



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 03:02 PM BST

PDB ID : 1JFP  
Title : Structure of bovine rhodopsin (dark adapted)  
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Deposited on : 2001-06-21

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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

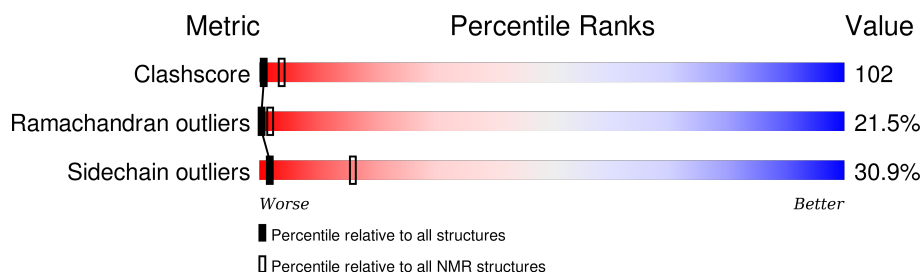
# 1 Overall quality at a glance

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.

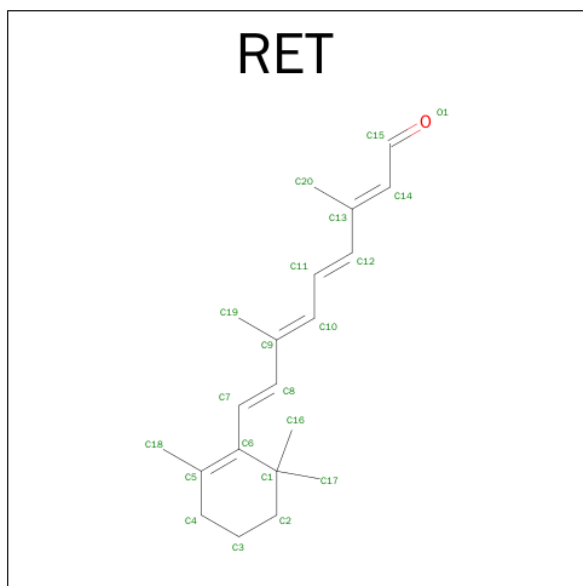
### 3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 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 (three-letter code: RET) (formula:  $C_{20}H_{28}O$ ).

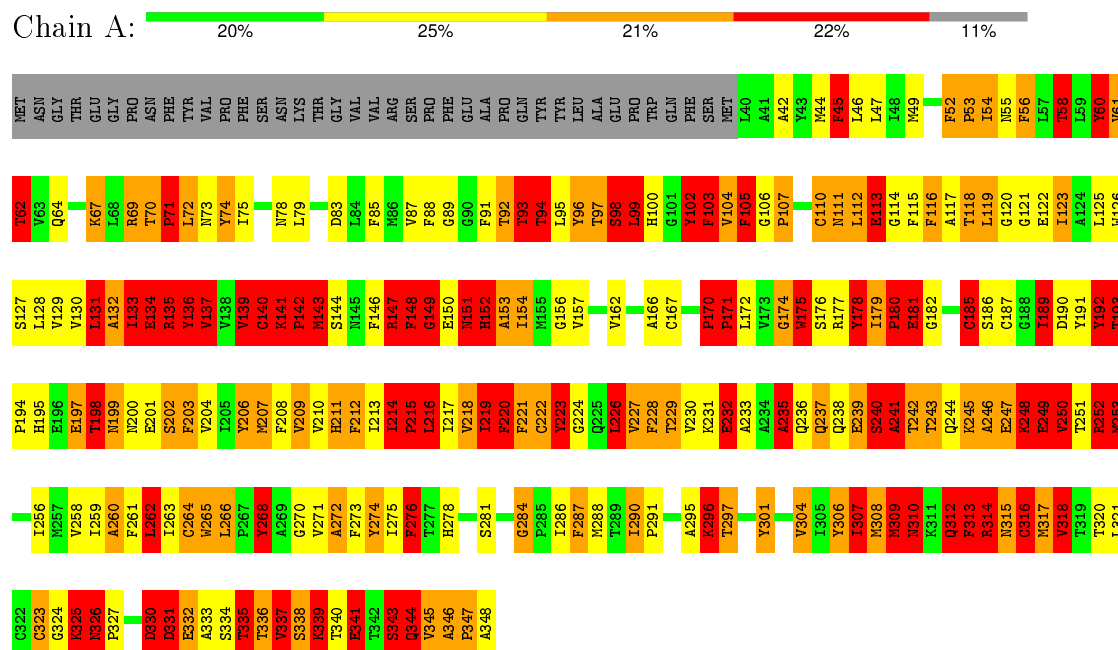


Mol	Chain	Residues	Atoms		
			Total	C	H
2	A	1	48	20	28

## 4 Residue-property plots

These plots are provided for all protein, RNA and DNA 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. No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality

### 6.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the (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	1.31	15/2496 (0.6%)	2.25	133/3401 (3.9%)
All	All	1.31	15/2496 (0.6%)	2.25	133/3401 (3.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	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	14.95	1.68	1.34
1	A	313	PHE	CA-CB	10.99	1.78	1.53
1	A	310	ASN	N-CA	9.89	1.66	1.46
1	A	253	MET	CA-CB	8.97	1.73	1.53
1	A	307	ILE	N-CA	8.86	1.64	1.46
1	A	331	ASP	N-CA	7.14	1.60	1.46
1	A	339	LYS	N-CA	6.58	1.59	1.46
1	A	113	GLU	C-N	6.49	1.44	1.33
1	A	344	GLN	N-CA	6.38	1.59	1.46
1	A	314	ARG	N-CA	5.69	1.57	1.46
1	A	141	LYS	C-N	5.62	1.45	1.34
1	A	345	VAL	CA-CB	5.56	1.66	1.54
1	A	315	ASN	CB-CG	5.48	1.63	1.51
1	A	246	ALA	CA-C	5.28	1.66	1.52
1	A	312	GLN	N-CA	5.03	1.56	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	TYR	CB-CG-CD1	-15.80	111.52	121.00
1	A	309	MET	CB-CA-C	-14.74	80.93	110.40
1	A	246	ALA	N-CA-CB	-14.20	90.22	110.10
1	A	140	CYS	CB-CA-C	-12.61	85.18	110.40
1	A	178	TYR	CG-CD1-CE1	-12.54	111.27	121.30
1	A	142	PRO	CB-CA-C	12.54	143.35	112.00
1	A	126	TRP	CE3-CZ3-CH2	-12.23	107.75	121.20
1	A	74	TYR	CB-CG-CD1	-12.20	113.68	121.00
1	A	126	TRP	CD2-CE3-CZ3	-11.41	103.97	118.80
1	A	113	GLU	O-C-N	-11.04	104.43	123.20
1	A	246	ALA	CB-CA-C	-10.69	94.07	110.10
1	A	175	TRP	CE2-CD2-CG	-10.06	99.25	107.30
1	A	215	PRO	CA-N-CD	-9.53	98.15	111.50
1	A	74	TYR	CB-CG-CD2	9.50	126.70	121.00
1	A	198	THR	CB-CA-C	-9.46	86.07	111.60
1	A	133	ILE	CB-CA-C	9.39	130.39	111.60
1	A	313	PHE	CG-CD1-CE1	-9.38	110.48	120.80
1	A	113	GLU	CA-C-N	9.26	134.73	116.20
1	A	126	TRP	CD1-NE1-CE2	-9.18	100.74	109.00
1	A	180	PRO	CA-N-CD	-8.93	99.00	111.50
1	A	249	GLU	CB-CA-C	8.82	128.05	110.40
1	A	96	TYR	CB-CG-CD1	-8.76	115.75	121.00
1	A	175	TRP	NE1-CE2-CD2	-8.76	98.54	107.30
1	A	215	PRO	N-CA-CB	-8.46	93.15	103.30
1	A	98	SER	N-CA-CB	-8.44	97.83	110.50
1	A	313	PHE	CB-CG-CD2	-8.43	114.90	120.80
1	A	126	TRP	CG-CD2-CE3	-8.00	126.70	133.90
1	A	331	ASP	CB-CG-OD2	-7.89	111.20	118.30
1	A	142	PRO	CA-N-CD	-7.68	100.75	111.50
1	A	306	TYR	CB-CG-CD1	7.53	125.52	121.00
1	A	306	TYR	CB-CG-CD2	-7.51	116.49	121.00
1	A	222	CYS	CB-CA-C	7.47	125.35	110.40
1	A	246	ALA	N-CA-C	7.44	131.08	111.00
1	A	136	TYR	CG-CD2-CE2	-7.38	115.39	121.30
1	A	142	PRO	N-CA-CB	-7.29	94.55	103.30
1	A	235	ALA	N-CA-CB	7.18	120.15	110.10
1	A	223	TYR	CA-CB-CG	7.07	126.83	113.40
1	A	232	GLU	CB-CA-C	7.06	124.52	110.40
1	A	175	TRP	CD1-NE1-CE2	-7.01	102.69	109.00
1	A	143	MET	N-CA-CB	-6.98	98.04	110.60
1	A	215	PRO	C-N-CA	6.92	139.00	121.70
1	A	331	ASP	O-C-N	-6.90	111.67	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247	GLU	C-N-CA	6.87	138.87	121.70
1	A	266	LEU	CB-CA-C	6.87	123.25	110.20
1	A	330	ASP	CA-CB-CG	-6.86	98.30	113.40
1	A	61	VAL	CB-CA-C	6.79	124.29	111.40
1	A	276	PHE	CB-CA-C	6.74	123.88	110.40
1	A	137	VAL	CB-CA-C	6.72	124.16	111.40
1	A	148	PHE	CB-CG-CD2	6.70	125.49	120.80
1	A	218	VAL	C-N-CA	6.59	138.17	121.70
1	A	315	ASN	CB-CA-C	-6.58	97.23	110.40
1	A	229	THR	N-CA-CB	6.57	122.79	110.30
1	A	248	LYS	N-CA-CB	6.53	122.35	110.60
1	A	331	ASP	N-CA-CB	-6.50	98.90	110.60
1	A	134	GLU	CA-C-N	-6.49	102.91	117.20
1	A	306	TYR	O-C-N	-6.47	112.34	122.70
1	A	310	ASN	N-CA-CB	6.46	122.23	110.60
1	A	135	ARG	N-CA-CB	-6.44	99.00	110.60
1	A	192	TYR	C-N-CA	-6.44	105.61	121.70
1	A	253	MET	N-CA-CB	6.35	122.04	110.60
1	A	314	ARG	O-C-N	-6.33	112.57	122.70
1	A	140	CYS	N-CA-CB	-6.33	99.21	110.60
1	A	136	TYR	CA-CB-CG	6.28	125.34	113.40
1	A	171	PRO	CA-N-CD	-6.26	102.73	111.50
1	A	175	TRP	CG-CD2-CE3	-6.25	128.27	133.90
1	A	178	TYR	CB-CG-CD2	-6.25	117.25	121.00
1	A	250	VAL	CA-CB-CG2	6.24	120.26	110.90
1	A	62	THR	CA-CB-CG2	6.20	121.08	112.40
1	A	175	TRP	CD2-CE2-CZ2	-6.15	114.92	122.30
1	A	113	GLU	C-N-CA	-6.14	109.40	122.30
1	A	142	PRO	CA-C-N	-6.13	103.72	117.20
1	A	223	TYR	CB-CG-CD1	6.05	124.63	121.00
1	A	268	TYR	CB-CG-CD1	6.05	124.63	121.00
1	A	312	GLN	CB-CA-C	6.04	122.48	110.40
1	A	216	LEU	N-CA-C	6.03	127.28	111.00
1	A	115	PHE	CA-C-N	-5.99	104.02	117.20
1	A	248	LYS	CB-CA-C	-5.99	98.42	110.40
1	A	135	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	248	LYS	CA-C-O	5.94	132.57	120.10
1	A	193	THR	N-CA-C	5.91	126.95	111.00
1	A	252	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	126	TRP	CZ3-CH2-CZ2	-5.84	114.59	121.60
1	A	253	MET	CA-CB-CG	-5.84	103.37	113.30
1	A	199	ASN	N-CA-CB	5.82	121.07	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	337	VAL	CB-CA-C	-5.81	100.36	111.40
1	A	175	TRP	CG-CD1-NE1	-5.79	104.31	110.10
1	A	341	GLU	N-CA-C	-5.74	95.50	111.00
1	A	69	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	A	102	TYR	N-CA-C	-5.70	95.62	111.00
1	A	148	PHE	CB-CA-C	5.60	121.61	110.40
1	A	226	LEU	CB-CA-C	5.57	120.79	110.20
1	A	223	TYR	CB-CG-CD2	-5.53	117.68	121.00
1	A	97	THR	CA-C-N	-5.53	105.03	117.20
1	A	331	ASP	CB-CA-C	5.53	121.46	110.40
1	A	332	GLU	N-CA-CB	5.53	120.55	110.60
1	A	232	GLU	N-CA-CB	5.49	120.49	110.60
1	A	192	TYR	CB-CG-CD2	-5.49	117.71	121.00
1	A	296	LYS	O-C-N	5.45	131.42	122.70
1	A	139	VAL	N-CA-CB	-5.41	99.60	111.50
1	A	248	LYS	CA-C-N	-5.39	105.34	117.20
1	A	272	ALA	N-CA-CB	5.38	117.64	110.10
1	A	152	HIS	CA-CB-CG	5.38	122.74	113.60
1	A	192	TYR	CB-CG-CD1	5.36	124.22	121.00
1	A	122	GLU	OE1-CD-OE2	5.35	129.72	123.30
1	A	71	PRO	CA-N-CD	-5.35	104.02	111.50
1	A	175	TRP	CB-CG-CD1	5.33	133.92	127.00
1	A	45	PHE	CB-CG-CD1	5.32	124.53	120.80
1	A	126	TRP	CB-CA-C	-5.31	99.79	110.40
1	A	253	MET	CA-C-N	-5.30	105.54	117.20
1	A	241	ALA	N-CA-CB	5.27	117.47	110.10
1	A	304	VAL	CB-CA-C	5.26	121.40	111.40
1	A	235	ALA	CB-CA-C	5.25	117.97	110.10
1	A	139	VAL	CB-CA-C	-5.24	101.44	111.40
1	A	174	GLY	N-CA-C	-5.24	100.01	113.10
1	A	148	PHE	CB-CG-CD1	-5.22	117.15	120.80
1	A	239	GLU	CB-CA-C	5.22	120.83	110.40
1	A	136	TYR	N-CA-C	-5.21	96.94	111.00
1	A	181	GLU	OE1-CD-OE2	5.20	129.53	123.30
1	A	135	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	A	141	LYS	CB-CA-C	-5.18	100.03	110.40
1	A	147	ARG	C-N-CA	-5.18	108.74	121.70
1	A	318	VAL	CB-CA-C	-5.18	101.55	111.40
1	A	343	SER	N-CA-C	-5.17	97.03	111.00
1	A	115	PHE	CA-C-O	5.16	130.94	120.10
1	A	268	TYR	CB-CG-CD2	-5.11	117.93	121.00
1	A	128	LEU	N-CA-C	5.08	124.72	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	A	313	PHE	N-CA-C	-5.07	97.30	111.00
1	A	85	PHE	CB-CG-CD1	5.06	124.34	120.80
1	A	140	CYS	O-C-N	-5.05	114.61	122.70
1	A	134	GLU	CA-C-O	5.02	130.64	120.10
1	A	239	GLU	CA-C-O	5.01	130.61	120.10
1	A	250	VAL	N-CA-CB	-5.01	100.48	111.50

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	103	PHE	Peptide
1	A	149	GLY	Peptide
1	A	198	THR	Mainchain,Peptide
1	A	309	MET	Peptide
1	A	264	CYS	Peptide
1	A	88	PHE	Peptide
1	A	219	ILE	Peptide
1	A	135	ARG	Peptide
1	A	202	SER	Peptide
1	A	91	PHE	Peptide
1	A	316	CYS	Peptide
1	A	93	THR	Peptide
1	A	94	THR	Peptide
1	A	210	VAL	Peptide
1	A	344	GLN	Peptide
1	A	224	GLY	Peptide
1	A	238	GLN	Peptide
1	A	204	VAL	Peptide
1	A	252	ARG	Peptide
1	A	42	ALA	Peptide
1	A	331	ASP	Peptide
1	A	98	SER	Peptide

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
1	A	278	HIS	Peptide
1	A	187	CYS	Peptide
1	A	45	PHE	Peptide
1	A	46	LEU	Peptide
1	A	215	PRO	Peptide
1	A	233	ALA	Peptide
1	A	47	LEU	Peptide
1	A	346	ALA	Peptide
1	A	226	LEU	Peptide
1	A	49	MET	Peptide
1	A	240	SER	Peptide
1	A	235	ALA	Peptide
1	A	276	PHE	Peptide
1	A	52	PHE	Peptide
1	A	220	PHE	Peptide
1	A	53	PRO	Peptide
1	A	54	ILE	Peptide
1	A	320	THR	Peptide
1	A	301	TYR	Sidechain
1	A	102	TYR	Peptide
1	A	211	HIS	Sidechain
1	A	268	TYR	Sidechain
1	A	274	TYR	Peptide
1	A	60	TYR	Peptide
1	A	61	VAL	Peptide
1	A	131	LEU	Peptide
1	A	347	PRO	Peptide
1	A	132	ALA	Peptide
1	A	133	ILE	Peptide
1	A	151	ASN	Peptide
1	A	284	GLY	Peptide
1	A	67	LYS	Peptide
1	A	241	ALA	Peptide
1	A	286	ILE	Peptide
1	A	207	MET	Peptide
1	A	281	SER	Peptide
1	A	343	SER	Peptide
1	A	107	PRO	Peptide
1	A	313	PHE	Sidechain
1	A	105	PHE	Peptide
1	A	136	TYR	Sidechain
1	A	148	PHE	Peptide

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
1	A	137	VAL	Peptide
1	A	290	ILE	Mainchain
1	A	166	ALA	Peptide
1	A	327	PRO	Peptide
1	A	72	LEU	Peptide
1	A	203	PHE	Sidechain
1	A	167	CYS	Peptide
1	A	262	LEU	Peptide
1	A	185	CYS	Peptide
1	A	97	THR	Peptide
1	A	140	CYS	Peptide
1	A	143	MET	Peptide
1	A	323	CYS	Peptide
1	A	141	LYS	Peptide
1	A	258	VAL	Mainchain,Peptide
1	A	178	TYR	Sidechain
1	A	153	ALA	Peptide
1	A	134	GLU	Peptide
1	A	249	GLU	Peptide
1	A	310	ASN	Peptide
1	A	222	CYS	Peptide
1	A	99	LEU	Peptide
1	A	176	SER	Peptide
1	A	287	PHE	Peptide
1	A	223	TYR	Peptide
1	A	197	GLU	Peptide
1	A	260	ALA	Peptide
1	A	100	HIS	Peptide
1	A	232	GLU	Peptide
1	A	83	ASP	Peptide
1	A	117	ALA	Peptide
1	A	312	GLN	Peptide
1	A	228	PHE	Peptide
1	A	79	LEU	Peptide
1	A	326	ASN	Peptide
1	A	146	PHE	Peptide
1	A	265	TRP	Peptide
1	A	186	SER	Peptide
1	A	170	PRO	Peptide
1	A	147	ARG	Peptide
1	A	308	MET	Peptide
1	A	189	ILE	Peptide

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Mol	Chain	Res	Type	Group
1	A	341	GLU	Peptide
1	A	221	PHE	Peptide
1	A	190	ASP	Peptide
1	A	227	VAL	Peptide
1	A	192	TYR	Peptide
1	A	314	ARG	Peptide
1	A	253	MET	Peptide
1	A	62	THR	Peptide
1	A	194	PRO	Peptide

## 6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in 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	499
2	A	20	28	24	25
All	All	2446	2444	2426	499

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 102.

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:CB	1:A:313:PHE:CA	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: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:296:LYS:C	1:A:297:THR:N	1.46	1.68
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
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
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: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:135:ARG:N	1:A:136:TYR:CG	1.27	1.68
1:A:125:LEU:HD21	2:A:400:RET:C17	1.27	1.37
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: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:318:VAL:CG1	1:A:331:ASP:HB3	1.21	1.65
1:A:317:MET:O	1:A:318:VAL:HG22	1.21	1.33
1:A:249:GLU:CB	1:A:313:PHE:HE2	1.21	1.47
1:A:98:SER:CB	1:A:102:TYR:CZ	1.21	1.95
1:A:248:LYS:H	1:A:250:VAL:CG2	1.21	1.40
1:A:72:LEU:HD22	1:A:134:GLU:OE2	1.21	1.02
1:A:246:ALA:HB2	1:A:310:ASN:C	1.21	1.57
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:94:THR:HA	1:A:98:SER:CB	1.19	1.66
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:316:CYS:O	1:A:343:SER:CB	1.17	1.92

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:339:LYS:CG	1:A:345:VAL:CA	1.17	2.22
1:A:309:MET:O	1:A:313:PHE:CD1	1.16	1.99
1:A:181:GLU:HG3	1:A:185:CYS:SG	1.15	1.81
1:A:248:LYS:C	1:A:250:VAL:HG22	1.15	1.58
1:A:103:PHE:CB	1:A:104:VAL:O	1.14	1.95
1:A:316:CYS:O	1:A:343:SER:OG	1.13	1.65
1:A:140:CYS:CB	1:A:141:LYS:CA	1.13	2.08
1:A:125:LEU:CD2	2:A:400:RET:H172	1.13	1.72
1:A:198:THR:HG21	1:A:199:ASN:OD1	1.13	1.40
1:A:246:ALA:C	1:A:313:PHE:HE1	1.11	1.48
1:A:309:MET:C	1:A:313:PHE:HB3	1.11	1.64
1:A:317:MET:C	1:A:318:VAL:HG22	1.09	1.66
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:317:MET:O	1:A:318:VAL:CG2	1.08	2.01
1:A:246:ALA:CB	1:A:310:ASN:C	1.08	2.19
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:248:LYS:CA	1:A:250:VAL:CG2	1.06	2.28
1:A:104:VAL:O	1:A:105:PHE:CD2	1.06	2.08
1:A:336:THR:O	1:A:337:VAL:HB	1.06	1.37
1:A:198:THR:CG2	1:A:199:ASN:CG	1.06	2.23
1:A:307:ILE:C	1:A:309:MET:HG2	1.05	1.48
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:295:ALA:C	1:A:296:LYS:HE3	1.04	1.72
1:A:246:ALA:CB	1:A:310:ASN:O	1.04	2.06
1:A:318:VAL:HB	1:A:331:ASP:CB	1.04	1.82
1:A:331:ASP:CG	1:A:332:GLU:HB2	1.04	1.72
1:A:98:SER:CB	1:A:102:TYR:OH	1.04	1.94
1:A:246:ALA:C	1:A:313:PHE:CE1	1.04	2.31
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
1:A:125:LEU:HD21	2:A:400:RET:H172	1.03	1.05
1:A:94:THR:CA	1:A:98:SER:HB2	1.03	1.82
1:A:240:SER:O	1:A:250:VAL:CG2	1.02	2.07
1:A:151:ASN:CG	1:A:152:HIS:C	1.02	2.17
1:A:236:GLN:CG	1:A:240:SER:HB2	1.02	1.82
1:A:181:GLU:CD	1:A:185:CYS:HB3	1.01	1.74
1:A:317:MET:SD	1:A:343:SER:HA	1.01	1.94

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:198:THR:CG2	1:A:199:ASN:OD1	1.01	2.07
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:103:PHE:HB2	1:A:104:VAL:C	1.00	1.77
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: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: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:134:GLU:CA	1:A:136:TYR:CB	0.98	2.42
1:A:136:TYR:CE1	1:A:253:MET:HE1	0.98	1.92
1:A:136:TYR:OH	1:A:253:MET:HE3	0.98	1.59
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:248:LYS:C	1:A:250:VAL:CG2	0.95	2.34
1:A:105:PHE:HB2	1:A:106:GLY:C	0.95	1.81
1:A:55:ASN:O	1:A:56:PHE:HD1	0.94	1.15
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:55:ASN:C	1:A:56:PHE:CD1	0.93	2.41
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
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:248:LYS:N	1:A:250:VAL:HG21	0.90	1.80
1:A:198:THR:HG21	1:A:199:ASN:CG	0.90	1.82
1:A:133:ILE:O	1:A:136:TYR:CB	0.89	2.16
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:246:ALA:O	1:A:313:PHE:HE1	0.87	1.53
1:A:103:PHE:HD1	1:A:104:VAL:H	0.87	1.08
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:317:MET:C	1:A:318:VAL:CG2	0.85	2.40
1:A:198:THR:HG23	1:A:199:ASN:CG	0.85	1.92
1:A:140:CYS:CB	1:A:141:LYS:CB	0.85	2.52
1:A:331:ASP:CG	1:A:332:GLU:CB	0.85	2.44
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:136:TYR:HE1	1:A:253:MET:HE1	0.84	1.32
1:A:318:VAL:HG23	1:A:330:ASP:N	0.84	1.66
1:A:246:ALA:O	1:A:313:PHE:CE1	0.84	2.31
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:136:TYR:CZ	1:A:253:MET:HE3	0.83	2.06
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:103:PHE:CD1	1:A:104:VAL:N	0.83	2.47
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
1:A:309:MET:CB	1:A:310:ASN:CB	0.82	2.57

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
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:246:ALA:HB1	1:A:310:ASN:HA	0.81	0.83
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: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:133:ILE:HG12	1:A:136:TYR:OH	0.80	1.75
1:A:309:MET:CA	1:A:313:PHE:HB3	0.80	2.06
1:A:265:TRP:CZ3	1:A:268:TYR:HB3	0.80	2.12
1:A:105:PHE:CG	1:A:107:PRO:HG3	0.80	2.12
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:307:ILE:C	1:A:309:MET:CG	0.79	2.40
1:A:236:GLN:HG3	1:A:240:SER:HB2	0.78	1.52
1:A:195:HIS:O	1:A:198:THR:CG2	0.78	2.30
1:A:151:ASN:CG	1:A:152:HIS:O	0.78	2.21
1:A:308:MET:N	1:A:309:MET:CG	0.78	2.46
1:A:136:TYR:OH	1:A:253:MET:CE	0.78	2.31
1:A:317:MET:CB	1:A:343:SER:HA	0.78	2.09
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: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:331:ASP:CB	1:A:332:GLU:HB3	0.75	2.10
1:A:125:LEU:HD13	2:A:400:RET:C3	0.75	2.10
1:A:93:THR:C	1:A:98:SER:HB2	0.75	2.02
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
1:A:249:GLU:CB	1:A:313:PHE:CD2	0.74	2.61
1:A:181:GLU:CD	1:A:185:CYS:CB	0.74	2.55
1:A:72:LEU:HD13	1:A:131:LEU:HD11	0.74	1.57

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:313:PHE:O	1:A:313:PHE:CD1	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:141:LYS:C	1:A:143:MET:H	0.72	1.82
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: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:CG1	1:A:139:VAL:O	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: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:295:ALA:O	2:A:400:RET:C15	0.69	2.40
1:A:93:THR:HA	1:A:98:SER:CB	0.69	2.16
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: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
1:A:317:MET:CG	1:A:348:ALA:HB1	0.67	2.20
1:A:236:GLN:CD	1:A:240:SER:HB2	0.66	2.11
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: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:313:PHE:CB	1:A:313:PHE:C	0.65	2.64

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
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:236:GLN:CD	1:A:240:SER:CB	0.64	2.66
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: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:337:VAL:HG12	1:A:339:LYS:H	0.62	1.53
1:A:198:THR:HG21	1:A:199:ASN:ND2	0.62	2.09
1:A:134:GLU:HA	1:A:137:VAL:N	0.61	2.08
1:A:151:ASN:CB	1:A:152:HIS:C	0.61	2.68
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:131:LEU:C	1:A:134:GLU:H	0.60	1.98
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:141:LYS:C	1:A:143:MET:N	0.60	2.53
1:A:313:PHE:O	1:A:313:PHE:CG	0.60	2.55
1:A:105:PHE:CB	1:A:107:PRO:N	0.60	2.60
1:A:134:GLU:C	1:A:136:TYR:HB2	0.59	2.15
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: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:316:CYS:C	1:A:343:SER:HB2	0.58	2.19
1:A:259:ILE:HG23	1:A:262:LEU:HG	0.58	1.75
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:313:PHE:CD1	1:A:313:PHE:C	0.57	2.77
1:A:72:LEU:HD12	1:A:72:LEU:O	0.57	2.00
1:A:140:CYS:CB	1:A:141:LYS:CG	0.57	2.82
1:A:130:VAL:O	1:A:133:ILE:C	0.57	2.42
1:A:339:LYS:HB2	1:A:341:GLU:O	0.57	1.99
1:A:198:THR:HG23	1:A:199:ASN:ND2	0.57	2.12
1:A:142:PRO:C	1:A:144:SER:HA	0.57	2.19
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:213:ILE:C	1:A:215:PRO:HD3	0.56	2.20
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:256:ILE:O	1:A:259:ILE:C	0.56	2.44
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: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:140:CYS:SG	1:A:141:LYS:HA	0.55	2.41
1:A:95:LEU:C	1:A:98:SER:OG	0.55	2.45
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:296:LYS:CA	1:A:296:LYS:HE3	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:251:THR:C	1:A:253:MET:N	0.54	2.60
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:251:THR:HA	1:A:253:MET:HB2	0.54	1.80
1:A:94:THR:N	1:A:98:SER:HB2	0.54	2.16
1:A:248:LYS:H	1:A:250:VAL:HG22	0.53	0.82
1:A:55:ASN:C	1:A:56:PHE:CG	0.53	2.81
1:A:94:THR:HA	1:A:98:SER:OG	0.53	2.03
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:338:SER:O	1:A:339:LYS:HB3	0.53	2.04

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:131:LEU:HA	1:A:134:GLU:HG2	0.53	1.80
1:A:268:TYR:O	1:A:272:ALA:HB3	0.53	2.04
1:A:239:GLU:O	1:A:240:SER:HB3	0.52	2.04
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: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:308:MET:CA	1:A:309:MET:HB2	0.52	2.34
1:A:105:PHE:HB2	1:A:107:PRO:HD3	0.52	1.60
1:A:72:LEU:CG	1:A:72:LEU:O	0.51	2.58
1:A:313:PHE:CG	1:A:313:PHE:C	0.51	2.83
1:A:118:THR:O	1:A:119:LEU:C	0.51	2.48
1:A:133:ILE:CD1	1:A:136:TYR:CE1	0.51	2.92
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:296:LYS:N	1:A:296:LYS:HE3	0.51	2.21
1:A:180:PRO:C	1:A:182:GLY:H	0.51	2.09
1:A:325:LYS:N	1:A:330:ASP:OD2	0.50	2.44
1:A:198:THR:CB	1:A:199:ASN:OD1	0.50	2.59
1:A:317:MET:HB2	1:A:343:SER:HB2	0.50	0.51
1:A:197:GLU:HA	1:A:201:GLU:HB2	0.50	1.83
1:A:265:TRP:CH2	1:A:268:TYR:CD2	0.50	2.99
1:A:317:MET:SD	1:A:343:SER:C	0.50	2.89
1:A:264:CYS:O	1:A:268:TYR:HB2	0.50	2.06
1:A:203:PHE:C	1:A:206:TYR:H	0.50	2.10
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: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:93:THR:C	1:A:98:SER:CB	0.49	2.79
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:189:ILE:CG2	1:A:192:TYR:C	0.48	2.82
1:A:247:GLU:CD	1:A:314:ARG:NH2	0.48	2.67
1:A:134:GLU:OE1	1:A:245:LYS:NZ	0.48	2.42
1:A:246:ALA:CA	1:A:314:ARG:HE	0.48	2.21
1:A:181:GLU:OE1	1:A:185:CYS:CB	0.48	2.61

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
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:264:CYS:CB	1:A:265:TRP:CZ2	0.48	2.96
1:A:170:PRO:O	1:A:172:LEU:N	0.48	2.47
1:A:215:PRO:HA	1:A:219:ILE:HG22	0.48	1.86
1:A:132:ALA:HB3	1:A:133:ILE:HB	0.47	1.86
1:A:55:ASN:O	1:A:56:PHE:CE1	0.47	2.54
1:A:245:LYS:C	1:A:314:ARG:NE	0.47	2.68
1:A:309:MET:HB3	1:A:310:ASN:CB	0.47	2.31
1:A:246:ALA:CB	1:A:310:ASN:OD1	0.47	2.62
1:A:337:VAL:N	1:A:338:SER:HA	0.47	2.23
1:A:152:HIS:C	1:A:156:GLY:H	0.47	2.12
1:A:246:ALA:O	1:A:310:ASN:HA	0.47	2.09
1:A:131:LEU:C	1:A:134:GLU:N	0.47	2.68
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:147:ARG:HB3	1:A:148:PHE:CB	0.47	2.39
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:232:GLU:HB3	1:A:235:ALA:C	0.46	2.30
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:245:LYS:O	1:A:314:ARG:NE	0.46	2.49
1:A:74:TYR:C	1:A:74:TYR:CD1	0.46	2.89
1:A:247:GLU:N	1:A:314:ARG:NE	0.46	2.64
1:A:92:THR:O	1:A:93:THR:HB	0.46	2.11
1:A:313:PHE:O	1:A:313:PHE:HD1	0.45	1.89
1:A:260:ALA:HA	1:A:263:ILE:HG22	0.45	1.87
1:A:72:LEU:HD11	1:A:131:LEU:HD11	0.45	1.83
1:A:135:ARG:HB2	1:A:253:MET:SD	0.45	2.51
1:A:103:PHE:CD1	1:A:105:PHE:CD2	0.45	3.05
1:A:89:GLY:O	1:A:94:THR:N	0.45	2.46
1:A:110:CYS:N	1:A:111:ASN:HA	0.45	2.26
1:A:250:VAL:N	1:A:313:PHE:CE2	0.45	2.84
1:A:105:PHE:CB	1:A:106:GLY:C	0.45	2.72
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:219:ILE:N	1:A:220:PHE:C	0.45	2.70
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
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:314:ARG:CG	1:A:347:PRO:O	0.44	2.66
1:A:203:PHE:HA	1:A:206:TYR:CB	0.44	2.43
1:A:136:TYR:O	1:A:140:CYS:N	0.44	2.51
1:A:316:CYS:C	1:A:343:SER:CB	0.44	2.79
1:A:60:TYR:O	1:A:64:GLN:N	0.44	2.51
1:A:116:PHE:O	1:A:120:GLY:HA3	0.43	2.13
1:A:247:GLU:CD	1:A:314:ARG:HH22	0.43	2.17
1:A:296:LYS:H	1:A:297:THR:N	0.43	2.11
1:A:125:LEU:CD1	2:A:400:RET:H32	0.43	2.23
1:A:52:PHE:HB3	1:A:53:PRO:HG3	0.43	1.89
1:A:55:ASN:HA	1:A:58:THR:HB	0.43	1.90
1:A:198:THR:OG1	1:A:199:ASN:CA	0.43	2.67
1:A:139:VAL:C	1:A:140:CYS:SG	0.43	2.97
1:A:226:LEU:HB2	1:A:229:THR:HG22	0.43	1.90
1:A:239:GLU:O	1:A:240:SER:CB	0.43	2.65
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:268:TYR:O	1:A:272:ALA:N	0.43	2.52
1:A:259:ILE:HG23	1:A:262:LEU:CG	0.43	2.42
1:A:175:TRP:C	1:A:175:TRP:CD1	0.43	2.91
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:247:GLU:OE1	1:A:314:ARG:NH1	0.42	2.52
1:A:103:PHE:C	1:A:104:VAL:HG23	0.42	2.34
1:A:250:VAL:O	1:A:253:MET:N	0.42	2.52
1:A:113:GLU:O	1:A:114:GLY:C	0.42	2.53
1:A:339:LYS:O	1:A:339:LYS:HG3	0.42	2.14
1:A:72:LEU:O	1:A:72:LEU:HG	0.42	2.14
1:A:148:PHE:C	1:A:150:GLU:N	0.42	2.72
1:A:125:LEU:O	1:A:129:VAL:HG13	0.42	2.14
1:A:245:LYS:O	1:A:314:ARG:CG	0.42	2.67
1:A:56:PHE:H	1:A:58:THR:N	0.42	2.13
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: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:315:ASN:CB	1:A:335:THR:OG1	0.42	2.68
1:A:92:THR:C	1:A:96:TYR:HB2	0.41	2.35
1:A:135:ARG:N	1:A:136:TYR:HB2	0.41	2.08
1:A:316:CYS:O	1:A:317:MET:CB	0.41	2.54

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:113:GLU:OE2	2:A:400:RET:H14	0.41	2.16
1:A:148:PHE:O	1:A:151:ASN:N	0.41	2.54
1:A:142:PRO:O	1:A:144:SER:HA	0.41	2.14
1:A:62:THR:HG22	1:A:62:THR:O	0.41	2.16
1:A:181:GLU:CD	1:A:185:CYS:SG	0.41	2.98
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:212:PHE:CG	2:A:400:RET:H31	0.41	2.49
1:A:309:MET:HG3	1:A:310:ASN:HB2	0.41	1.93
1:A:147:ARG:NE	1:A:150:GLU:OE1	0.41	2.49
1:A:151:ASN:C	1:A:153:ALA:N	0.41	2.74
1:A:214:ILE:N	1:A:215:PRO:CD	0.41	2.83
1:A:250:VAL:O	1:A:253:MET:HA	0.41	2.14
1:A:103:PHE:C	1:A:104:VAL:CG2	0.41	2.86
1:A:93:THR:N	1:A:102:TYR:OH	0.41	2.46
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:228:PHE:HA	1:A:232:GLU:CD	0.40	2.36
1:A:112:LEU:O	1:A:113:GLU:C	0.40	2.58
1:A:272:ALA:CA	1:A:275:ILE:H	0.40	2.30

## 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	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	219	ILE
1	A	99	LEU
1	A	171	PRO
1	A	253	MET
1	A	240	SER
1	A	103	PHE
1	A	110	CYS
1	A	119	LEU
1	A	140	CYS
1	A	139	VAL
1	A	326	ASN
1	A	288	MET
1	A	193	THR
1	A	121	GLY
1	A	290	ILE
1	A	284	GLY
1	A	235	ALA
1	A	325	LYS
1	A	136	TYR
1	A	56	PHE
1	A	220	PHE
1	A	215	PRO
1	A	314	ARG
1	A	242	THR
1	A	334	SER
1	A	318	VAL
1	A	216	LEU
1	A	261	PHE
1	A	209	VAL
1	A	180	PRO
1	A	266	LEU
1	A	244	GLN
1	A	310	ASN
1	A	152	HIS
1	A	170	PRO
1	A	307	ILE
1	A	335	THR
1	A	316	CYS
1	A	67	LYS
1	A	181	GLU
1	A	336	THR
1	A	250	VAL
1	A	58	THR

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Mol	Chain	Res	Type
1	A	337	VAL
1	A	178	TYR
1	A	142	PRO
1	A	346	ALA
1	A	339	LYS
1	A	118	THR
1	A	151	ASN
1	A	321	LEU
1	A	105	PHE
1	A	271	VAL
1	A	227	VAL
1	A	270	GLY
1	A	93	THR
1	A	98	SER
1	A	214	ILE
1	A	70	THR
1	A	102	TYR
1	A	287	PHE
1	A	133	ILE
1	A	71	PRO
1	A	104	VAL
1	A	248	LYS
1	A	149	GLY

### 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	262/296 (89%)	181 (69%)	81 (31%)	2	16
All	All	262/296 (89%)	181 (69%)	81 (31%)	2	16

All 81 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	116	PHE
1	A	99	LEU

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Mol	Chain	Res	Type
1	A	69	ARG
1	A	309	MET
1	A	87	VAL
1	A	137	VAL
1	A	274	TYR
1	A	276	PHE
1	A	296	LYS
1	A	123	ILE
1	A	73	ASN
1	A	223	TYR
1	A	312	GLN
1	A	141	LYS
1	A	171	PRO
1	A	193	THR
1	A	94	THR
1	A	208	PHE
1	A	306	TYR
1	A	177	ARG
1	A	297	THR
1	A	330	ASP
1	A	326	ASN
1	A	237	GLN
1	A	325	LYS
1	A	135	ARG
1	A	341	GLU
1	A	262	LEU
1	A	252	ARG
1	A	217	ILE
1	A	215	PRO
1	A	242	THR
1	A	318	VAL
1	A	131	LEU
1	A	189	ILE
1	A	191	TYR
1	A	211	HIS
1	A	152	HIS
1	A	209	VAL
1	A	113	GLU
1	A	338	SER
1	A	112	LEU
1	A	206	TYR
1	A	337	VAL

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Mol	Chain	Res	Type
1	A	273	PHE
1	A	230	VAL
1	A	313	PHE
1	A	111	ASN
1	A	54	ILE
1	A	243	THR
1	A	58	THR
1	A	179	ILE
1	A	78	ASN
1	A	142	PRO
1	A	212	PHE
1	A	339	LYS
1	A	245	LYS
1	A	317	MET
1	A	134	GLU
1	A	220	PHE
1	A	340	THR
1	A	148	PHE
1	A	291	PRO
1	A	154	ILE
1	A	207	MET
1	A	136	TYR
1	A	214	ILE
1	A	45	PHE
1	A	70	THR
1	A	102	TYR
1	A	200	ASN
1	A	44	MET
1	A	198	THR
1	A	71	PRO
1	A	60	TYR
1	A	221	PHE
1	A	162	VAL
1	A	175	TRP
1	A	231	LYS
1	A	185	CYS
1	A	92	THR

### 6.3.3 RNA ⓘ

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 carbohydrates 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	19,20,21	0.43	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	1	27,27,28	0.74	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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 6.7 Other polymers

There are no such molecules in this entry.

## 6.8 Polymer linkage issues

There are no chain breaks in this entry.



## 7 Chemical shift validation

No chemical shift data were provided