



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:13 PM UTC

PDB ID : 2V12 / pdb_00002v12
Title : Crystal Structure of Renin with Inhibitor 8
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Stutz, S.; Cumin, F.; Fuhrer, W.; Wood, J.M.; Grutter, M.G.
Deposited on : 2007-05-21
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray 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/XrayValidationReportHelp>

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)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

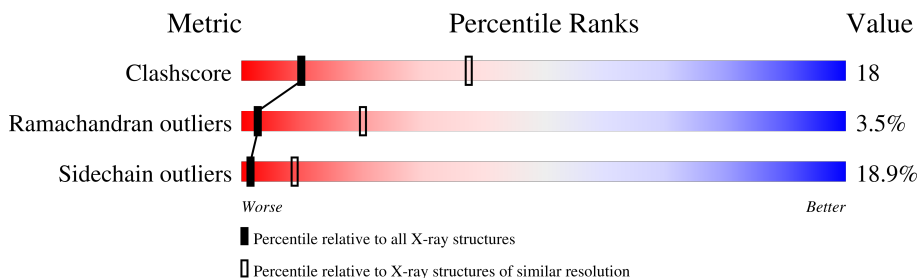
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	340	 44% 33% 17% . .
1	O	340	 40% 35% 19% . .

2 Entry composition [i](#)

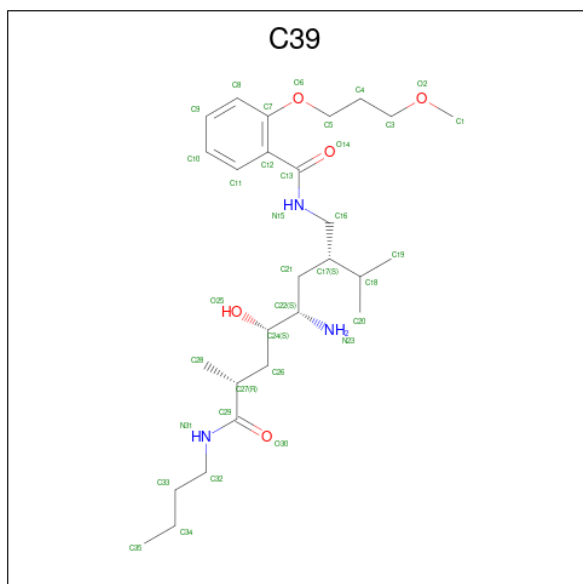
There are 2 unique types of molecules in this entry. The entry contains 5194 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called RENIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	334	Total	C	N	O	S	0	0	1
			2567	1639	416	498	14			
1	O	332	Total	C	N	O	S	0	0	1
			2557	1634	414	495	14			

- Molecule 2 is N-[(2S,4S,5S,7R)-4-AMINO-8-(BUTYLAMINO)-5-HYDROXY-7-METHYL-2-(1-METHYLETHYL)-8-OXOOCTYL]-2-(3-METHOXYPROPOXY)BENZAMIDE (CCD ID: C39) (formula: C₂₇H₄₇N₃O₅).



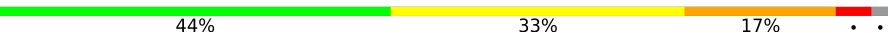
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			35	27	3	5		
2	O	1	Total	C	N	O	0	0
			35	27	3	5		

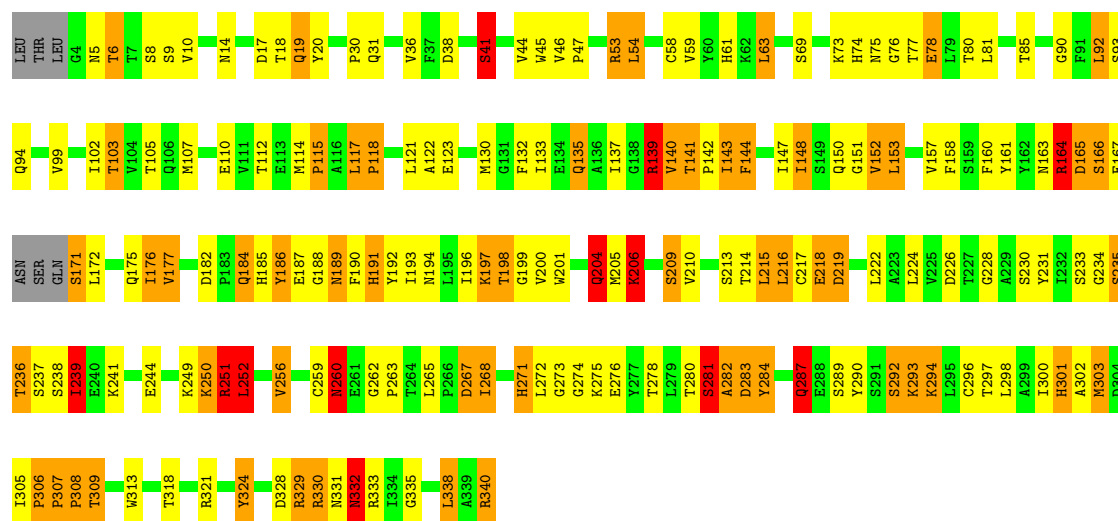
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

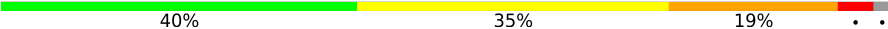
Note EDS was not executed.

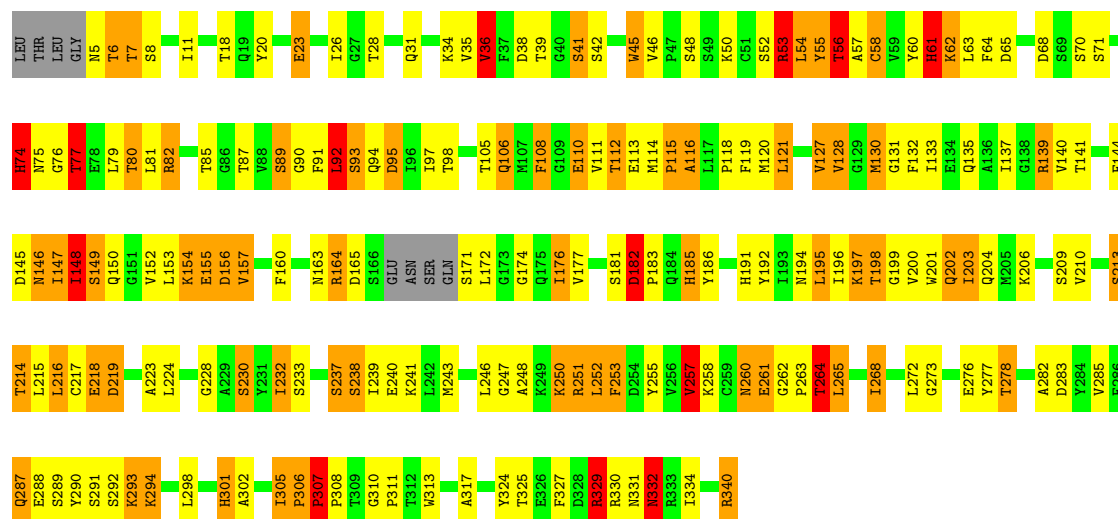
• Molecule 1: RENIN

Chain C: 



• Molecule 1: RENIN

Chain O: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	142.90 Å 142.90 Å 142.90 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.20	Depositor
% Data completeness (in resolution range)	92.0 (10.00-3.20)	Depositor
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.236 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5194	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: C39

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	C	1.42	16/2626 (0.6%)	2.23	122/3560 (3.4%)
1	O	1.42	19/2616 (0.7%)	2.29	141/3547 (4.0%)
All	All	1.42	35/5242 (0.7%)	2.26	263/7107 (3.7%)

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 outliers	#Planarity outliers
1	C	0	1
1	O	0	4
All	All	0	5

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	271	HIS	CD2-NE2	-7.08	1.30	1.37
1	O	185	HIS	CD2-NE2	-6.94	1.30	1.37
1	C	301	HIS	CD2-NE2	-6.86	1.30	1.37
1	C	61	HIS	CD2-NE2	-6.83	1.30	1.37
1	C	18	THR	CA-CB	-6.56	1.43	1.53
1	O	111	VAL	CA-CB	-6.47	1.46	1.54
1	C	338	LEU	CA-CB	-6.28	1.43	1.53
1	O	53	ARG	NE-CZ	5.96	1.39	1.33
1	O	61	HIS	CG-ND1	-5.93	1.31	1.38
1	O	191	HIS	CD2-NE2	-5.90	1.31	1.37
1	O	61	HIS	CD2-NE2	-5.88	1.31	1.37
1	C	233	SER	CA-C	-5.74	1.46	1.52
1	O	204	GLN	CA-CB	-5.70	1.45	1.53
1	O	74	HIS	CD2-NE2	-5.70	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	61	HIS	CG-ND1	-5.67	1.32	1.38
1	C	191	HIS	CA-C	-5.62	1.46	1.52
1	O	64	PHE	CA-CB	-5.60	1.45	1.53
1	C	185	HIS	CD2-NE2	-5.58	1.31	1.37
1	C	191	HIS	CD2-NE2	-5.56	1.31	1.37
1	O	8	SER	CA-CB	-5.54	1.45	1.53
1	O	261	GLU	C-N	-5.39	1.30	1.34
1	C	10	VAL	CA-CB	-5.37	1.47	1.54
1	O	324	TYR	CA-CB	-5.36	1.45	1.53
1	C	210	VAL	CA-CB	-5.35	1.48	1.54
1	O	185	HIS	CG-ND1	-5.34	1.32	1.38
1	C	166	SER	C-N	-5.32	1.25	1.33
1	O	301	HIS	CD2-NE2	-5.26	1.32	1.37
1	C	309	THR	CA-CB	5.22	1.60	1.52
1	O	165	ASP	C-N	-5.18	1.26	1.33
1	C	214	THR	CA-CB	5.18	1.59	1.52
1	O	85	THR	CA-CB	-5.14	1.46	1.54
1	C	268	ILE	CA-CB	-5.12	1.48	1.54
1	O	56	THR	CA-CB	5.07	1.61	1.53
1	O	139	ARG	NE-CZ	5.06	1.38	1.33
1	O	198	THR	CA-CB	5.05	1.61	1.53

All (263) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	191	HIS	CA-CB-CG	-12.32	101.48	113.80
1	C	165	ASP	CA-CB-CG	12.01	124.61	112.60
1	C	165	ASP	O-C-N	10.83	136.13	122.81
1	O	154	LYS	N-CA-C	10.42	126.08	113.16
1	O	65	ASP	CA-CB-CG	-9.37	103.23	112.60
1	C	226	ASP	CA-CB-CG	9.29	121.89	112.60
1	O	324	TYR	CA-C-O	-9.22	110.10	120.70
1	O	7	THR	N-CA-C	-8.99	92.77	108.69
1	C	282	ALA	N-CA-C	-8.99	91.66	110.80
1	O	106	GLN	CG-CD-NE2	8.81	129.61	116.40
1	C	184	GLN	N-CA-C	-8.76	100.47	113.61
1	O	290	TYR	N-CA-C	-8.58	100.93	112.26
1	C	5	ASN	CA-CB-CG	-8.55	104.05	112.60
1	C	331	ASN	CA-CB-CG	-8.34	104.26	112.60
1	C	59	VAL	N-CA-C	-8.30	102.72	110.53
1	C	92	LEU	N-CA-C	8.16	122.55	110.48
1	C	250	LYS	N-CA-C	8.12	123.19	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	103	THR	CA-CB-OG1	-8.12	97.43	109.60
1	C	6	THR	CA-CB-OG1	-8.11	97.43	109.60
1	O	23	GLU	N-CA-C	8.07	122.55	108.75
1	O	210	VAL	CA-C-O	8.04	127.37	120.22
1	O	253	PHE	N-CA-C	-8.04	98.38	110.28
1	O	265	LEU	N-CA-C	7.90	119.67	109.64
1	O	106	GLN	OE1-CD-NE2	-7.88	114.72	122.60
1	C	152	VAL	N-CA-CB	-7.82	101.26	110.64
1	O	61	HIS	CA-CB-CG	-7.81	105.99	113.80
1	O	185	HIS	N-CA-C	7.70	121.98	112.59
1	C	177	VAL	N-CA-C	-7.69	97.40	108.48
1	O	140	VAL	N-CA-C	-7.67	98.78	109.21
1	O	154	LYS	CA-CB-CG	-7.61	98.88	114.10
1	O	38	ASP	CA-CB-CG	7.59	120.19	112.60
1	O	194	ASN	CA-CB-CG	7.58	120.18	112.60
1	C	153	LEU	N-CA-C	7.52	120.84	110.24
1	C	61	HIS	CA-CB-CG	-7.47	106.33	113.80
1	O	268	ILE	N-CA-C	-7.45	97.57	108.89
1	O	163	ASN	CA-CB-CG	7.43	120.03	112.60
1	O	148	ILE	CA-C-O	-7.43	113.69	121.41
1	C	69	SER	N-CA-C	-7.39	97.19	109.46
1	O	252	LEU	N-CA-C	-7.39	96.37	108.12
1	C	164	ARG	CB-CG-CD	7.37	128.25	111.30
1	C	182	ASP	O-C-N	-7.36	115.27	121.23
1	O	85	THR	N-CA-CB	-7.35	101.22	111.00
1	C	164	ARG	N-CA-C	-7.33	99.18	110.10
1	O	121	LEU	N-CA-C	-7.29	104.19	113.23
1	C	38	ASP	CA-C-O	-7.28	113.35	120.92
1	O	144	PHE	CA-CB-CG	-7.21	106.59	113.80
1	O	182	ASP	CA-C-O	7.19	126.21	119.59
1	C	139	ARG	CA-CB-CG	-7.18	99.74	114.10
1	O	144	PHE	CA-C-O	-7.17	113.32	120.70
1	O	174	GLY	CA-C-O	-7.15	111.67	122.54
1	C	331	ASN	OD1-CG-ND2	-7.14	115.46	122.60
1	C	14	ASN	CA-C-O	-7.13	113.12	120.54
1	O	232	ILE	N-CA-C	-7.12	98.04	108.87
1	O	145	ASP	CA-CB-CG	7.12	119.72	112.60
1	C	5	ASN	OD1-CG-ND2	-7.08	115.52	122.60
1	C	297	THR	CA-CB-OG1	-7.08	98.98	109.60
1	C	54	LEU	N-CA-C	-7.08	103.61	111.82
1	C	8	SER	CA-CB-OG	-7.03	97.04	111.10
1	C	239	ILE	N-CA-C	-7.01	103.64	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	290	TYR	O-C-N	-6.95	113.30	122.20
1	O	287	GLN	OE1-CD-NE2	-6.92	115.68	122.60
1	C	300	ILE	N-CA-C	-6.92	98.16	108.12
1	O	276	GLU	CA-CB-CG	-6.87	100.36	114.10
1	O	287	GLN	CG-CD-NE2	6.84	126.66	116.40
1	O	287	GLN	N-CA-C	6.84	119.88	109.62
1	C	163	ASN	CA-CB-CG	6.83	119.42	112.60
1	C	110	GLU	N-CA-C	-6.81	96.56	108.20
1	O	38	ASP	N-CA-C	6.76	119.75	108.20
1	C	148	ILE	CA-C-O	-6.74	113.94	120.95
1	C	331	ASN	CB-CG-ND2	6.72	126.49	116.40
1	C	249	LYS	CB-CG-CD	6.72	126.75	111.30
1	O	8	SER	N-CA-C	-6.70	98.28	109.07
1	O	264	THR	N-CA-CB	-6.70	100.25	110.16
1	O	202	GLN	OE1-CD-NE2	-6.69	115.91	122.60
1	O	247	GLY	N-CA-C	-6.67	107.15	115.08
1	O	302	ALA	CA-C-O	-6.65	113.82	121.47
1	C	6	THR	CA-CB-CG2	6.61	121.73	110.50
1	O	182	ASP	CA-CB-CG	6.61	119.21	112.60
1	O	92	LEU	N-CA-C	6.58	120.60	110.20
1	O	264	THR	CA-CB-OG1	-6.57	99.75	109.60
1	O	105	THR	N-CA-C	-6.53	98.58	108.96
1	O	219	ASP	N-CA-C	-6.49	96.97	110.80
1	C	189	ASN	CB-CG-ND2	6.42	126.04	116.40
1	O	260	ASN	CA-CB-CG	6.42	119.02	112.60
1	O	6	THR	CA-C-O	6.40	127.93	120.89
1	O	313	TRP	N-CA-C	-6.39	100.17	110.32
1	O	251	ARG	N-CA-C	-6.38	97.21	110.80
1	O	108	PHE	CA-CB-CG	6.38	120.17	113.80
1	O	46	VAL	O-C-N	-6.37	117.26	121.72
1	O	331	ASN	OD1-CG-ND2	-6.36	116.24	122.60
1	O	149	SER	CA-CB-OG	6.34	123.78	111.10
1	O	55	TYR	N-CA-C	-6.31	96.88	107.99
1	O	115	PRO	O-C-N	6.31	131.16	122.64
1	O	198	THR	CB-CA-C	6.30	120.18	109.53
1	O	214	THR	CA-CB-OG1	-6.29	100.16	109.60
1	C	267	ASP	CA-CB-CG	6.28	118.88	112.60
1	O	264	THR	N-CA-C	6.28	118.20	111.36
1	O	155	GLU	CA-CB-CG	6.27	126.64	114.10
1	O	257	VAL	O-C-N	-6.25	116.01	122.95
1	C	58	CYS	N-CA-C	-6.25	105.14	112.89
1	O	265	LEU	CA-C-N	6.24	127.64	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	265	LEU	C-N-CA	6.24	127.64	119.84
1	C	143	ILE	CA-C-O	-6.23	114.47	120.95
1	C	31	GLN	N-CA-C	-6.22	98.59	108.73
1	C	198	THR	CA-CB-OG1	-6.21	100.28	109.60
1	O	257	VAL	N-CA-C	-6.21	99.65	108.65
1	C	18	THR	CA-CB-OG1	-6.17	100.34	109.60
1	O	54	LEU	N-CA-CB	-6.17	101.46	110.53
1	O	156	ASP	CA-CB-CG	6.16	118.76	112.60
1	C	122	ALA	N-CA-C	6.12	118.67	108.20
1	O	53	ARG	NE-CZ-NH1	6.12	127.62	121.50
1	C	78	GLU	CB-CG-CD	6.11	122.99	112.60
1	O	197	LYS	N-CA-C	-6.11	99.24	108.46
1	O	45	TRP	CB-CG-CD1	-6.09	117.76	126.90
1	C	290	TYR	CA-C-O	6.08	126.84	119.78
1	C	219	ASP	N-CA-CB	6.08	120.77	110.49
1	C	251	ARG	N-CA-C	6.08	123.74	110.80
1	O	18	THR	N-CA-C	-6.07	106.20	113.97
1	C	324	TYR	CA-C-O	-6.07	114.00	120.92
1	C	204	GLN	OE1-CD-NE2	-6.07	116.53	122.60
1	O	294	LYS	N-CA-C	6.06	118.91	109.52
1	C	152	VAL	N-CA-C	6.05	116.25	110.74
1	C	301	HIS	CB-CG-CD2	-6.05	123.34	131.20
1	O	68	ASP	N-CA-C	-6.05	106.23	113.97
1	C	171	SER	CA-C-O	-6.04	110.53	120.80
1	O	71	SER	N-CA-C	6.03	120.24	113.01
1	C	19	GLN	CA-CB-CG	-6.01	102.08	114.10
1	O	128	VAL	N-CA-C	-5.99	99.79	108.71
1	O	34	LYS	CA-C-O	-5.99	113.55	120.49
1	C	281	SER	N-CA-C	5.96	121.60	113.37
1	C	216	LEU	N-CA-CB	-5.96	101.70	111.66
1	C	209	SER	CA-C-N	-5.95	115.43	122.93
1	C	209	SER	C-N-CA	-5.95	115.43	122.93
1	O	329	ARG	CA-CB-CG	-5.94	102.22	114.10
1	O	334	ILE	O-C-N	-5.93	116.75	123.10
1	O	75	ASN	CA-C-O	-5.93	112.03	120.51
1	C	191	HIS	CB-CG-CD2	-5.89	123.54	131.20
1	O	147	ILE	N-CA-C	-5.89	104.77	110.72
1	C	206	LYS	CB-CA-C	-5.89	102.81	111.77
1	C	332	ASN	OD1-CG-ND2	-5.89	116.71	122.60
1	C	189	ASN	OD1-CG-ND2	-5.89	116.71	122.60
1	O	75	ASN	O-C-N	-5.87	114.78	122.59
1	C	103	THR	CA-CB-CG2	5.87	120.48	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	112	THR	CA-CB-OG1	-5.87	100.79	109.60
1	C	201	TRP	CG-CD2-CE3	5.86	139.76	133.90
1	O	154	LYS	CG-CD-CE	5.86	124.78	111.30
1	O	130	MET	N-CA-C	-5.86	105.89	113.16
1	C	292	SER	N-CA-C	-5.85	104.82	111.14
1	O	31	GLN	CA-C-O	-5.84	113.20	120.57
1	O	218	GLU	N-CA-C	-5.83	102.28	110.50
1	O	62	LYS	N-CA-C	-5.81	100.42	109.72
1	C	185	HIS	CB-CG-CD2	-5.81	123.65	131.20
1	O	176	ILE	CA-CB-CG1	-5.81	100.53	110.40
1	C	313	TRP	CG-CD2-CE3	5.78	139.68	133.90
1	C	260	ASN	OD1-CG-ND2	-5.78	116.82	122.60
1	C	284	TYR	CA-C-O	-5.78	112.44	119.32
1	O	213	SER	N-CA-CB	-5.75	100.78	110.49
1	C	233	SER	CB-CA-C	-5.73	98.88	109.37
1	O	82	ARG	CB-CG-CD	5.73	124.48	111.30
1	C	18	THR	N-CA-CB	-5.71	102.11	110.40
1	O	287	GLN	CB-CG-CD	5.71	122.30	112.60
1	O	325	THR	CA-CB-OG1	-5.70	101.05	109.60
1	C	301	HIS	ND1-CG-CD2	5.70	111.80	106.10
1	C	190	PHE	CA-CB-CG	-5.69	108.11	113.80
1	C	164	ARG	CA-CB-CG	5.67	125.44	114.10
1	O	332	ASN	CB-CG-ND2	-5.67	107.90	116.40
1	O	283	ASP	CA-CB-CG	5.66	118.26	112.60
1	O	172	LEU	CA-C-O	-5.66	114.43	120.42
1	C	206	LYS	N-CA-C	5.63	120.37	107.48
1	O	257	VAL	N-CA-CB	-5.62	103.97	112.35
1	C	75	ASN	CB-CG-ND2	5.62	124.83	116.40
1	C	329	ARG	CA-CB-CG	-5.61	102.88	114.10
1	C	244	GLU	CB-CG-CD	5.59	122.10	112.60
1	O	61	HIS	N-CA-C	5.58	122.70	110.80
1	C	10	VAL	N-CA-C	-5.57	100.34	108.97
1	O	53	ARG	CA-C-O	5.57	128.47	120.51
1	C	30	PRO	O-C-N	5.56	130.06	123.06
1	O	192	TYR	N-CA-C	5.55	119.14	110.32
1	C	148	ILE	O-C-N	-5.54	116.50	121.87
1	O	110	GLU	N-CA-C	-5.52	98.23	107.99
1	C	176	ILE	CB-CA-C	-5.51	102.08	110.95
1	C	151	GLY	CA-C-O	5.50	126.73	119.58
1	O	238	SER	N-CA-C	-5.50	105.20	111.14
1	O	45	TRP	CG-CD2-CE3	5.49	139.39	133.90
1	O	81	LEU	N-CA-CB	-5.48	101.34	110.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	287	GLN	O-C-N	-5.47	115.31	122.59
1	O	327	PHE	CA-C-O	5.47	126.94	120.70
1	C	272	LEU	O-C-N	5.46	129.74	123.02
1	O	56	THR	N-CA-C	-5.46	104.72	111.33
1	O	198	THR	CA-CB-OG1	-5.44	101.44	109.60
1	O	53	ARG	N-CA-C	5.43	122.36	110.80
1	C	41	SER	CA-CB-OG	5.42	121.93	111.10
1	C	256	VAL	N-CA-CB	-5.42	102.48	111.36
1	C	301	HIS	CA-CB-CG	-5.41	108.39	113.80
1	O	194	ASN	OD1-CG-ND2	-5.40	117.20	122.60
1	C	233	SER	CA-CB-OG	5.39	121.88	111.10
1	O	111	VAL	CA-CB-CG2	-5.39	101.24	110.40
1	C	36	VAL	O-C-N	-5.38	117.06	123.03
1	C	252	LEU	N-CA-C	5.37	122.23	110.80
1	O	157	VAL	N-CA-C	-5.36	100.12	108.81
1	C	5	ASN	CB-CA-C	-5.36	103.34	110.79
1	C	144	PHE	CA-CB-CG	-5.36	108.44	113.80
1	O	7	THR	CB-CA-C	5.35	119.02	109.65
1	O	257	VAL	CA-C-O	-5.35	116.40	121.64
1	C	233	SER	N-CA-CB	5.34	119.40	110.85
1	O	111	VAL	O-C-N	5.34	128.74	122.81
1	C	99	VAL	N-CA-C	-5.34	97.10	106.61
1	C	135	GLN	OE1-CD-NE2	-5.32	117.28	122.60
1	C	46	VAL	O-C-N	-5.30	118.01	121.72
1	C	275	LYS	O-C-N	-5.29	115.74	122.78
1	C	74	HIS	CB-CG-CD2	-5.29	124.33	131.20
1	O	53	ARG	CA-CB-CG	5.28	124.66	114.10
1	O	156	ASP	CA-C-O	5.28	127.49	121.58
1	C	105	THR	N-CA-C	-5.27	102.68	110.48
1	C	85	THR	CA-CB-OG1	-5.26	101.72	109.60
1	C	186	TYR	CA-CB-CG	5.25	123.35	113.90
1	O	201	TRP	CG-CD2-CE3	5.25	139.15	133.90
1	O	156	ASP	O-C-N	5.25	129.25	122.43
1	C	99	VAL	O-C-N	5.24	127.79	122.71
1	O	77	THR	OG1-CB-CG2	5.23	119.77	109.30
1	C	115	PRO	CA-C-O	5.23	126.99	121.03
1	C	6	THR	O-C-N	5.22	129.53	122.59
1	O	282	ALA	CB-CA-C	-5.21	101.82	110.68
1	O	278	THR	CA-CB-OG1	-5.21	101.79	109.60
1	C	278	THR	CA-CB-OG1	-5.20	101.80	109.60
1	O	111	VAL	N-CA-CB	-5.20	104.86	110.53
1	C	31	GLN	OE1-CD-NE2	-5.19	117.41	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	219	ASP	CA-CB-CG	5.19	117.79	112.60
1	C	239	ILE	CA-C-O	-5.19	115.35	120.85
1	O	332	ASN	N-CA-CB	-5.19	103.46	111.65
1	C	188	GLY	CA-C-N	-5.18	113.70	122.67
1	C	188	GLY	C-N-CA	-5.18	113.70	122.67
1	O	201	TRP	CB-CG-CD1	-5.17	119.14	126.90
1	O	163	ASN	N-CA-CB	-5.17	102.56	110.42
1	O	215	LEU	CA-C-N	-5.17	113.72	123.27
1	O	215	LEU	C-N-CA	-5.17	113.72	123.27
1	C	201	TRP	CB-CG-CD1	-5.16	119.15	126.90
1	O	94	GLN	N-CA-C	5.16	117.47	108.76
1	C	44	VAL	O-C-N	-5.15	117.89	123.14
1	O	288	GLU	CA-C-N	5.10	131.28	121.54
1	O	288	GLU	C-N-CA	5.10	131.28	121.54
1	O	36	VAL	CA-C-O	-5.09	114.43	121.51
1	O	191	HIS	CB-CG-CD2	-5.08	124.59	131.20
1	O	141	THR	CA-C-N	5.08	125.01	119.78
1	O	141	THR	C-N-CA	5.08	125.01	119.78
1	C	76	GLY	N-CA-C	5.08	122.12	115.47
1	C	313	TRP	CB-CG-CD1	-5.08	119.28	126.90
1	O	92	LEU	CA-C-O	-5.06	115.28	121.05
1	C	38	ASP	N-CA-C	5.06	116.89	107.99
1	C	61	HIS	CB-CG-CD2	-5.05	124.63	131.20
1	C	14	ASN	OD1-CG-ND2	-5.05	117.55	122.60
1	O	305	ILE	CA-C-N	5.05	125.58	120.38
1	O	305	ILE	C-N-CA	5.05	125.58	120.38
1	C	271	HIS	CB-CG-CD2	-5.05	124.64	131.20
1	C	305	ILE	CA-C-O	5.05	124.67	119.82
1	O	307	PRO	O-C-N	-5.03	115.52	121.46
1	C	141	THR	CA-CB-OG1	-5.03	102.05	109.60
1	O	58	CYS	N-CA-C	-5.03	104.75	111.24
1	C	236	THR	CA-CB-OG1	-5.03	102.06	109.60
1	O	258	LYS	CB-CG-CD	-5.02	99.75	111.30
1	O	163	ASN	OD1-CG-ND2	-5.01	117.59	122.60
1	O	152	VAL	N-CA-CB	-5.00	102.97	111.23
1	O	93	SER	N-CA-C	5.00	115.64	108.74

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	307	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	O	182	ASP	Peptide
1	O	277	TYR	Sidechain
1	O	306	PRO	Peptide
1	O	307	PRO	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2567	0	2498	91	0
1	O	2557	0	2490	89	0
2	C	35	0	47	6	0
2	O	35	0	47	5	0
All	All	5194	0	5082	180	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (180) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:5:ASN:HA	1:O:154:LYS:HD3	1.28	1.07
1:O:148:ILE:HD11	1:O:156:ASP:HB3	1.56	0.87
1:C:293:LYS:HG3	1:C:294:LYS:HG2	1.58	0.85
1:O:243:MET:HE1	1:O:298:LEU:HD12	1.61	0.83
1:O:285:VAL:HG22	1:O:298:LEU:HD22	1.64	0.79
1:C:260:ASN:OD1	1:C:292:SER:HA	1.87	0.74
1:O:55:TYR:HB2	1:O:58:CYS:SG	2.30	0.71
1:O:6:THR:HB	1:O:153:LEU:HA	1.73	0.70
1:O:80:THR:HG23	1:O:89:SER:HB3	1.73	0.70
1:C:197:LYS:N	1:C:197:LYS:HD2	2.08	0.68
1:O:53:ARG:HH11	1:O:53:ARG:HB3	1.59	0.67
1:C:20:TYR:HD1	2:C:350:C39:H1C1	1.60	0.67
1:C:197:LYS:HD2	1:C:197:LYS:H	1.60	0.66
1:C:53:ARG:NE	1:C:53:ARG:H	1.94	0.66
1:C:204:GLN:HE21	1:C:205:MET:N	1.93	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:PHE:HB3	1:C:329:ARG:NH2	2.13	0.64
1:C:193:ILE:HD12	1:C:273:GLY:HA3	1.79	0.63
1:O:230:SER:O	1:O:317:ALA:HB3	1.99	0.63
1:C:293:LYS:HZ2	1:C:294:LYS:H	1.46	0.62
1:O:200:VAL:HG12	1:O:202:GLN:HB2	1.81	0.62
1:C:81:LEU:HD23	1:C:137:ILE:HD12	1.81	0.61
1:C:157:VAL:HG12	1:C:328:ASP:HA	1.81	0.60
1:C:204:GLN:HE21	1:C:205:MET:H	1.49	0.60
1:C:186:TYR:HA	1:C:338:LEU:O	2.01	0.60
1:O:5:ASN:OD1	1:O:154:LYS:HE2	2.02	0.60
1:O:216:LEU:HB3	1:O:241:LYS:HE2	1.83	0.59
1:O:147:ILE:O	1:O:150:GLN:HG2	2.02	0.59
1:O:228:GLY:HA2	2:O:350:C39:H3C1	1.84	0.59
1:C:239:ILE:HB	1:C:302:ALA:HB2	1.85	0.59
1:C:164:ARG:NH1	1:C:164:ARG:H	2.00	0.59
1:C:196:ILE:HD11	1:C:204:GLN:HB2	1.85	0.58
1:C:139:ARG:HH11	1:C:139:ARG:HG2	1.69	0.58
1:O:233:SER:HA	1:O:301:HIS:O	2.03	0.58
1:O:53:ARG:HB3	1:O:53:ARG:NH1	2.17	0.58
1:O:139:ARG:NH1	1:O:139:ARG:H	2.02	0.57
1:O:216:LEU:N	1:O:241:LYS:HZ3	2.01	0.57
1:O:209:SER:HA	1:O:214:THR:HA	1.87	0.57
1:O:216:LEU:HB3	1:O:241:LYS:NZ	2.20	0.57
1:O:132:PHE:HD2	1:O:199:GLY:C	2.13	0.56
1:C:53:ARG:N	1:C:53:ARG:HE	2.03	0.56
1:C:293:LYS:HE3	1:C:294:LYS:HD2	1.88	0.56
1:O:139:ARG:HH11	1:O:139:ARG:HG2	1.71	0.56
1:O:307:PRO:HA	1:O:310:GLY:O	2.06	0.56
1:O:26:ILE:HG23	1:O:97:ILE:HG12	1.86	0.56
1:O:202:GLN:HA	1:O:223:ALA:O	2.06	0.56
1:O:11:ILE:HD12	1:O:11:ILE:H	1.71	0.55
1:O:41:SER:HB3	2:O:350:C39:H331	1.89	0.54
1:C:213:SER:O	1:C:215:LEU:HD23	2.07	0.54
1:O:291:SER:HB3	1:O:294:LYS:HG3	1.90	0.54
1:C:259:CYS:SG	1:C:296:CYS:N	2.82	0.53
1:O:79:LEU:HD13	1:O:92:LEU:HD13	1.90	0.53
1:C:133:ILE:HG12	1:C:139:ARG:HH12	1.73	0.53
1:C:187:GLU:HB3	1:C:340:ARG:HE	1.74	0.53
1:C:192:TYR:HB3	1:C:333:ARG:HD3	1.91	0.52
1:C:330:ARG:O	1:C:330:ARG:HD3	2.09	0.52
1:O:155:GLU:HB3	1:O:157:VAL:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:GLU:N	1:C:171:SER:N	2.58	0.52
1:O:248:ALA:HA	1:O:257:VAL:HG23	1.92	0.52
1:O:216:LEU:HB3	1:O:241:LYS:CE	2.40	0.52
1:C:47:PRO:HB2	1:C:63:LEU:HD23	1.92	0.52
1:C:53:ARG:H	1:C:53:ARG:HE	1.57	0.52
1:C:102:ILE:HG21	1:C:147:ILE:HG23	1.92	0.52
1:O:250:LYS:HA	1:O:255:TYR:HA	1.91	0.51
1:C:206:LYS:H	1:C:206:LYS:HD2	1.76	0.51
1:O:127:VAL:HG11	2:O:350:C39:H201	1.91	0.51
1:C:144:PHE:HB3	1:C:329:ARG:HH21	1.76	0.51
1:O:246:LEU:HD21	1:O:268:ILE:HD11	1.92	0.51
1:O:5:ASN:HA	1:O:154:LYS:CD	2.20	0.51
1:C:107:MET:HB2	1:C:140:VAL:HG13	1.92	0.51
1:O:216:LEU:HB3	1:O:241:LYS:HZ3	1.76	0.50
1:C:271:HIS:CD2	1:C:276:GLU:HG3	2.46	0.50
1:C:267:ASP:OD1	1:C:280:THR:HG22	2.10	0.50
1:C:20:TYR:CD1	2:C:350:C39:H1C1	2.45	0.50
1:C:301:HIS:HE1	1:C:303:MET:HG3	1.76	0.50
1:C:216:LEU:HD13	1:C:241:LYS:CE	2.42	0.50
1:C:234:GLY:O	1:C:302:ALA:HA	2.11	0.49
1:O:95:ASP:HB2	1:O:108:PHE:HE2	1.77	0.49
1:O:156:ASP:OD1	1:O:330:ARG:HB3	2.13	0.49
1:O:261:GLU:O	1:O:264:THR:HB	2.13	0.49
1:O:185:HIS:HA	1:O:340:ARG:O	2.11	0.49
1:C:150:GLN:O	1:C:152:VAL:HG23	2.13	0.49
1:O:196:ILE:HB	1:O:197:LYS:HG2	1.94	0.49
1:C:301:HIS:CE1	1:C:303:MET:HG3	2.48	0.48
1:C:250:LYS:O	1:C:250:LYS:HD3	2.14	0.48
1:O:182:ASP:HA	1:O:183:PRO:HD3	1.56	0.48
1:C:132:PHE:HB2	1:C:199:GLY:O	2.13	0.48
1:O:183:PRO:HA	1:O:186:TYR:CE1	2.49	0.48
1:C:191:HIS:O	1:C:335:GLY:HA2	2.14	0.48
1:O:195:LEU:HB2	1:O:332:ASN:O	2.13	0.48
1:O:257:VAL:HG21	1:O:265:LEU:HD21	1.95	0.48
1:O:56:THR:HB	1:O:120:MET:SD	2.53	0.47
1:C:17:ASP:HB3	1:C:321:ARG:CZ	2.44	0.47
1:O:74:HIS:HA	1:O:93:SER:HB2	1.96	0.47
1:O:57:ALA:HB2	1:O:116:ALA:HA	1.97	0.47
1:O:305:ILE:O	1:O:310:GLY:HA3	2.14	0.47
1:C:148:ILE:HD13	1:C:153:LEU:HD12	1.97	0.47
1:C:176:ILE:HG22	1:C:177:VAL:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:SER:HB2	2:C:350:C39:H353	1.95	0.47
1:C:216:LEU:HD12	1:C:217:CYS:H	1.80	0.47
1:O:62:LYS:C	1:O:63:LEU:HD12	2.40	0.47
1:C:135:GLN:O	2:C:350:C39:H352	2.15	0.46
2:C:350:C39:H193	2:C:350:C39:H15	1.80	0.46
1:O:237:SER:HA	1:O:240:GLU:HB2	1.97	0.46
1:O:61:HIS:HE1	1:O:119:PHE:O	1.98	0.46
1:O:216:LEU:HD21	1:O:238:SER:OG	2.16	0.46
1:C:340:ARG:NH2	1:O:7:THR:HG22	2.31	0.46
1:C:139:ARG:HH11	1:C:139:ARG:CG	2.28	0.46
1:O:90:GLY:HA2	1:O:112:THR:HB	1.96	0.46
1:C:45:TRP:HZ3	1:C:114:MET:HE3	1.81	0.46
1:O:164:ARG:HH11	1:O:164:ARG:HD2	1.63	0.46
1:C:340:ARG:HH11	1:C:340:ARG:HG3	1.81	0.46
1:O:5:ASN:CA	1:O:154:LYS:HD3	2.20	0.46
1:C:47:PRO:HG3	1:C:114:MET:HE1	1.98	0.45
1:C:268:ILE:HG12	1:C:284:TYR:CE2	2.51	0.45
2:O:350:C39:H193	2:O:350:C39:H15	1.80	0.45
1:C:280:THR:O	1:C:283:ASP:HB2	2.16	0.45
1:O:82:ARG:HA	1:O:87:THR:OG1	2.16	0.45
1:C:338:LEU:HD23	1:C:338:LEU:HA	1.72	0.45
1:C:228:GLY:HA2	2:C:350:C39:H3C1	1.98	0.45
1:C:282:ALA:O	1:C:283:ASP:C	2.59	0.45
1:C:308:PRO:HB2	1:C:309:THR:HG23	1.99	0.45
1:C:73:LYS:HB2	1:C:94:GLN:HB3	1.97	0.45
1:C:340:ARG:HH22	1:O:7:THR:HG22	1.82	0.45
1:O:139:ARG:NH1	1:O:139:ARG:N	2.65	0.45
1:O:11:ILE:HD12	1:O:11:ILE:N	2.32	0.44
1:C:328:ASP:HB3	1:C:333:ARG:O	2.18	0.44
1:O:36:VAL:HG11	2:O:350:C39:H192	2.00	0.44
1:C:53:ARG:H	1:C:53:ARG:CD	2.29	0.44
1:C:218:GLU:H	1:C:218:GLU:CD	2.25	0.44
1:O:39:THR:HG22	1:O:130:MET:HB2	2.00	0.44
1:C:90:GLY:HA2	1:C:112:THR:OG1	2.17	0.44
1:C:196:ILE:HD12	1:C:222:LEU:HD23	1.99	0.44
1:O:48:SER:HB2	1:O:110:GLU:HB3	2.00	0.44
1:C:141:THR:HA	1:C:142:PRO:HD3	1.56	0.44
1:C:194:ASN:HA	1:C:333:ARG:HB3	2.00	0.43
1:O:154:LYS:HA	1:O:154:LYS:HD2	1.43	0.43
1:O:203:ILE:HG13	1:O:223:ALA:HB3	1.99	0.43
1:C:239:ILE:HD13	1:C:239:ILE:HA	1.69	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:LYS:O	1:C:252:LEU:N	2.51	0.43
1:C:161:TYR:HB2	1:C:324:TYR:CE2	2.53	0.43
1:O:90:GLY:HA3	1:O:110:GLU:O	2.18	0.43
1:C:19:GLN:OE1	1:C:123:GLU:N	2.52	0.43
1:O:60:TYR:HD1	1:O:120:MET:HG3	1.83	0.43
1:C:265:LEU:HB2	1:C:281:SER:OG	2.19	0.43
1:O:243:MET:SD	1:O:246:LEU:HD12	2.59	0.43
1:C:289:SER:OG	1:C:294:LYS:HG3	2.19	0.43
1:O:146:ASN:O	1:O:149:SER:HB3	2.17	0.43
1:O:305:ILE:HA	1:O:306:PRO:HD3	1.84	0.43
1:O:114:MET:HA	1:O:115:PRO:HD3	1.84	0.43
1:C:194:ASN:HD22	1:C:194:ASN:N	2.17	0.42
1:O:77:THR:O	1:O:91:PHE:HA	2.18	0.42
1:C:333:ARG:HD2	1:C:333:ARG:C	2.44	0.42
1:O:7:THR:HG23	1:O:177:VAL:CG1	2.49	0.42
1:C:192:TYR:HA	1:C:335:GLY:HA2	2.01	0.42
1:C:213:SER:O	1:C:215:LEU:N	2.52	0.42
1:O:35:VAL:HG21	1:O:128:VAL:HG23	2.02	0.42
1:C:306:PRO:HG2	1:C:308:PRO:HG2	2.02	0.42
1:O:132:PHE:HE1	1:O:329:ARG:CZ	2.33	0.42
1:O:217:CYS:SG	1:O:217:CYS:O	2.78	0.42
1:O:45:TRP:NE1	1:O:127:VAL:HG13	2.36	0.41
1:C:158:PHE:HD2	1:C:160:PHE:HE2	1.69	0.41
1:C:117:LEU:HA	1:C:118:PRO:HA	1.80	0.41
1:O:42:SER:OG	1:O:135:GLN:HB2	2.21	0.41
1:C:139:ARG:O	1:C:141:THR:N	2.54	0.41
1:C:239:ILE:CB	1:C:302:ALA:HB2	2.51	0.41
1:O:160:PHE:CE1	1:O:176:ILE:HD11	2.55	0.41
1:O:292:SER:HB2	1:O:293:LYS:NZ	2.36	0.41
1:C:206:LYS:NZ	1:C:274:GLY:H	2.19	0.41
1:O:89:SER:OG	1:O:113:GLU:HB2	2.21	0.41
1:O:239:ILE:HD13	1:O:239:ILE:HA	1.88	0.41
1:O:251:ARG:HB3	1:O:252:LEU:H	1.60	0.41
1:O:262:GLY:HA2	1:O:265:LEU:HD12	2.03	0.41
1:C:217:CYS:SG	1:C:217:CYS:O	2.79	0.40
1:O:146:ASN:HD22	1:O:146:ASN:HA	1.71	0.40
1:C:47:PRO:HG3	1:C:114:MET:CE	2.51	0.40
1:C:231:TYR:HD2	1:C:301:HIS:CD2	2.40	0.40
1:O:79:LEU:HD22	1:O:92:LEU:HD12	2.02	0.40
1:C:198:THR:OG1	1:C:332:ASN:ND2	2.54	0.40
1:O:285:VAL:HG22	1:O:298:LEU:CD2	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:LEU:HA	1:C:137:ILE:HD12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 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 X-ray entries followed by that with respect to entries of similar resolution.

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	C	330/340 (97%)	296 (90%)	23 (7%)	11 (3%)	3	21
1	O	328/340 (96%)	281 (86%)	35 (11%)	12 (4%)	2	18
All	All	658/680 (97%)	577 (88%)	58 (9%)	23 (4%)	3	20

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	166	SER
1	C	251	ARG
1	O	50	LYS
1	O	116	ALA
1	C	140	VAL
1	C	219	ASP
1	C	262	GLY
1	O	53	ARG
1	O	61	HIS
1	O	273	GLY
1	O	289	SER
1	O	308	PRO
1	C	235	SER
1	C	294	LYS
1	C	283	ASP
1	O	76	GLY
1	O	77	THR

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Mol	Chain	Res	Type
1	C	287	GLN
1	O	131	GLY
1	C	308	PRO
1	C	263	PRO
1	O	307	PRO
1	O	137	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	C	283/290 (98%)	229 (81%)	54 (19%)	1	9
1	O	282/290 (97%)	229 (81%)	53 (19%)	1	9
All	All	565/580 (97%)	458 (81%)	107 (19%)	1	9

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	6	THR
1	C	9	SER
1	C	41	SER
1	C	53	ARG
1	C	54	LEU
1	C	63	LEU
1	C	77	THR
1	C	78	GLU
1	C	80	THR
1	C	92	LEU
1	C	93	SER
1	C	103	THR
1	C	115	PRO
1	C	117	LEU
1	C	118	PRO
1	C	121	LEU
1	C	130	MET

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Mol	Chain	Res	Type
1	C	139	ARG
1	C	143	ILE
1	C	164	ARG
1	C	165	ASP
1	C	172	LEU
1	C	175	GLN
1	C	184	GLN
1	C	189	ASN
1	C	197	LYS
1	C	200	VAL
1	C	204	GLN
1	C	206	LYS
1	C	209	SER
1	C	215	LEU
1	C	218	GLU
1	C	224	LEU
1	C	230	SER
1	C	235	SER
1	C	236	THR
1	C	237	SER
1	C	238	SER
1	C	239	ILE
1	C	251	ARG
1	C	252	LEU
1	C	256	VAL
1	C	260	ASN
1	C	281	SER
1	C	287	GLN
1	C	293	LYS
1	C	298	LEU
1	C	303	MET
1	C	306	PRO
1	C	307	PRO
1	C	318	THR
1	C	330	ARG
1	C	332	ASN
1	C	340	ARG
1	O	20	TYR
1	O	23	GLU
1	O	28	THR
1	O	36	VAL
1	O	41	SER

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Mol	Chain	Res	Type
1	O	52	SER
1	O	53	ARG
1	O	54	LEU
1	O	56	THR
1	O	70	SER
1	O	74	HIS
1	O	80	THR
1	O	89	SER
1	O	92	LEU
1	O	95	ASP
1	O	98	THR
1	O	106	GLN
1	O	118	PRO
1	O	121	LEU
1	O	127	VAL
1	O	133	ILE
1	O	146	ASN
1	O	148	ILE
1	O	164	ARG
1	O	171	SER
1	O	181	SER
1	O	182	ASP
1	O	195	LEU
1	O	198	THR
1	O	203	ILE
1	O	206	LYS
1	O	213	SER
1	O	216	LEU
1	O	218	GLU
1	O	219	ASP
1	O	224	LEU
1	O	230	SER
1	O	232	ILE
1	O	237	SER
1	O	250	LYS
1	O	253	PHE
1	O	257	VAL
1	O	260	ASN
1	O	263	PRO
1	O	264	THR
1	O	272	LEU
1	O	278	THR

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Mol	Chain	Res	Type
1	O	287	GLN
1	O	293	LYS
1	O	311	PRO
1	O	329	ARG
1	O	332	ASN
1	O	340	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	175	GLN
1	C	189	ASN
1	C	194	ASN
1	C	204	GLN
1	C	301	HIS
1	C	331	ASN
1	C	332	ASN
1	O	31	GLN
1	O	146	ASN
1	O	185	HIS
1	O	202	GLN
1	O	271	HIS
1	O	332	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	C39	O	350	-	35,35,35	1.29	2 (5%)	35,44,44	1.89	8 (22%)
2	C39	C	350	-	35,35,35	1.40	2 (5%)	35,44,44	1.89	7 (20%)

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	C39	O	350	-	-	14/40/40/40	0/1/1/1
2	C39	C	350	-	-	15/40/40/40	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	350	C39	C12-C13	-5.99	1.38	1.50
2	O	350	C39	C12-C13	-5.51	1.39	1.50
2	C	350	C39	C11-C12	-2.32	1.36	1.39
2	O	350	C39	O6-C7	2.23	1.41	1.37

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	350	C39	O6-C7-C8	-4.94	113.17	123.95
2	O	350	C39	O6-C7-C12	4.82	127.57	116.97
2	C	350	C39	O6-C7-C12	4.68	127.28	116.97
2	C	350	C39	C27-C29-N31	4.39	122.37	116.68
2	O	350	C39	O6-C7-C8	-4.31	114.55	123.95
2	O	350	C39	C7-C12-C13	-3.82	119.35	126.24
2	O	350	C39	C11-C12-C7	3.68	123.04	118.21
2	C	350	C39	C7-C12-C13	-3.51	119.92	126.24
2	O	350	C39	C28-C27-C26	-3.19	105.22	111.52
2	O	350	C39	O25-C24-C22	-2.94	103.90	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	350	C39	O25-C24-C22	-2.75	104.25	109.48
2	C	350	C39	C11-C12-C7	2.36	121.32	118.21
2	O	350	C39	C16-N15-C13	-2.30	118.30	122.54
2	O	350	C39	C26-C27-C29	2.30	114.26	109.84
2	C	350	C39	O30-C29-N31	-2.10	118.55	122.98

There are no chirality outliers.

All (29) torsion outliers are listed below:

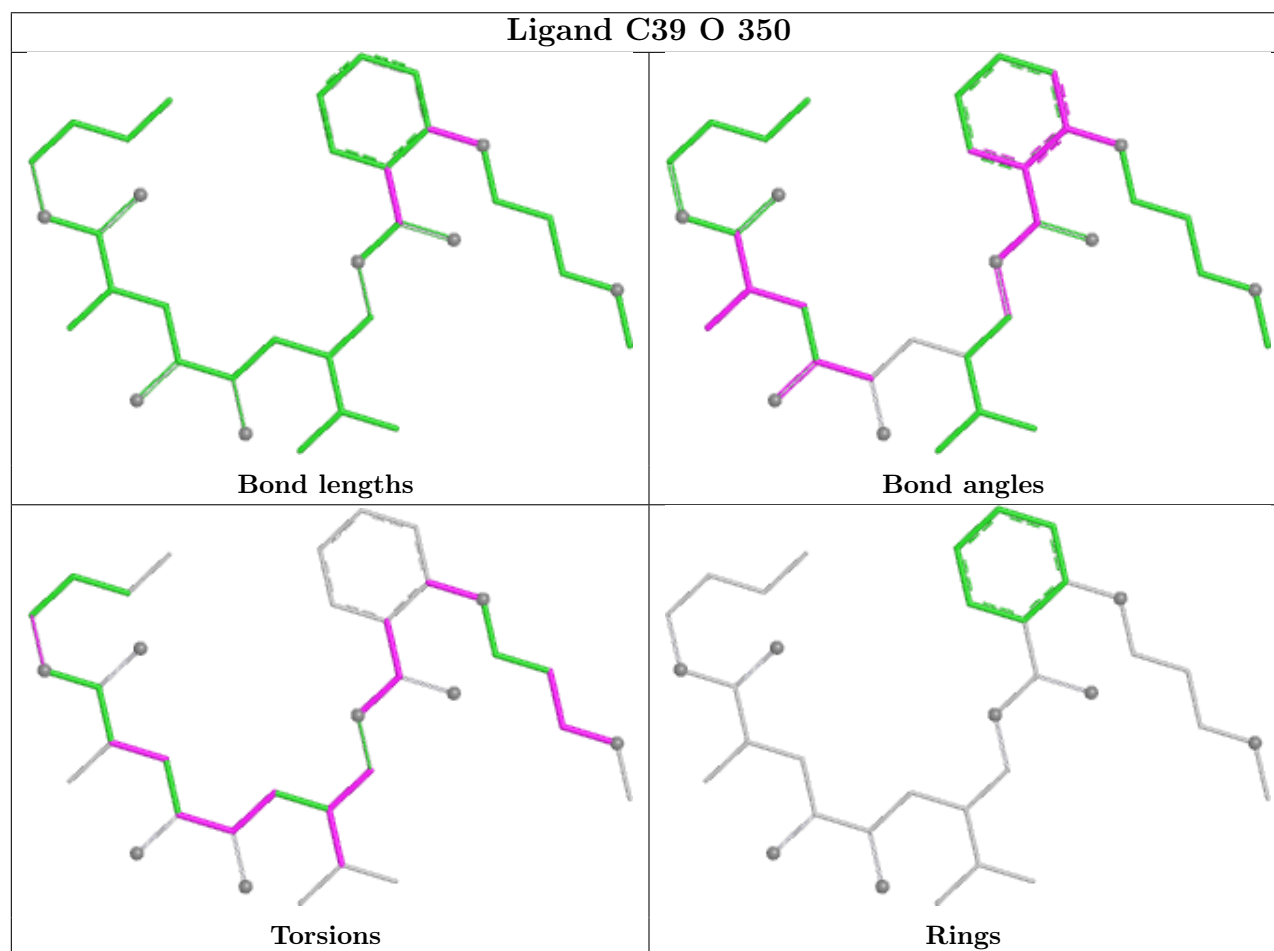
Mol	Chain	Res	Type	Atoms
2	C	350	C39	C17-C21-C22-N23
2	C	350	C39	O30-C29-N31-C32
2	O	350	C39	C17-C21-C22-N23
2	O	350	C39	C12-C13-N15-C16
2	C	350	C39	O2-C3-C4-C5
2	C	350	C39	C4-C3-O2-C1
2	O	350	C39	C7-C12-C13-O14
2	O	350	C39	C4-C3-O2-C1
2	O	350	C39	O2-C3-C4-C5
2	C	350	C39	C27-C29-N31-C32
2	C	350	C39	C32-C33-C34-C35
2	O	350	C39	C21-C22-C24-O25
2	C	350	C39	N15-C16-C17-C18
2	O	350	C39	N15-C16-C17-C18
2	O	350	C39	O14-C13-N15-C16
2	O	350	C39	C24-C26-C27-C29
2	C	350	C39	C7-C12-C13-O14
2	C	350	C39	C16-C17-C21-C22
2	C	350	C39	C8-C7-O6-C5
2	O	350	C39	C8-C7-O6-C5
2	O	350	C39	C7-C12-C13-N15
2	O	350	C39	C12-C7-O6-C5
2	O	350	C39	C33-C32-N31-C29
2	C	350	C39	C21-C22-C24-O25
2	O	350	C39	C21-C17-C18-C19
2	C	350	C39	C12-C7-O6-C5
2	C	350	C39	C12-C13-N15-C16
2	C	350	C39	C21-C17-C18-C19
2	C	350	C39	C16-C17-C18-C19

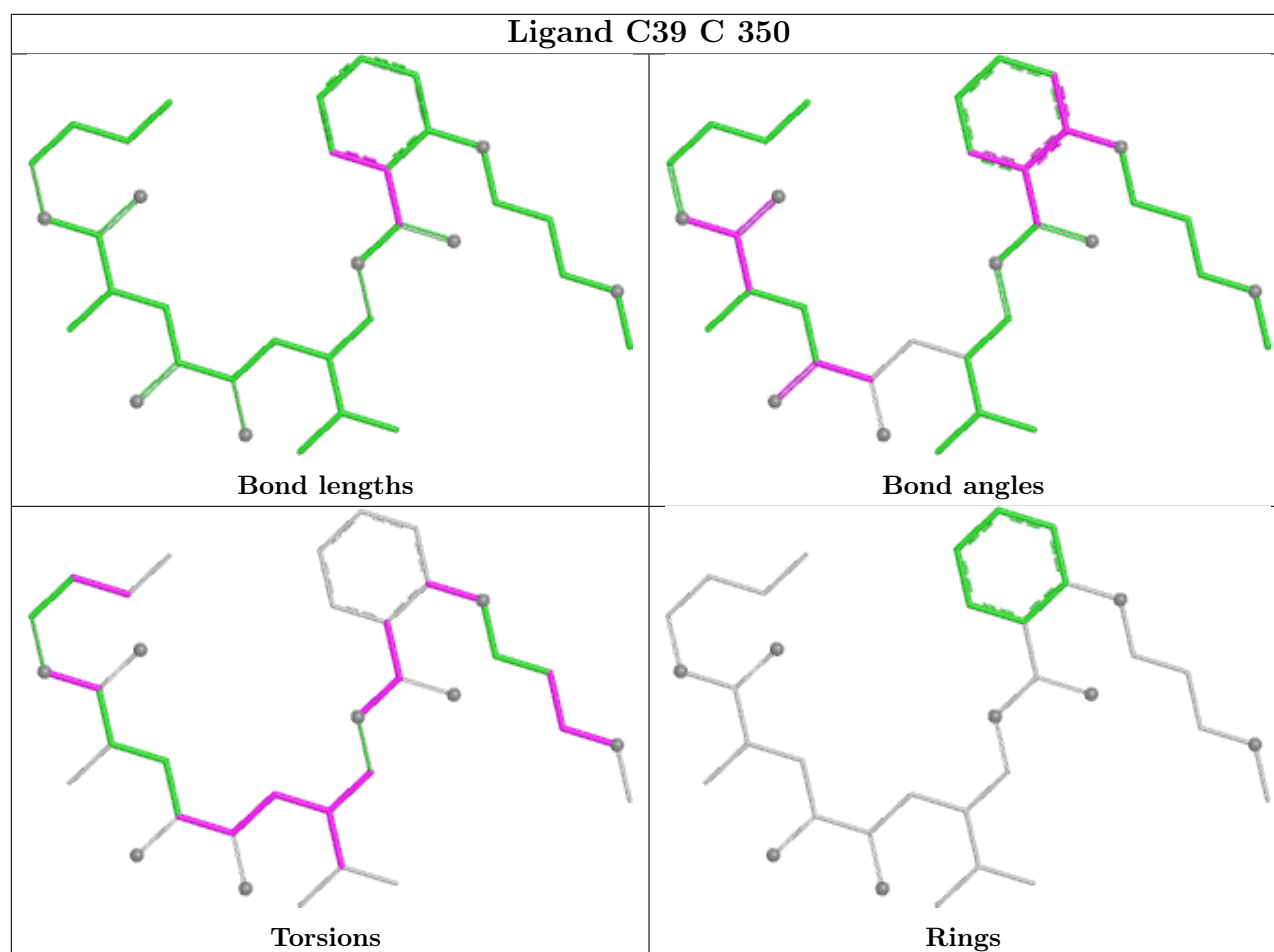
There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	350	C39	5	0
2	C	350	C39	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.