	2:A:400:RET:H31	0.69	2.21
1:A:249:GLU:N	1:A:250:VAL:HG22	0.69	2.02
1:A:95:LEU:CA	1:A:98:SER:OG	0.69	2.41
1:A:93:THR:HA	1:A:98:SER:CB	0.69	2.16
1:A:295:ALA:O	2:A:400:RET:C15	0.69	2.40
1:A:136:TYR:OH	1:A:253:MET:CE	0.69	2.31
1:A:236:GLN:CD	1:A:240:SER:CB	0.68	2.66
1:A:136:TYR:HH	1:A:253:MET:HE3	0.68	1.44
1:A:103:PHE:HA	1:A:104:VAL:HB	0.68	1.66
1:A:144:SER:H	1:A:149:GLY:N	0.68	1.83
1:A:308:MET:N	1:A:309:MET:CB	0.67	2.58
1:A:333:ALA:CB	1:A:343:SER:CB	0.67	2.72
1:A:151:ASN:CB	1:A:152:HIS:C	0.67	2.68
1:A:313:PHE:CA	1:A:313:PHE:CG	0.67	2.74
1:A:140:CYS:HB3	1:A:141:LYS:HA	0.67	0.67
1:A:249:GLU:N	1:A:313:PHE:HE2	0.67	1.81

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:317:MET:CG	1:A:348:ALA:HB1	0.67	2.20
1:A:104:VAL:CG1	1:A:105:PHE:H	0.66	2.00
1:A:181:GLU:CG	1:A:185:CYS:HB3	0.66	2.21
1:A:134:GLU:C	1:A:136:TYR:HB2	0.65	2.15
1:A:141:LYS:C	1:A:143:MET:N	0.65	2.53
1:A:135:ARG:HH12	1:A:139:VAL:HG21	0.65	0.96
1:A:135:ARG:HH12	1:A:139:VAL:HG23	0.65	1.47
1:A:248:LYS:H	1:A:250:VAL:CB	0.65	1.96
1:A:131:LEU:C	1:A:134:GLU:H	0.65	1.98
1:A:309:MET:CG	1:A:310:ASN:HB2	0.65	2.22
1:A:226:LEU:HA	1:A:229:THR:HG22	0.64	1.69
1:A:295:ALA:CB	2:A:400:RET:C15	0.64	2.75
1:A:296:LYS:CA	1:A:297:THR:N	0.64	2.60
1:A:181:GLU:CG	1:A:185:CYS:CB	0.64	2.76
1:A:105:PHE:HD2	1:A:107:PRO:HD3	0.64	0.85
1:A:295:ALA:HB3	2:A:400:RET:C15	0.64	2.23
1:A:295:ALA:CB	2:A:400:RET:H201	0.63	2.22
1:A:317:MET:CG	1:A:343:SER:HA	0.63	2.23
1:A:313:PHE:CB	1:A:313:PHE:N	0.63	2.61
1:A:316:CYS:C	1:A:343:SER:HB2	0.63	2.19
1:A:140:CYS:HB2	1:A:141:LYS:CG	0.62	2.22
1:A:247:GLU:CA	1:A:313:PHE:CZ	0.62	2.82
1:A:103:PHE:HD1	1:A:104:VAL:N	0.62	1.81
1:A:125:LEU:HD22	2:A:400:RET:H22	0.62	0.65
1:A:198:THR:HG21	1:A:199:ASN:ND2	0.62	2.09
1:A:313:PHE:CD1	1:A:313:PHE:C	0.62	2.77
1:A:337:VAL:HG12	1:A:339:LYS:H	0.62	1.53
1:A:130:VAL:O	1:A:133:ILE:C	0.62	2.42
1:A:134:GLU:HA	1:A:137:VAL:N	0.61	2.08
1:A:142:PRO:C	1:A:144:SER:HA	0.61	2.19
1:A:213:ILE:C	1:A:215:PRO:HD3	0.61	2.20
1:A:214:ILE:N	1:A:215:PRO:HD3	0.61	2.11
1:A:133:ILE:CG1	1:A:136:TYR:OH	0.61	2.42
1:A:264:CYS:HB2	1:A:265:TRP:CE2	0.61	2.31
1:A:313:PHE:CB	1:A:323:CYS:O	0.61	2.49
1:A:93:THR:CB	1:A:102:TYR:OH	0.60	2.49
1:A:72:LEU:HD13	1:A:131:LEU:CD1	0.60	2.26
1:A:198:THR:HG23	1:A:199:ASN:H	0.60	1.53
1:A:339:LYS:HG3	1:A:345:VAL:CA	0.60	2.17
1:A:256:ILE:O	1:A:259:ILE:C	0.60	2.44
1:A:105:PHE:CB	1:A:107:PRO:N	0.60	2.60
1:A:313:PHE:CG	1:A:313:PHE:O	0.60	2.55

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:95:LEU:C	1:A:98:SER:OG	0.59	2.45
1:A:246:ALA:HA	1:A:314:ARG:HB3	0.59	1.75
1:A:94:THR:CA	1:A:98:SER:CB	0.59	2.59
1:A:134:GLU:C	1:A:136:TYR:CG	0.58	2.74
1:A:125:LEU:CD1	2:A:400:RET:C3	0.58	2.78
1:A:198:THR:OG1	1:A:199:ASN:HA	0.58	1.99
1:A:153:ALA:O	1:A:157:VAL:HG23	0.58	1.98
1:A:331:ASP:CB	1:A:332:GLU:HB2	0.58	2.22
1:A:251:THR:C	1:A:253:MET:N	0.58	2.60
1:A:259:ILE:HG23	1:A:262:LEU:HG	0.58	1.75
1:A:55:ASN:C	1:A:56:PHE:CG	0.58	2.81
1:A:135:ARG:NH1	1:A:139:VAL:HG23	0.58	2.03
1:A:179:ILE:H	1:A:181:GLU:H	0.58	1.41
1:A:72:LEU:O	1:A:72:LEU:HD12	0.57	2.00
1:A:140:CYS:CB	1:A:141:LYS:CG	0.57	2.82
1:A:198:THR:HG23	1:A:199:ASN:ND2	0.57	2.12
1:A:339:LYS:HB2	1:A:341:GLU:O	0.57	1.99
1:A:313:PHE:CD2	1:A:323:CYS:O	0.57	2.58
1:A:331:ASP:OD1	1:A:332:GLU:CB	0.56	2.27
1:A:229:THR:HA	1:A:232:GLU:HB2	0.56	1.77
1:A:140:CYS:CB	1:A:141:LYS:HG3	0.56	2.24
1:A:198:THR:OG1	1:A:199:ASN:OD1	0.56	2.23
1:A:105:PHE:HB3	1:A:107:PRO:HG3	0.56	1.77
1:A:237:GLN:O	1:A:241:ALA:HB3	0.56	2.00
1:A:264:CYS:CB	1:A:265:TRP:CE2	0.56	2.89
1:A:301:TYR:HA	1:A:304:VAL:HG13	0.56	1.77
1:A:265:TRP:CZ3	1:A:268:TYR:CD2	0.56	2.94
1:A:313:PHE:CG	1:A:313:PHE:C	0.56	2.83
1:A:317:MET:SD	1:A:343:SER:C	0.56	2.89
1:A:247:GLU:O	1:A:325:LYS:HD2	0.55	2.00
1:A:125:LEU:CD1	2:A:400:RET:C2	0.55	2.52
1:A:103:PHE:O	1:A:104:VAL:HG23	0.55	2.01
1:A:118:THR:O	1:A:119:LEU:C	0.55	2.48
1:A:180:PRO:C	1:A:182:GLY:H	0.55	2.09
1:A:203:PHE:C	1:A:206:TYR:H	0.55	2.10
1:A:309:MET:HB2	1:A:310:ASN:CA	0.55	2.29
1:A:103:PHE:CG	1:A:104:VAL:O	0.55	2.58
1:A:93:THR:C	1:A:98:SER:CB	0.55	2.79
1:A:140:CYS:SG	1:A:141:LYS:HA	0.55	2.41
1:A:179:ILE:N	1:A:181:GLU:H	0.55	2.00
1:A:198:THR:O	1:A:202:SER:N	0.55	2.40
1:A:309:MET:C	1:A:313:PHE:CB	0.55	2.56

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:296:LYS:HE3	1:A:296:LYS:CA	0.55	2.32
1:A:216:LEU:N	1:A:219:ILE:O	0.54	2.40
1:A:236:GLN:CG	1:A:240:SER:CB	0.54	2.72
1:A:136:TYR:CE1	1:A:253:MET:HE3	0.54	2.11
1:A:246:ALA:N	1:A:314:ARG:NH2	0.54	2.55
1:A:265:TRP:CE3	1:A:268:TYR:HB3	0.54	2.36
1:A:94:THR:N	1:A:98:SER:HB2	0.54	2.16
1:A:251:THR:HA	1:A:253:MET:HB2	0.54	1.80
1:A:248:LYS:H	1:A:250:VAL:HG22	0.53	0.82
1:A:105:PHE:CB	1:A:106:GLY:C	0.53	2.72
1:A:94:THR:HA	1:A:98:SER:OG	0.53	2.03
1:A:136:TYR:CE1	1:A:253:MET:HE1	0.53	2.34
1:A:189:ILE:CG2	1:A:192:TYR:C	0.53	2.82
1:A:313:PHE:O	1:A:325:LYS:NZ	0.53	2.42
1:A:308:MET:N	1:A:309:MET:HB2	0.53	2.19
1:A:247:GLU:CD	1:A:314:ARG:NH2	0.53	2.67
1:A:338:SER:O	1:A:339:LYS:HB3	0.53	2.04
1:A:131:LEU:HA	1:A:134:GLU:HG2	0.53	1.80
1:A:152:HIS:C	1:A:156:GLY:H	0.53	2.12
1:A:268:TYR:O	1:A:272:ALA:HB3	0.53	2.04
1:A:134:GLU:OE1	1:A:245:LYS:NZ	0.52	2.42
1:A:239:GLU:O	1:A:240:SER:HB3	0.52	2.04
1:A:113:GLU:O	1:A:114:GLY:C	0.52	2.53
1:A:240:SER:O	1:A:248:LYS:N	0.52	2.43
1:A:265:TRP:CZ3	1:A:268:TYR:CB	0.52	2.91
1:A:245:LYS:C	1:A:314:ARG:NE	0.52	2.68
1:A:324:GLY:O	1:A:325:LYS:HD3	0.52	2.05
1:A:93:THR:CA	1:A:98:SER:CB	0.52	2.87
1:A:105:PHE:HB2	1:A:107:PRO:HD3	0.52	1.60
1:A:308:MET:CA	1:A:309:MET:HB2	0.52	2.34
1:A:131:LEU:C	1:A:134:GLU:N	0.51	2.68
1:A:133:ILE:CD1	1:A:136:TYR:CE1	0.51	2.92
1:A:232:GLU:HB3	1:A:235:ALA:C	0.51	2.30
1:A:130:VAL:O	1:A:134:GLU:N	0.51	2.43
1:A:237:GLN:NE2	1:A:251:THR:OG1	0.51	2.43
1:A:72:LEU:O	1:A:72:LEU:CG	0.51	2.58
1:A:136:TYR:HE1	1:A:253:MET:CE	0.50	2.13
1:A:325:LYS:N	1:A:330:ASP:OD2	0.50	2.44
1:A:74:TYR:CD1	1:A:74:TYR:C	0.50	2.89
1:A:198:THR:CB	1:A:199:ASN:OD1	0.50	2.59
1:A:197:GLU:HA	1:A:201:GLU:HB2	0.50	1.83
1:A:317:MET:HB2	1:A:343:SER:HB2	0.50	0.51

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:265:TRP:CH2	1:A:268:TYR:CD2	0.50	2.99
1:A:296:LYS:C	1:A:297:THR:CA	0.50	2.77
1:A:264:CYS:O	1:A:268:TYR:HB2	0.50	2.06
1:A:318:VAL:HG11	1:A:331:ASP:CA	0.50	2.35
1:A:296:LYS:N	1:A:297:THR:N	0.50	2.60
1:A:295:ALA:O	1:A:296:LYS:HE2	0.49	1.93
1:A:212:PHE:CD1	2:A:400:RET:H32	0.49	2.42
1:A:219:ILE:N	1:A:220:PHE:C	0.49	2.70
1:A:141:LYS:O	1:A:143:MET:N	0.49	2.46
1:A:232:GLU:O	1:A:236:GLN:N	0.49	2.45
1:A:247:GLU:HB2	1:A:314:ARG:CZ	0.49	2.38
1:A:264:CYS:SG	1:A:265:TRP:CZ2	0.49	3.06
1:A:103:PHE:CG	1:A:105:PHE:CD2	0.49	2.99
1:A:125:LEU:HD11	2:A:400:RET:C6	0.49	1.99
1:A:136:TYR:O	1:A:139:VAL:N	0.49	2.45
1:A:316:CYS:C	1:A:343:SER:CB	0.48	2.79
1:A:246:ALA:CA	1:A:314:ARG:HE	0.48	2.21
1:A:104:VAL:C	1:A:105:PHE:CG	0.48	2.90
1:A:181:GLU:OE1	1:A:185:CYS:CB	0.48	2.61
1:A:247:GLU:CD	1:A:314:ARG:HH22	0.48	2.17
1:A:119:LEU:O	1:A:123:ILE:HB	0.48	2.09
1:A:214:ILE:O	1:A:218:VAL:N	0.48	2.33
1:A:170:PRO:O	1:A:172:LEU:N	0.48	2.47
1:A:264:CYS:CB	1:A:265:TRP:CZ2	0.48	2.96
1:A:215:PRO:HA	1:A:219:ILE:HG22	0.48	1.86
1:A:55:ASN:O	1:A:56:PHE:CE1	0.47	2.54
1:A:132:ALA:HB3	1:A:133:ILE:HB	0.47	1.86
1:A:139:VAL:C	1:A:140:CYS:SG	0.47	2.97
1:A:175:TRP:CD1	1:A:175:TRP:C	0.47	2.91
1:A:246:ALA:CB	1:A:310:ASN:OD1	0.47	2.62
1:A:309:MET:HB3	1:A:310:ASN:CB	0.47	2.31
1:A:337:VAL:N	1:A:338:SER:HA	0.47	2.23
1:A:246:ALA:O	1:A:310:ASN:HA	0.47	2.09
1:A:103:PHE:C	1:A:104:VAL:HG23	0.47	2.34
1:A:147:ARG:HB3	1:A:148:PHE:CB	0.47	2.39
1:A:148:PHE:C	1:A:150:GLU:N	0.47	2.72
1:A:245:LYS:H	1:A:314:ARG:CZ	0.47	2.23
1:A:313:PHE:CG	1:A:323:CYS:O	0.47	2.67
1:A:119:LEU:HD12	1:A:119:LEU:H	0.47	1.68
1:A:247:GLU:HA	1:A:313:PHE:CE1	0.46	2.40
1:A:93:THR:CA	1:A:102:TYR:HH	0.46	1.98
1:A:92:THR:C	1:A:96:TYR:HB2	0.46	2.35

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:72:LEU:CD1	1:A:72:LEU:O	0.46	2.63
1:A:75:ILE:HG22	1:A:127:SER:HB3	0.46	1.88
1:A:136:TYR:HE1	1:A:253:MET:HE1	0.46	1.68
1:A:181:GLU:CD	1:A:185:CYS:SG	0.46	2.98
1:A:245:LYS:O	1:A:314:ARG:NE	0.46	2.49
1:A:92:THR:O	1:A:93:THR:HB	0.46	2.11
1:A:247:GLU:N	1:A:314:ARG:NE	0.46	2.64
1:A:151:ASN:C	1:A:153:ALA:N	0.45	2.74
1:A:260:ALA:HA	1:A:263:ILE:HG22	0.45	1.87
1:A:313:PHE:O	1:A:313:PHE:HD1	0.45	1.89
1:A:72:LEU:HD11	1:A:131:LEU:HD11	0.45	1.83
1:A:103:PHE:C	1:A:104:VAL:CG2	0.45	2.86
1:A:135:ARG:HB2	1:A:253:MET:SD	0.45	2.51
1:A:228:PHE:HA	1:A:232:GLU:CD	0.45	2.36
1:A:89:GLY:O	1:A:94:THR:N	0.45	2.46
1:A:103:PHE:CD1	1:A:105:PHE:CD2	0.45	3.05
1:A:110:CYS:N	1:A:111:ASN:HA	0.45	2.26
1:A:112:LEU:O	1:A:113:GLU:C	0.45	2.58
1:A:250:VAL:N	1:A:313:PHE:CE2	0.45	2.84
1:A:96:TYR:N	1:A:98:SER:HG	0.45	2.07
1:A:243:THR:H	1:A:314:ARG:HH11	0.45	1.54
1:A:148:PHE:HA	1:A:150:GLU:H	0.45	1.72
1:A:135:ARG:NH1	1:A:139:VAL:CB	0.44	2.76
1:A:250:VAL:HG13	1:A:313:PHE:HZ	0.44	1.61
1:A:226:LEU:CA	1:A:229:THR:HG22	0.44	2.41
1:A:125:LEU:HD21	2:A:400:RET:C2	0.44	1.68
1:A:189:ILE:HG22	1:A:192:TYR:C	0.44	2.37
1:A:203:PHE:HA	1:A:206:TYR:CB	0.44	2.43
1:A:314:ARG:CG	1:A:347:PRO:O	0.44	2.66
1:A:136:TYR:O	1:A:140:CYS:N	0.44	2.51
1:A:60:TYR:O	1:A:64:GLN:N	0.44	2.51
1:A:180:PRO:C	1:A:182:GLY:N	0.44	2.75
1:A:103:PHE:CB	1:A:104:VAL:C	0.43	2.71
1:A:116:PHE:O	1:A:120:GLY:HA3	0.43	2.13
1:A:296:LYS:H	1:A:297:THR:N	0.43	2.11
1:A:52:PHE:HB3	1:A:53:PRO:HG3	0.43	1.89
1:A:56:PHE:C	1:A:58:THR:H	0.43	2.20
1:A:125:LEU:CD1	2:A:400:RET:H32	0.43	2.23
1:A:55:ASN:HA	1:A:58:THR:HB	0.43	1.90
1:A:132:ALA:O	1:A:136:TYR:OH	0.43	2.24
1:A:198:THR:OG1	1:A:199:ASN:CA	0.43	2.67
1:A:226:LEU:HB2	1:A:229:THR:HG22	0.43	1.90

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:239:GLU:O	1:A:240:SER:CB	0.43	2.65
1:A:268:TYR:O	1:A:272:ALA:N	0.43	2.52
1:A:314:ARG:HG3	1:A:347:PRO:O	0.43	2.14
1:A:317:MET:CE	1:A:348:ALA:HB1	0.43	2.43
1:A:259:ILE:HG23	1:A:262:LEU:CG	0.43	2.42
1:A:135:ARG:HH11	1:A:139:VAL:CG2	0.42	1.95
1:A:249:GLU:OE2	1:A:252:ARG:NH2	0.42	2.51
1:A:95:LEU:C	1:A:98:SER:HG	0.42	2.22
1:A:247:GLU:OE1	1:A:314:ARG:NH1	0.42	2.52
1:A:247:GLU:C	1:A:325:LYS:HD2	0.42	2.39
1:A:250:VAL:O	1:A:253:MET:N	0.42	2.52
1:A:339:LYS:HG3	1:A:339:LYS:O	0.42	2.14
1:A:72:LEU:O	1:A:72:LEU:HG	0.42	2.14
1:A:125:LEU:O	1:A:129:VAL:HG13	0.42	2.14
1:A:56:PHE:H	1:A:58:THR:N	0.42	2.13
1:A:214:ILE:C	1:A:217:ILE:N	0.42	2.78
1:A:245:LYS:O	1:A:314:ARG:CG	0.42	2.67
1:A:338:SER:O	1:A:339:LYS:CB	0.42	2.66
1:A:170:PRO:O	1:A:174:GLY:N	0.42	2.53
1:A:200:ASN:C	1:A:200:ASN:HD22	0.42	2.22
1:A:296:LYS:HE3	1:A:296:LYS:N	0.42	2.21
1:A:308:MET:C	1:A:310:ASN:N	0.42	2.77
1:A:131:LEU:O	1:A:136:TYR:CD2	0.42	2.73
1:A:136:TYR:CZ	1:A:253:MET:SD	0.42	3.12
1:A:249:GLU:C	1:A:313:PHE:CE2	0.42	2.97
1:A:315:ASN:CB	1:A:335:THR:OG1	0.42	2.68
1:A:139:VAL:C	1:A:140:CYS:HG	0.41	2.23
1:A:315:ASN:CG	1:A:335:THR:OG1	0.41	2.63
1:A:152:HIS:C	1:A:156:GLY:N	0.41	2.77
1:A:113:GLU:OE2	2:A:400:RET:H14	0.41	2.16
1:A:135:ARG:N	1:A:136:TYR:HB2	0.41	2.08
1:A:148:PHE:O	1:A:151:ASN:N	0.41	2.54
1:A:316:CYS:O	1:A:317:MET:CB	0.41	2.54
1:A:62:THR:O	1:A:62:THR:HG22	0.41	2.16
1:A:142:PRO:O	1:A:144:SER:HA	0.41	2.14
1:A:212:PHE:CG	2:A:400:RET:H31	0.41	2.49
1:A:232:GLU:HB3	1:A:235:ALA:CA	0.41	2.45
1:A:317:MET:HB3	1:A:343:SER:CA	0.41	2.26
1:A:147:ARG:NE	1:A:150:GLU:OE1	0.41	2.49
1:A:214:ILE:N	1:A:215:PRO:CD	0.41	2.83
1:A:309:MET:HG3	1:A:310:ASN:HB2	0.41	1.93
1:A:93:THR:N	1:A:102:TYR:OH	0.41	2.46

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:250:VAL:O	1:A:253:MET:HA	0.41	2.14
1:A:132:ALA:CB	1:A:133:ILE:HB	0.40	2.46
1:A:245:LYS:N	1:A:314:ARG:CZ	0.40	2.84
1:A:72:LEU:HD23	1:A:134:GLU:OE2	0.40	1.96
1:A:154:ILE:O	1:A:157:VAL:N	0.40	2.48
1:A:268:TYR:O	1:A:272:ALA:CB	0.40	2.69
1:A:272:ALA:CA	1:A:275:ILE:H	0.40	2.30

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	307/348 (88%)	147 (48%)	94 (31%)	66 (21%)	0	2
All	All	307/348 (88%)	147 (48%)	94 (31%)	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	56	PHE
1	A	58	THR
1	A	67	LYS
1	A	70	THR
1	A	71	PRO
1	A	93	THR
1	A	98	SER
1	A	99	LEU
1	A	102	TYR
1	A	103	PHE
1	A	104	VAL
1	A	105	PHE
1	A	110	CYS
1	A	118	THR
1	A	119	LEU
1	A	121	GLY

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Mol	Chain	Res	Type
1	A	133	ILE
1	A	136	TYR
1	A	139	VAL
1	A	140	CYS
1	A	142	PRO
1	A	149	GLY
1	A	151	ASN
1	A	152	HIS
1	A	170	PRO
1	A	171	PRO
1	A	178	TYR
1	A	180	PRO
1	A	181	GLU
1	A	193	THR
1	A	209	VAL
1	A	214	ILE
1	A	215	PRO
1	A	216	LEU
1	A	219	ILE
1	A	220	PHE
1	A	227	VAL
1	A	235	ALA
1	A	240	SER
1	A	242	THR
1	A	244	GLN
1	A	248	LYS
1	A	250	VAL
1	A	253	MET
1	A	261	PHE
1	A	266	LEU
1	A	270	GLY
1	A	271	VAL
1	A	284	GLY
1	A	287	PHE
1	A	288	MET
1	A	290	ILE
1	A	307	ILE
1	A	310	ASN
1	A	314	ARG
1	A	316	CYS
1	A	318	VAL
1	A	321	LEU

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Mol	Chain	Res	Type
1	A	325	LYS
1	A	326	ASN
1	A	334	SER
1	A	335	THR
1	A	336	THR
1	A	337	VAL
1	A	339	LYS
1	A	346	ALA

6.3.2 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 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	0	-	-	-
All	All	0	-	-	-

There are no protein residues with a non-rotameric sidechain to report.

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

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	1	20,20,21	0.65	1 (5%)

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	1	27,27,28	0.75	0 (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	400	1	-	0,13,30,31	0,1,1,1

All bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	RET	C14-C13	2.13	1.35	1.33

There are no bond-angle outliers.

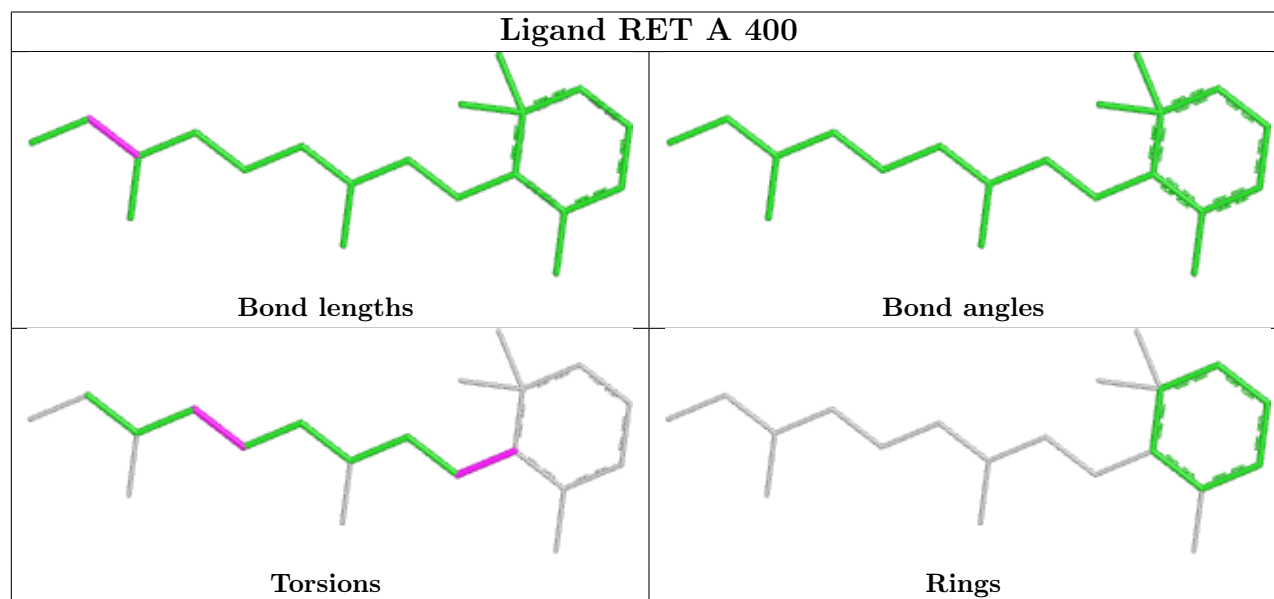
There are no chirality outliers.

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	296:LYS	C	297:THR	N	1.68

7 Chemical shift validation

No chemical shift data were provided