



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:14 AM UTC

PDB ID : 1Z6P / pdb_00001z6p
Title : Glycogen phosphorylase AMP site inhibitor complex
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Deposited on : 2005-03-23
Resolution : 2.40 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

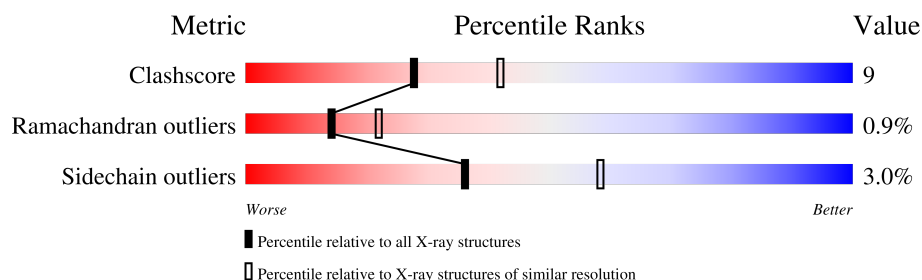
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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	A	842	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6794 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.

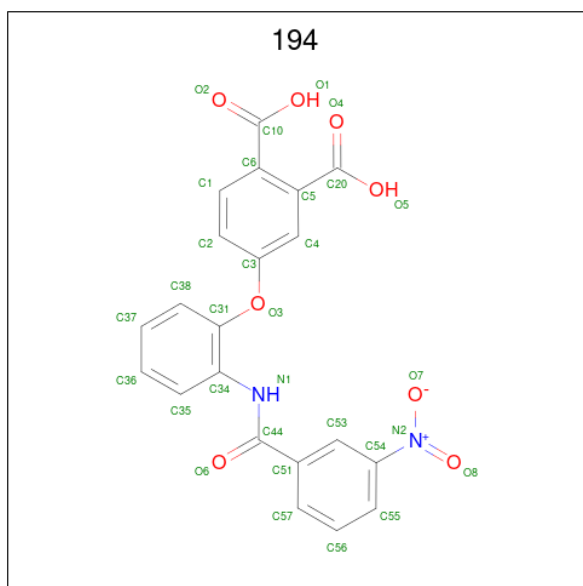
- Molecule 1 is a protein called Glycogen phosphorylase, muscle form.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	813	6642	4232	1173	1207	1	29	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	conflict	UNP P00489
A	680	LLP	LYS	modified residue	UNP P00489

- Molecule 2 is 4-{2-[(3-NITROBENZOYL)AMINO]PHENOXY}PHTHALIC ACID (CCD ID: 194) (formula: C₂₁H₁₄N₂O₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	31	21	2	8	0	0

- Molecule 3 is water.

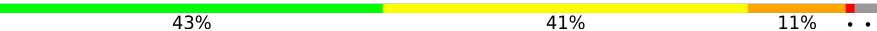
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	121	Total 121	O 121	0	0

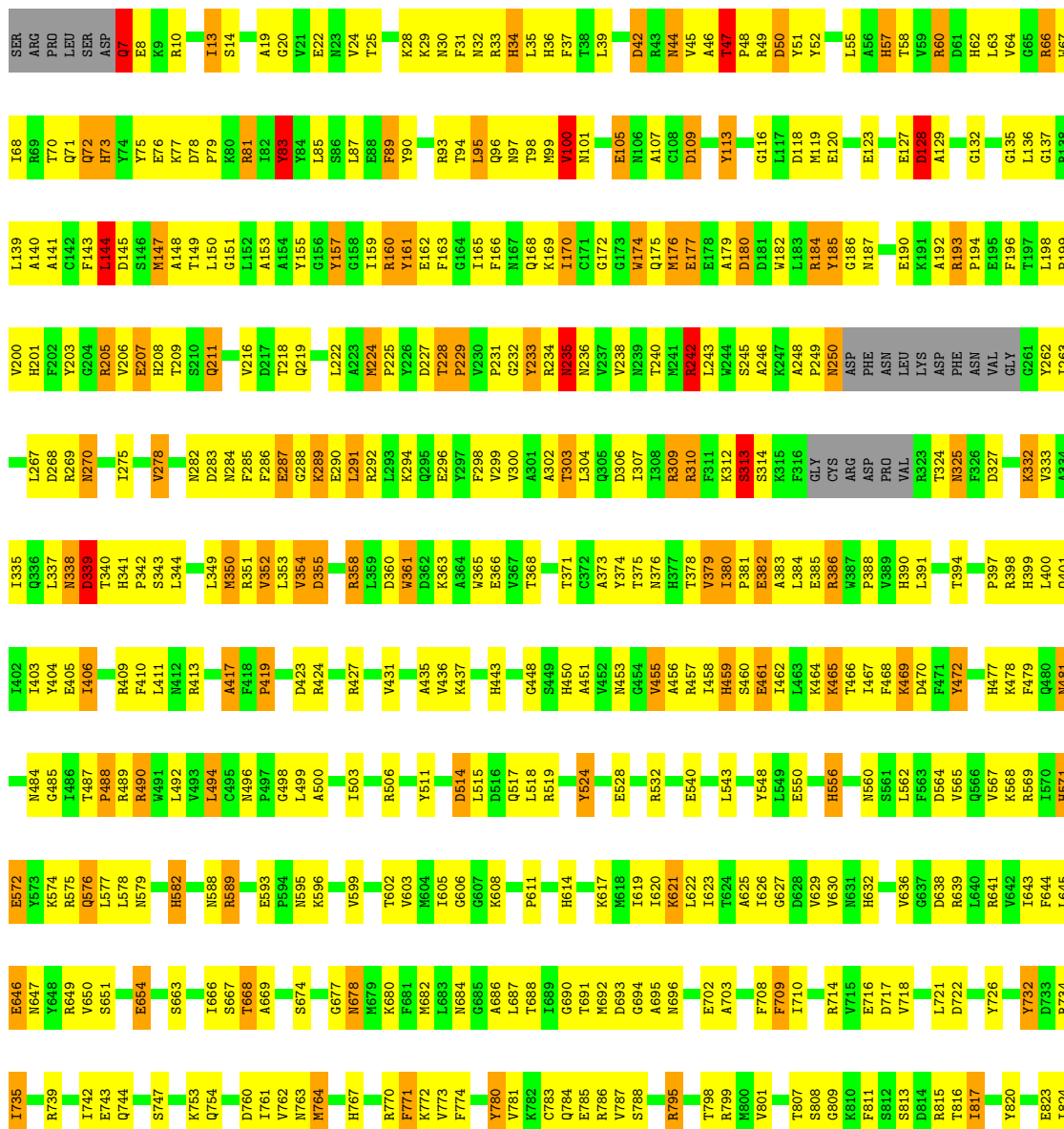
3 Residue-property plots

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: Glycogen phosphorylase, muscle form

Chain A: 



W825	G826	S830	R831	Q832	R833	L834	P835	ALA	PRO	ASP	GLU	LYS	ILE	PRO
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4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	127.47Å 127.47Å 115.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40	Depositor
% Data completeness (in resolution range)	97.0 (20.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.200 , 0.260	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6794	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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: 194, LLP

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	A	2.05	171/6764 (2.5%)	2.38	391/9147 (4.3%)

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	A	0	18

All (171) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	284	ASN	C-N	13.67	1.52	1.33
1	A	341	HIS	CA-C	11.68	1.67	1.52
1	A	284	ASN	CA-C	11.40	1.69	1.53
1	A	469	LYS	CA-C	9.53	1.65	1.52
1	A	90	TYR	CA-CB	9.17	1.64	1.52
1	A	314	SER	CA-C	9.10	1.65	1.52
1	A	380	ILE	CA-C	9.07	1.62	1.52
1	A	248	ALA	CA-C	8.98	1.62	1.53
1	A	703	ALA	CA-C	8.70	1.64	1.52
1	A	284	ASN	N-CA	8.59	1.59	1.46
1	A	599	VAL	CA-C	8.54	1.61	1.52
1	A	773	VAL	CA-C	8.50	1.62	1.52
1	A	824	ILE	CA-C	8.49	1.63	1.52
1	A	285	PHE	CA-C	8.16	1.63	1.52
1	A	621	LYS	CA-C	8.13	1.63	1.52
1	A	477	HIS	CG-CD2	8.07	1.44	1.35
1	A	176	MET	CA-C	8.06	1.62	1.52
1	A	132	GLY	CA-C	8.00	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	787	VAL	CA-CB	7.86	1.63	1.54
1	A	684	ASN	CA-C	7.83	1.63	1.52
1	A	355	ASP	CA-C	7.74	1.62	1.52
1	A	709	PHE	CA-C	7.72	1.61	1.53
1	A	300	VAL	CA-CB	7.69	1.62	1.54
1	A	174	TRP	CA-C	7.65	1.62	1.52
1	A	567	VAL	CA-C	7.65	1.62	1.52
1	A	81	ARG	CA-C	-7.61	1.43	1.52
1	A	623	ILE	CA-C	-7.59	1.43	1.52
1	A	19	ALA	C-N	7.59	1.40	1.33
1	A	229	PRO	CA-C	7.56	1.61	1.52
1	A	761	ILE	CA-C	7.53	1.61	1.52
1	A	373	ALA	CA-C	7.52	1.61	1.52
1	A	398	ARG	CA-C	7.52	1.62	1.52
1	A	64	VAL	CA-CB	7.49	1.63	1.54
1	A	79	PRO	CA-C	7.47	1.63	1.52
1	A	170	ILE	CA-C	-7.47	1.43	1.52
1	A	668	THR	N-CA	7.40	1.55	1.46
1	A	817	ILE	CA-CB	7.33	1.63	1.54
1	A	151	GLY	CA-C	-7.31	1.42	1.51
1	A	386	ARG	CA-C	7.30	1.62	1.53
1	A	168	GLN	CA-C	7.29	1.61	1.52
1	A	543	LEU	CA-C	7.21	1.62	1.52
1	A	283	ASP	CA-C	7.16	1.61	1.52
1	A	443	HIS	CG-CD2	7.15	1.43	1.35
1	A	588	ASN	CA-C	7.15	1.62	1.52
1	A	686	ALA	CA-C	-7.14	1.44	1.52
1	A	830	SER	CA-C	6.98	1.61	1.52
1	A	49	ARG	CA-C	-6.97	1.43	1.52
1	A	290	GLU	CA-C	6.93	1.62	1.52
1	A	352	VAL	CA-CB	-6.93	1.47	1.54
1	A	34	HIS	CG-ND1	-6.92	1.30	1.38
1	A	820	TYR	N-CA	6.92	1.54	1.46
1	A	490	ARG	N-CA	6.91	1.54	1.46
1	A	605	ILE	CA-CB	6.91	1.62	1.54
1	A	157	TYR	CA-C	-6.88	1.44	1.52
1	A	64	VAL	N-CA	6.73	1.54	1.46
1	A	813	SER	CA-C	6.72	1.62	1.52
1	A	479	PHE	CA-C	6.71	1.61	1.52
1	A	686	ALA	C-N	6.67	1.42	1.33
1	A	532	ARG	CA-C	6.66	1.61	1.52
1	A	589	ARG	CA-C	-6.66	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	459	HIS	CD2-NE2	-6.65	1.30	1.37
1	A	809	GLY	CA-C	6.61	1.59	1.51
1	A	630	VAL	CA-CB	6.58	1.62	1.54
1	A	35	LEU	C-N	6.57	1.42	1.33
1	A	190	GLU	CA-C	6.54	1.61	1.52
1	A	366	GLU	CA-C	6.52	1.61	1.52
1	A	735	ILE	CA-C	-6.48	1.46	1.52
1	A	784	GLN	CA-C	6.47	1.61	1.52
1	A	144	LEU	CA-C	6.40	1.61	1.52
1	A	582	HIS	CG-CD2	6.40	1.42	1.35
1	A	385	GLU	CA-C	-6.38	1.44	1.52
1	A	457	ARG	CA-C	6.33	1.61	1.52
1	A	199	PRO	CA-C	6.33	1.59	1.52
1	A	488	PRO	C-N	6.30	1.42	1.33
1	A	249	PRO	CA-C	6.28	1.60	1.52
1	A	787	VAL	CA-C	-6.25	1.45	1.52
1	A	349	LEU	CA-C	6.23	1.61	1.52
1	A	404	TYR	CA-C	6.23	1.61	1.52
1	A	250	ASN	CA-C	6.22	1.66	1.52
1	A	582	HIS	ND1-CE1	6.21	1.38	1.32
1	A	403	ILE	CA-C	6.20	1.60	1.52
1	A	574	LYS	CA-C	6.17	1.61	1.52
1	A	184	ARG	CA-CB	6.15	1.63	1.53
1	A	435	ALA	CA-C	6.15	1.60	1.52
1	A	625	ALA	CA-C	6.06	1.60	1.52
1	A	575	ARG	CA-C	6.04	1.60	1.53
1	A	578	LEU	CA-C	6.04	1.60	1.52
1	A	603	VAL	CA-C	6.03	1.60	1.52
1	A	494	LEU	C-N	5.96	1.42	1.34
1	A	196	PHE	CA-C	5.95	1.60	1.52
1	A	291	LEU	CA-C	5.94	1.60	1.52
1	A	468	PHE	CA-CB	5.89	1.61	1.53
1	A	496	ASN	CA-CB	5.89	1.60	1.53
1	A	674	SER	CB-OG	5.88	1.53	1.42
1	A	813	SER	N-CA	5.85	1.53	1.46
1	A	93	ARG	CA-C	5.84	1.61	1.53
1	A	184	ARG	CA-C	5.84	1.60	1.52
1	A	242	ARG	C-N	5.78	1.41	1.33
1	A	708	PHE	CA-C	5.78	1.59	1.52
1	A	341	HIS	CD2-NE2	-5.76	1.31	1.37
1	A	153	ALA	CA-CB	5.75	1.60	1.52
1	A	296	GLU	CA-C	5.70	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	744	GLN	N-CA	5.69	1.53	1.46
1	A	245	SER	CA-C	5.68	1.59	1.52
1	A	72	GLN	CA-C	5.64	1.60	1.52
1	A	722	ASP	CA-CB	5.64	1.62	1.53
1	A	678	ASN	CA-C	5.64	1.60	1.52
1	A	36	HIS	CG-CD2	5.60	1.42	1.35
1	A	187	ASN	C-N	5.60	1.40	1.34
1	A	368	THR	N-CA	5.60	1.52	1.46
1	A	161	TYR	C-N	5.59	1.40	1.33
1	A	571	HIS	CG-CD2	5.57	1.42	1.35
1	A	543	LEU	N-CA	5.56	1.53	1.46
1	A	182	TRP	NE1-CE2	5.53	1.43	1.37
1	A	275	ILE	CA-CB	-5.53	1.48	1.54
1	A	639	ARG	CA-C	5.52	1.60	1.52
1	A	209	THR	CA-C	5.51	1.58	1.53
1	A	55	LEU	N-CA	5.49	1.53	1.46
1	A	288	GLY	CA-C	5.48	1.59	1.51
1	A	288	GLY	N-CA	5.48	1.53	1.45
1	A	333	VAL	CA-CB	5.47	1.61	1.54
1	A	383	ALA	CA-C	5.46	1.60	1.52
1	A	224	MET	CA-C	5.45	1.58	1.52
1	A	488	PRO	CA-C	5.45	1.61	1.52
1	A	579	ASN	N-CA	5.43	1.52	1.46
1	A	669	ALA	N-CA	-5.42	1.39	1.46
1	A	678	ASN	N-CA	5.42	1.52	1.46
1	A	278	VAL	CA-CB	5.42	1.61	1.54
1	A	764	MET	CA-C	5.41	1.59	1.52
1	A	606	GLY	N-CA	5.40	1.51	1.45
1	A	95	LEU	CA-C	5.40	1.60	1.52
1	A	419	PRO	CA-C	5.38	1.59	1.52
1	A	399	HIS	CG-CD2	5.36	1.41	1.35
1	A	66	ARG	CA-C	5.35	1.59	1.52
1	A	771	PHE	CA-C	5.33	1.59	1.52
1	A	489	ARG	CZ-NH2	-5.33	1.26	1.33
1	A	565	VAL	C-N	5.31	1.41	1.33
1	A	453	ASN	CA-C	5.30	1.59	1.52
1	A	517	GLN	CA-C	5.30	1.59	1.52
1	A	617	LYS	C-N	5.30	1.40	1.33
1	A	459	HIS	CB-CG	5.29	1.57	1.50
1	A	294	LYS	N-CA	5.28	1.52	1.46
1	A	240	THR	C-N	5.27	1.41	1.33
1	A	33	ARG	NE-CZ	5.24	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	262	TYR	CA-C	5.22	1.59	1.52
1	A	375	THR	C-N	5.22	1.40	1.33
1	A	172	GLY	N-CA	5.21	1.53	1.45
1	A	14	SER	CA-CB	5.20	1.61	1.53
1	A	344	LEU	CA-C	5.19	1.59	1.52
1	A	400	LEU	CA-C	5.18	1.59	1.52
1	A	228	THR	CA-C	5.17	1.57	1.52
1	A	702	GLU	CA-C	-5.17	1.46	1.52
1	A	406	ILE	CA-C	5.16	1.59	1.52
1	A	687	LEU	N-CA	5.13	1.52	1.45
1	A	185	TYR	C-N	5.11	1.39	1.33
1	A	431	VAL	CA-C	5.11	1.59	1.52
1	A	299	VAL	CA-CB	5.09	1.59	1.54
1	A	801	VAL	C-N	5.09	1.40	1.33
1	A	627	GLY	CA-C	5.09	1.57	1.51
1	A	691	THR	CA-C	5.08	1.60	1.53
1	A	528	GLU	CA-C	5.07	1.59	1.52
1	A	107	ALA	C-N	5.06	1.40	1.34
1	A	83	TYR	CA-C	5.05	1.58	1.52
1	A	304	LEU	C-N	5.05	1.40	1.33
1	A	576	GLN	C-N	5.04	1.40	1.33
1	A	386	ARG	NE-CZ	5.02	1.38	1.33
1	A	186	GLY	N-CA	5.01	1.50	1.45
1	A	477	HIS	ND1-CE1	5.01	1.37	1.32
1	A	556	HIS	CG-CD2	5.01	1.41	1.35
1	A	100	VAL	CA-C	5.00	1.59	1.52
1	A	361	TRP	CA-C	5.00	1.60	1.52

All (391) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	ARG	NE-CZ-NH2	13.34	131.21	119.20
1	A	206	VAL	CA-C-N	12.01	139.86	123.05
1	A	206	VAL	C-N-CA	12.01	139.86	123.05
1	A	283	ASP	N-CA-CB	-11.62	91.36	110.52
1	A	753	LYS	CA-C-N	-10.92	112.21	122.37
1	A	753	LYS	C-N-CA	-10.92	112.21	122.37
1	A	774	PHE	CA-CB-CG	10.62	124.42	113.80
1	A	688	THR	CA-CB-OG1	10.46	125.29	109.60
1	A	564	ASP	CA-CB-CG	10.45	123.05	112.60
1	A	786	ARG	CA-C-N	10.42	133.90	120.56
1	A	786	ARG	C-N-CA	10.42	133.90	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	470	ASP	CA-CB-CG	10.38	122.98	112.60
1	A	632	HIS	CA-CB-CG	-10.19	103.61	113.80
1	A	399	HIS	CA-CB-CG	-10.18	103.62	113.80
1	A	770	ARG	NE-CZ-NH2	10.18	128.36	119.20
1	A	94	THR	N-CA-CB	-10.05	97.72	110.98
1	A	270	ASN	CA-CB-CG	-9.61	102.99	112.60
1	A	518	LEU	CA-C-N	9.55	134.03	120.28
1	A	518	LEU	C-N-CA	9.55	134.03	120.28
1	A	572	GLU	N-CA-C	9.32	121.44	111.28
1	A	773	VAL	N-CA-C	9.24	119.84	110.23
1	A	263	ILE	CA-C-N	9.21	132.62	120.28
1	A	263	ILE	C-N-CA	9.21	132.62	120.28
1	A	649	ARG	NE-CZ-NH1	9.17	130.67	121.50
1	A	391	LEU	CB-CA-C	9.09	125.26	110.90
1	A	485	GLY	CA-C-N	8.93	135.35	122.94
1	A	485	GLY	C-N-CA	8.93	135.35	122.94
1	A	97	ASN	CA-CB-CG	-8.85	103.75	112.60
1	A	47	THR	CA-C-N	-8.53	110.86	119.56
1	A	47	THR	C-N-CA	-8.53	110.86	119.56
1	A	424	ARG	NE-CZ-NH1	8.42	129.92	121.50
1	A	830	SER	N-CA-C	8.35	121.06	108.46
1	A	716	GLU	CB-CG-CD	8.24	126.61	112.60
1	A	193	ARG	CD-NE-CZ	-8.20	112.92	124.40
1	A	593	GLU	CB-CG-CD	-8.19	98.67	112.60
1	A	487	THR	CA-CB-CG2	8.18	124.41	110.50
1	A	644	PHE	CA-CB-CG	-8.18	105.62	113.80
1	A	34	HIS	CA-CB-CG	-8.12	105.68	113.80
1	A	79	PRO	CB-CA-C	8.11	124.94	111.56
1	A	379	VAL	CB-CA-C	-8.10	103.93	111.06
1	A	663	SER	N-CA-C	8.08	121.90	108.73
1	A	717	ASP	CA-CB-CG	7.92	120.53	112.60
1	A	375	THR	N-CA-C	7.85	121.71	109.07
1	A	666	ILE	N-CA-C	7.83	119.91	111.77
1	A	582	HIS	CA-CB-CG	-7.77	106.03	113.80
1	A	136	LEU	N-CA-CB	-7.75	98.78	110.01
1	A	571	HIS	CA-CB-CG	-7.72	106.08	113.80
1	A	668	THR	OG1-CB-CG2	-7.70	93.89	109.30
1	A	175	GLN	CA-C-N	7.70	133.82	123.05
1	A	175	GLN	C-N-CA	7.70	133.82	123.05
1	A	192	ALA	CA-C-N	-7.68	114.07	123.21
1	A	192	ALA	C-N-CA	-7.68	114.07	123.21
1	A	543	LEU	N-CA-C	7.65	119.70	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	HIS	CA-CB-CG	-7.62	106.18	113.80
1	A	325	ASN	CA-CB-CG	7.61	120.21	112.60
1	A	826	GLY	O-C-N	7.61	130.30	122.54
1	A	37	PHE	CA-CB-CG	-7.55	106.25	113.80
1	A	208	HIS	CA-CB-CG	-7.53	106.27	113.80
1	A	519	ARG	NE-CZ-NH1	-7.49	114.01	121.50
1	A	743	GLU	CA-C-N	7.47	130.62	120.54
1	A	743	GLU	C-N-CA	7.47	130.62	120.54
1	A	762	VAL	N-CA-CB	-7.44	102.25	110.51
1	A	232	GLY	CA-C-N	-7.42	110.94	121.99
1	A	232	GLY	C-N-CA	-7.42	110.94	121.99
1	A	128	ASP	CA-CB-CG	7.41	120.01	112.60
1	A	139	LEU	CA-C-N	7.40	131.92	120.82
1	A	139	LEU	C-N-CA	7.40	131.92	120.82
1	A	718	VAL	O-C-N	7.38	129.14	121.91
1	A	32	ASN	CA-CB-CG	-7.34	105.26	112.60
1	A	484	ASN	CA-CB-CG	7.33	119.93	112.60
1	A	458	ILE	CA-C-N	7.33	129.97	120.44
1	A	458	ILE	C-N-CA	7.33	129.97	120.44
1	A	378	THR	CA-CB-OG1	7.33	120.59	109.60
1	A	290	GLU	N-CA-C	7.31	121.11	111.75
1	A	285	PHE	CA-CB-CG	-7.29	106.51	113.80
1	A	360	ASP	CA-CB-CG	-7.28	105.32	112.60
1	A	760	ASP	CA-CB-CG	7.27	119.87	112.60
1	A	312	LYS	O-C-N	-7.26	111.83	122.43
1	A	234	ARG	CD-NE-CZ	7.21	134.50	124.40
1	A	37	PHE	N-CA-C	7.11	120.06	111.82
1	A	216	VAL	CA-C-N	7.08	132.44	122.46
1	A	216	VAL	C-N-CA	7.08	132.44	122.46
1	A	285	PHE	N-CA-C	7.08	125.88	110.80
1	A	282	ASN	CB-CG-ND2	-7.06	105.81	116.40
1	A	451	ALA	CA-C-N	7.04	132.46	123.10
1	A	451	ALA	C-N-CA	7.04	132.46	123.10
1	A	283	ASP	CA-CB-CG	-7.02	105.58	112.60
1	A	470	ASP	CA-C-N	7.01	129.97	120.44
1	A	470	ASP	C-N-CA	7.01	129.97	120.44
1	A	129	ALA	CA-C-N	6.98	135.09	121.41
1	A	129	ALA	C-N-CA	6.98	135.09	121.41
1	A	686	ALA	O-C-N	6.97	132.29	123.23
1	A	22	GLU	CB-CG-CD	-6.96	100.76	112.60
1	A	287	GLU	O-C-N	-6.94	115.08	123.27
1	A	33	ARG	CD-NE-CZ	6.94	134.11	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	572	GLU	CB-CG-CD	-6.93	100.82	112.60
1	A	66	ARG	CD-NE-CZ	-6.87	114.78	124.40
1	A	177	GLU	CB-CG-CD	6.85	124.25	112.60
1	A	283	ASP	CA-C-N	-6.85	112.47	122.40
1	A	283	ASP	C-N-CA	-6.85	112.47	122.40
1	A	815	ARG	NE-CZ-NH2	6.85	125.36	119.20
1	A	816	THR	CA-CB-OG1	6.84	119.87	109.60
1	A	245	SER	N-CA-CB	-6.81	98.67	111.00
1	A	691	THR	N-CA-CB	-6.80	100.11	110.45
1	A	285	PHE	CA-C-N	6.76	131.63	122.84
1	A	285	PHE	C-N-CA	6.76	131.63	122.84
1	A	519	ARG	NE-CZ-NH2	6.74	125.27	119.20
1	A	371	THR	N-CA-C	6.74	118.71	111.36
1	A	30	ASN	CA-CB-CG	-6.72	105.88	112.60
1	A	219	GLN	CB-CG-CD	6.72	124.03	112.60
1	A	193	ARG	NH1-CZ-NH2	-6.72	110.56	119.30
1	A	81	ARG	O-C-N	6.71	131.73	123.21
1	A	275	ILE	N-CA-C	6.71	116.86	110.42
1	A	24	VAL	CA-CB-CG1	6.70	121.80	110.40
1	A	62	HIS	CA-CB-CG	-6.68	107.12	113.80
1	A	299	VAL	N-CA-CB	6.65	117.87	110.62
1	A	466	THR	CA-CB-OG1	6.64	119.57	109.60
1	A	500	ALA	N-CA-C	-6.61	104.16	111.36
1	A	654	GLU	N-CA-C	6.58	120.41	112.38
1	A	650	VAL	N-CA-CB	6.57	117.80	110.51
1	A	292	ARG	N-CA-C	6.56	119.02	111.02
1	A	494	LEU	O-C-N	6.53	129.08	122.03
1	A	595	ASN	CA-CB-CG	-6.52	106.08	112.60
1	A	579	ASN	CA-CB-CG	6.51	119.11	112.60
1	A	781	VAL	N-CA-C	6.51	116.67	110.42
1	A	302	ALA	CB-CA-C	6.50	121.21	110.81
1	A	560	ASN	CA-CB-CG	-6.50	106.10	112.60
1	A	391	LEU	N-CA-CB	-6.50	100.65	110.07
1	A	28	LYS	N-CA-CB	-6.49	100.33	110.06
1	A	207	GLU	CA-C-O	6.49	127.45	120.32
1	A	289	LYS	N-CA-CB	-6.48	100.19	109.85
1	A	378	THR	OG1-CB-CG2	-6.46	96.38	109.30
1	A	472	TYR	N-CA-CB	-6.46	100.62	110.12
1	A	427	ARG	CD-NE-CZ	6.46	133.44	124.40
1	A	419	PRO	CB-CA-C	6.45	119.83	111.64
1	A	269	ARG	NE-CZ-NH2	-6.44	113.40	119.20
1	A	296	GLU	N-CA-C	6.42	118.28	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	310	ARG	CD-NE-CZ	-6.42	115.41	124.40
1	A	207	GLU	CB-CA-C	-6.41	99.68	110.19
1	A	394	THR	CA-CB-OG1	6.34	119.11	109.60
1	A	688	THR	OG1-CB-CG2	-6.31	96.67	109.30
1	A	129	ALA	N-CA-CB	-6.29	101.52	110.58
1	A	180	ASP	N-CA-CB	-6.29	100.08	110.53
1	A	238	VAL	O-C-N	6.29	130.43	122.57
1	A	162	GLU	CA-CB-CG	-6.28	101.53	114.10
1	A	248	ALA	CB-CA-C	6.24	119.39	109.52
1	A	145	ASP	CA-CB-CG	6.24	118.84	112.60
1	A	228	THR	CA-CB-OG1	6.24	118.96	109.60
1	A	795	ARG	O-C-N	6.24	129.26	122.15
1	A	286	PHE	CA-C-N	6.23	131.77	123.05
1	A	286	PHE	C-N-CA	6.23	131.77	123.05
1	A	105	GLU	N-CA-C	6.23	118.07	111.28
1	A	462	ILE	N-CA-C	6.21	116.96	110.62
1	A	629	VAL	O-C-N	6.19	128.57	121.94
1	A	400	LEU	O-C-N	-6.19	115.56	122.12
1	A	494	LEU	CB-CA-C	-6.16	101.40	110.95
1	A	747	SER	CA-C-O	6.16	126.48	119.27
1	A	51	TYR	CB-CA-C	6.16	120.71	110.92
1	A	32	ASN	CB-CG-ND2	-6.14	107.19	116.40
1	A	338	ASN	CA-CB-CG	-6.14	106.46	112.60
1	A	398	ARG	CG-CD-NE	-6.13	98.51	112.00
1	A	339	ASP	CA-CB-CG	6.13	118.73	112.60
1	A	696	ASN	CA-CB-CG	6.12	118.72	112.60
1	A	160	ARG	CD-NE-CZ	6.12	132.96	124.40
1	A	20	GLY	CA-C-N	6.11	129.14	120.53
1	A	20	GLY	C-N-CA	6.11	129.14	120.53
1	A	42	ASP	CB-CA-C	6.11	123.94	111.11
1	A	754	GLN	O-C-N	6.10	125.64	121.19
1	A	638	ASP	N-CA-CB	-6.08	101.64	110.70
1	A	187	ASN	OD1-CG-ND2	-6.08	116.52	122.60
1	A	469	LYS	O-C-N	-6.08	115.81	122.07
1	A	101	ASN	OD1-CG-ND2	-6.07	116.53	122.60
1	A	246	ALA	O-C-N	6.02	130.08	123.22
1	A	211	GLN	CB-CG-CD	5.99	122.78	112.60
1	A	767	HIS	CA-CB-CG	-5.98	107.82	113.80
1	A	313	SER	N-CA-C	5.94	121.26	113.30
1	A	233	TYR	CB-CA-C	-5.94	100.85	110.77
1	A	198	LEU	O-C-N	-5.93	116.31	121.35
1	A	218	THR	OG1-CB-CG2	-5.93	97.43	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	423	ASP	CA-CB-CG	-5.93	106.67	112.60
1	A	677	GLY	N-CA-C	-5.91	105.64	112.73
1	A	695	ALA	CA-C-N	5.91	128.52	120.54
1	A	695	ALA	C-N-CA	5.91	128.52	120.54
1	A	291	LEU	N-CA-C	5.90	118.19	111.11
1	A	135	GLY	CA-C-N	5.89	128.10	120.44
1	A	135	GLY	C-N-CA	5.89	128.10	120.44
1	A	206	VAL	O-C-N	5.89	129.62	123.26
1	A	808	SER	CA-C-N	5.89	127.55	120.13
1	A	808	SER	C-N-CA	5.89	127.55	120.13
1	A	722	ASP	CA-CB-CG	-5.89	106.71	112.60
1	A	288	GLY	CA-C-N	5.87	129.17	120.95
1	A	288	GLY	C-N-CA	5.87	129.17	120.95
1	A	98	THR	CA-CB-OG1	5.85	118.38	109.60
1	A	42	ASP	CA-CB-CG	5.85	118.45	112.60
1	A	645	LEU	CA-C-O	5.85	126.98	120.43
1	A	298	PHE	N-CA-CB	-5.83	101.25	109.94
1	A	120	GLU	CA-C-O	5.82	126.72	120.55
1	A	58	THR	CA-CB-OG1	5.81	118.31	109.60
1	A	772	LYS	N-CA-C	5.80	119.43	111.54
1	A	350	MET	CA-C-N	5.80	128.85	120.79
1	A	350	MET	C-N-CA	5.80	128.85	120.79
1	A	692	MET	CG-SD-CE	-5.77	88.21	100.90
1	A	243	LEU	CA-C-O	-5.76	114.13	120.36
1	A	569	ARG	NE-CZ-NH2	-5.76	114.02	119.20
1	A	87	LEU	N-CA-C	-5.75	106.03	113.16
1	A	375	THR	CA-CB-OG1	5.75	118.22	109.60
1	A	303	THR	N-CA-C	5.75	117.22	111.07
1	A	89	PHE	CA-CB-CG	-5.74	108.06	113.80
1	A	455	VAL	CA-C-O	5.73	125.19	119.97
1	A	667	SER	N-CA-CB	-5.73	101.92	110.17
1	A	771	PHE	CA-CB-CG	-5.71	108.08	113.80
1	A	602	THR	OG1-CB-CG2	-5.71	97.88	109.30
1	A	620	ILE	N-CA-CB	5.71	118.31	110.54
1	A	638	ASP	CB-CA-C	5.69	120.33	110.94
1	A	34	HIS	CE1-NE2-CD2	-5.68	103.32	109.00
1	A	184	ARG	CB-CG-CD	5.68	124.36	111.30
1	A	380	ILE	CA-CB-CG1	5.67	120.04	110.40
1	A	148	ALA	N-CA-CB	-5.67	101.74	110.13
1	A	47	THR	CA-CB-OG1	5.66	118.09	109.60
1	A	278	VAL	CA-CB-CG1	5.66	120.02	110.40
1	A	478	LYS	N-CA-C	5.65	118.21	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	GLN	O-C-N	5.65	129.88	122.93
1	A	543	LEU	CA-C-N	5.65	128.16	120.54
1	A	543	LEU	C-N-CA	5.65	128.16	120.54
1	A	646	GLU	CA-C-N	-5.64	114.35	122.36
1	A	646	GLU	C-N-CA	-5.64	114.35	122.36
1	A	13	ILE	CA-C-N	5.64	127.83	120.28
1	A	13	ILE	C-N-CA	5.64	127.83	120.28
1	A	7	GLN	CB-CG-CD	5.63	122.16	112.60
1	A	682	MET	CA-C-N	5.63	128.59	120.38
1	A	682	MET	C-N-CA	5.63	128.59	120.38
1	A	833	ARG	CB-CA-C	5.62	118.67	109.90
1	A	90	TYR	CB-CA-C	5.62	120.55	112.12
1	A	785	GLU	CA-C-O	5.62	126.38	120.42
1	A	567	VAL	CB-CA-C	5.61	118.74	110.77
1	A	390	HIS	CA-C-O	5.61	126.42	119.97
1	A	499	LEU	O-C-N	5.61	129.84	122.33
1	A	788	SER	N-CA-CB	-5.60	101.68	110.30
1	A	34	HIS	N-CA-C	5.60	117.83	111.11
1	A	332	LYS	CB-CA-C	5.59	118.41	109.02
1	A	562	LEU	CB-CA-C	5.58	119.16	110.67
1	A	619	ILE	O-C-N	5.58	127.28	121.87
1	A	349	LEU	CA-C-O	5.58	126.40	120.10
1	A	718	VAL	CA-C-N	5.57	127.75	120.28
1	A	718	VAL	C-N-CA	5.57	127.75	120.28
1	A	514	ASP	N-CA-CB	-5.57	101.08	110.49
1	A	337	LEU	N-CA-C	5.57	117.81	108.23
1	A	250	ASN	CA-CB-CG	5.57	118.17	112.60
1	A	832	GLN	N-CA-CB	5.56	118.30	109.51
1	A	450	HIS	CE1-NE2-CD2	-5.54	103.46	109.00
1	A	576	GLN	O-C-N	5.53	127.98	122.12
1	A	744	GLN	N-CA-CB	5.53	118.17	109.94
1	A	762	VAL	N-CA-C	5.52	116.16	110.36
1	A	324	THR	CA-CB-OG1	5.52	117.88	109.60
1	A	349	LEU	N-CA-CB	-5.52	101.72	110.22
1	A	684	ASN	N-CA-CB	-5.52	102.18	110.73
1	A	185	TYR	CB-CG-CD1	-5.51	112.54	120.80
1	A	324	THR	CA-C-O	5.51	127.09	120.92
1	A	127	GLU	N-CA-CB	5.50	118.48	109.95
1	A	355	ASP	CB-CA-C	5.50	119.52	110.88
1	A	200	VAL	CA-C-N	5.50	130.75	123.05
1	A	200	VAL	C-N-CA	5.50	130.75	123.05
1	A	314	SER	N-CA-CB	-5.50	101.20	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	284	ASN	OD1-CG-ND2	-5.50	117.10	122.60
1	A	240	THR	CA-CB-OG1	5.50	117.84	109.60
1	A	160	ARG	NE-CZ-NH1	-5.49	116.01	121.50
1	A	245	SER	CB-CA-C	5.49	120.22	109.35
1	A	742	ILE	CA-CB-CG2	5.49	119.83	110.50
1	A	325	ASN	CB-CA-C	5.48	121.33	110.42
1	A	572	GLU	CA-CB-CG	-5.48	103.14	114.10
1	A	608	LYS	O-C-N	5.47	130.05	123.16
1	A	621	LYS	CA-C-O	5.47	126.35	120.55
1	A	743	GLU	CB-CA-C	5.47	119.87	110.79
1	A	60	ARG	CD-NE-CZ	5.46	132.05	124.40
1	A	187	ASN	CA-CB-CG	5.46	118.06	112.60
1	A	309	ARG	CD-NE-CZ	-5.44	116.79	124.40
1	A	413	ARG	CD-NE-CZ	5.44	132.01	124.40
1	A	250	ASN	CA-C-O	5.43	130.03	120.80
1	A	614	HIS	CB-CG-CD2	-5.43	124.14	131.20
1	A	162	GLU	N-CA-C	5.43	117.62	111.11
1	A	145	ASP	N-CA-C	5.42	117.61	111.11
1	A	556	HIS	CA-CB-CG	-5.41	108.39	113.80
1	A	487	THR	N-CA-C	5.40	117.44	109.50
1	A	44	ASN	CA-CB-CG	-5.40	107.20	112.60
1	A	313	SER	N-CA-CB	-5.38	102.49	110.61
1	A	235	ASN	OD1-CG-ND2	-5.38	117.22	122.60
1	A	798	THR	CA-CB-OG1	5.36	117.63	109.60
1	A	709	PHE	N-CA-C	5.35	117.25	109.71
1	A	262	TYR	CA-C-N	-5.35	112.83	120.42
1	A	262	TYR	C-N-CA	-5.35	112.83	120.42
1	A	160	ARG	NE-CZ-NH2	5.34	124.01	119.20
1	A	180	ASP	CB-CA-C	5.34	120.60	111.68
1	A	381	PRO	CA-C-O	5.34	125.96	118.86
1	A	42	ASP	N-CA-CB	-5.32	102.82	111.22
1	A	767	HIS	CA-C-N	-5.32	113.40	121.53
1	A	767	HIS	C-N-CA	-5.32	113.40	121.53
1	A	461	GLU	N-CA-C	5.30	116.75	111.07
1	A	817	ILE	N-CA-CB	5.30	117.36	110.57
1	A	417	ALA	CA-C-N	-5.30	116.95	122.89
1	A	417	ALA	C-N-CA	-5.30	116.95	122.89
1	A	87	LEU	CB-CA-C	5.30	119.55	110.01
1	A	222	LEU	O-C-N	5.29	129.19	123.10
1	A	170	ILE	N-CA-C	-5.29	100.79	108.36
1	A	596	LYS	CA-C-N	-5.29	113.36	120.87
1	A	596	LYS	C-N-CA	-5.29	113.36	120.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	344	LEU	CA-C-N	5.28	131.63	121.54
1	A	344	LEU	C-N-CA	5.28	131.63	121.54
1	A	636	VAL	CA-C-O	5.28	127.24	120.96
1	A	116	GLY	O-C-N	5.28	127.92	122.54
1	A	763	ASN	OD1-CG-ND2	-5.28	117.32	122.60
1	A	577	LEU	N-CA-C	5.27	117.02	111.28
1	A	668	THR	CA-C-O	-5.27	115.75	121.44
1	A	113	TYR	O-C-N	5.27	127.49	122.07
1	A	481	ASN	CA-C-O	-5.26	115.02	120.70
1	A	815	ARG	NH1-CZ-NH2	-5.26	112.46	119.30
1	A	424	ARG	NE-CZ-NH2	-5.25	114.47	119.20
1	A	302	ALA	CA-C-N	-5.25	113.62	120.44
1	A	302	ALA	C-N-CA	-5.25	113.62	120.44
1	A	575	ARG	N-CA-C	5.25	118.82	111.74
1	A	386	ARG	CG-CD-NE	-5.24	100.47	112.00
1	A	225	PRO	CA-C-N	5.24	131.04	123.13
1	A	225	PRO	C-N-CA	5.24	131.04	123.13
1	A	179	ALA	CA-C-O	-5.24	115.30	121.16
1	A	385	GLU	CA-CB-CG	-5.24	103.63	114.10
1	A	490	ARG	N-CA-CB	5.23	117.60	110.01
1	A	411	LEU	N-CA-C	5.23	117.73	111.71
1	A	405	GLU	CA-C-O	5.22	125.95	119.79
1	A	283	ASP	CB-CA-C	5.22	118.25	109.48
1	A	73	HIS	CA-CB-CG	-5.22	108.58	113.80
1	A	461	GLU	CB-CG-CD	5.22	121.47	112.60
1	A	830	SER	CA-C-O	5.21	126.20	120.31
1	A	81	ARG	CA-CB-CG	-5.21	103.68	114.10
1	A	368	THR	OG1-CB-CG2	-5.20	98.89	109.30
1	A	645	LEU	CA-C-N	5.20	128.23	120.95
1	A	645	LEU	C-N-CA	5.20	128.23	120.95
1	A	235	ASN	N-CA-C	5.20	120.27	113.30
1	A	721	LEU	O-C-N	5.19	127.62	122.12
1	A	33	ARG	CA-C-N	-5.19	113.53	120.54
1	A	33	ARG	C-N-CA	-5.19	113.53	120.54
1	A	528	GLU	N-CA-CB	-5.19	102.23	110.22
1	A	353	LEU	N-CA-CB	5.18	117.66	109.94
1	A	208	HIS	ND1-CG-CD2	5.18	111.28	106.10
1	A	219	GLN	N-CA-CB	-5.17	101.99	110.41
1	A	268	ASP	CA-CB-CG	5.15	117.75	112.60
1	A	457	ARG	NE-CZ-NH2	-5.15	114.56	119.20
1	A	224	MET	N-CA-CB	-5.15	102.50	110.01
1	A	248	ALA	N-CA-CB	-5.15	101.90	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	550	GLU	CA-C-O	5.15	126.22	120.82
1	A	638	ASP	CA-CB-CG	5.15	117.75	112.60
1	A	726	TYR	CB-CA-C	5.12	118.69	110.29
1	A	358	ARG	NE-CZ-NH1	-5.12	116.38	121.50
1	A	641	ARG	NE-CZ-NH1	-5.12	116.38	121.50
1	A	410	PHE	CA-C-N	5.12	127.64	120.28
1	A	410	PHE	C-N-CA	5.12	127.64	120.28
1	A	287	GLU	N-CA-CB	-5.11	102.52	110.55
1	A	678	ASN	CA-C-N	5.11	130.90	121.70
1	A	678	ASN	C-N-CA	5.11	130.90	121.70
1	A	823	GLU	CA-C-N	5.11	131.16	121.97
1	A	823	GLU	C-N-CA	5.11	131.16	121.97
1	A	147	MET	N-CA-CB	-5.10	102.37	110.28
1	A	109	ASP	CA-C-O	5.10	125.82	120.42
1	A	409	ARG	NE-CZ-NH2	-5.10	114.61	119.20
1	A	540	GLU	CB-CG-CD	5.10	121.27	112.60
1	A	686	ALA	N-CA-C	-5.09	101.10	109.40
1	A	381	PRO	O-C-N	5.08	129.44	122.38
1	A	807	THR	CA-CB-CG2	5.08	119.14	110.50
1	A	90	TYR	N-CA-C	-5.08	102.00	109.62
1	A	282	ASN	OD1-CG-ND2	5.07	127.67	122.60
1	A	588	ASN	CA-C-N	5.07	127.33	120.44
1	A	588	ASN	C-N-CA	5.07	127.33	120.44
1	A	477	HIS	CA-CB-CG	-5.06	108.74	113.80
1	A	118	ASP	N-CA-CB	-5.06	101.84	109.94
1	A	300	VAL	N-CA-C	5.06	115.21	110.30
1	A	203	TYR	N-CA-CB	-5.06	101.94	110.49
1	A	811	PHE	CA-C-O	5.06	125.48	119.56
1	A	225	PRO	CA-C-O	-5.05	115.41	121.48
1	A	107	ALA	CA-C-O	-5.05	115.70	121.00
1	A	761	ILE	N-CA-C	5.05	115.19	110.30
1	A	832	GLN	OE1-CD-NE2	-5.04	117.56	122.60
1	A	75	TYR	CB-CA-C	5.04	119.15	110.79
1	A	57	HIS	CA-CB-CG	-5.04	108.77	113.80
1	A	46	ALA	N-CA-C	-5.03	103.76	110.55
1	A	50	ASP	CB-CA-C	-5.03	102.30	110.85
1	A	296	GLU	N-CA-CB	-5.03	102.72	110.12
1	A	34	HIS	ND1-CE1-NE2	5.03	113.43	108.40
1	A	786	ARG	CD-NE-CZ	-5.03	117.36	124.40
1	A	25	THR	CA-CB-CG2	5.02	119.04	110.50
1	A	45	VAL	N-CA-C	5.02	117.05	112.43
1	A	456	ALA	CA-C-O	5.02	126.38	120.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	340	THR	CA-CB-OG1	5.02	117.13	109.60
1	A	286	PHE	O-C-N	5.00	129.00	123.05

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	TYR	Sidechain
1	A	157	TYR	Sidechain
1	A	160	ARG	Sidechain
1	A	205	ARG	Sidechain
1	A	233	TYR	Sidechain
1	A	242	ARG	Sidechain
1	A	374	TYR	Sidechain
1	A	472	TYR	Sidechain
1	A	52	TYR	Sidechain
1	A	524	TYR	Sidechain
1	A	548	TYR	Sidechain
1	A	589	ARG	Sidechain
1	A	63	LEU	Peptide
1	A	66	ARG	Sidechain
1	A	732	TYR	Sidechain
1	A	780	TYR	Sidechain
1	A	81	ARG	Sidechain
1	A	83	TYR	Sidechain

5.2 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 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	A	6642	0	6593	118	0
2	A	31	0	13	5	0
3	A	121	0	0	15	0
All	All	6794	0	6606	119	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 9.

All (119) 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:A:141:ALA:O	3:A:1036:HOH:O	1.90	0.88
1:A:100:VAL:HG21	1:A:494:LEU:HD22	1.64	0.80
1:A:231:PRO:O	3:A:1022:HOH:O	2.02	0.77
1:A:556:HIS:O	3:A:1109:HOH:O	2.04	0.75
1:A:351:ARG:HG2	3:A:1034:HOH:O	1.93	0.69
1:A:211:GLN:HB3	1:A:358:ARG:HH12	1.61	0.65
1:A:235:ASN:H	1:A:235:ASN:HD22	1.47	0.63
1:A:732:TYR:CZ	1:A:739:ARG:HG3	2.36	0.60
1:A:668:THR:HG21	3:A:1045:HOH:O	2.03	0.58
1:A:70:THR:O	1:A:73:HIS:HB3	2.05	0.57
1:A:34:HIS:CD2	1:A:57:HIS:HB3	2.40	0.57
1:A:147:MET:HB2	3:A:1089:HOH:O	2.06	0.56
1:A:100:VAL:HG21	1:A:494:LEU:CD2	2.33	0.56
1:A:205:ARG:HH12	1:A:207:GLU:HG3	1.70	0.56
1:A:235:ASN:H	1:A:235:ASN:ND2	2.03	0.55
1:A:461:GLU:OE1	1:A:465:LYS:NZ	2.39	0.55
1:A:643:ILE:HA	3:A:1052:HOH:O	2.06	0.55
1:A:310:ARG:HG3	1:A:310:ARG:NH1	2.21	0.54
1:A:351:ARG:CG	3:A:1034:HOH:O	2.54	0.54
1:A:44:ASN:ND2	3:A:1058:HOH:O	2.40	0.53
1:A:384:LEU:HB2	1:A:386:ARG:NH1	2.24	0.53
1:A:39:LEU:CD1	1:A:50:ASP:O	2.56	0.53
1:A:380:ILE:CG2	1:A:382:GLU:CD	2.82	0.53
1:A:678:ASN:ND2	3:A:1001:HOH:O	2.41	0.53
1:A:490:ARG:HA	1:A:494:LEU:HG	1.91	0.52
1:A:100:VAL:CG2	1:A:494:LEU:HD22	2.37	0.52
1:A:170:ILE:HA	1:A:174:TRP:O	2.09	0.52
1:A:95:LEU:HD23	1:A:123:GLU:HG2	1.92	0.52
1:A:287:GLU:HG2	1:A:289:LYS:HG2	1.91	0.52
1:A:71:GLN:HB2	2:A:843:194:H57	1.93	0.51
1:A:105:GLU:O	1:A:109:ASP:HB2	2.09	0.51
1:A:184:ARG:NE	1:A:185:TYR:CZ	2.79	0.51
1:A:379:VAL:O	3:A:1107:HOH:O	2.19	0.51
1:A:174:TRP:CE2	1:A:621:LYS:HD3	2.46	0.50
1:A:72:GLN:HG3	2:A:843:194:C36	2.42	0.50
1:A:228:THR:HG23	1:A:229:PRO:HD2	1.94	0.49
1:A:571:HIS:ND1	1:A:572:GLU:N	2.60	0.49
1:A:68:ILE:HA	2:A:843:194:C57	2.43	0.48
1:A:455:VAL:H	1:A:459:HIS:HD2	1.61	0.48
1:A:235:ASN:HD22	1:A:235:ASN:N	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:646:GLU:O	1:A:647:ASN:C	2.55	0.48
1:A:95:LEU:HD23	1:A:123:GLU:CG	2.43	0.48
1:A:85:LEU:HD13	1:A:335:ILE:HG23	1.95	0.48
1:A:327:ASP:OD1	1:A:363:LYS:NZ	2.48	0.47
1:A:361:TRP:C	1:A:361:TRP:CD1	2.91	0.47
1:A:376:ASN:OD1	1:A:459:HIS:CE1	2.67	0.47
1:A:78:ASP:O	1:A:332:LYS:NZ	2.47	0.47
1:A:193:ARG:CZ	2:A:843:194:O7	2.63	0.47
1:A:350:MET:O	1:A:354:VAL:HB	2.14	0.47
1:A:7:GLN:HG2	1:A:8:GLU:HG3	1.96	0.46
1:A:100:VAL:HG11	1:A:494:LEU:HD23	1.98	0.46
1:A:163:PHE:O	1:A:278:VAL:HA	2.16	0.46
1:A:211:GLN:CB	1:A:358:ARG:HH12	2.26	0.46
1:A:709:PHE:HB3	1:A:783:CYS:SG	2.56	0.46
1:A:193:ARG:O	1:A:194:PRO:C	2.57	0.46
1:A:417:ALA:C	1:A:419:PRO:HD3	2.42	0.45
1:A:380:ILE:HG23	1:A:382:GLU:OE1	2.16	0.45
1:A:303:THR:O	1:A:307:ILE:HG13	2.16	0.45
1:A:137:GLY:O	1:A:140:ALA:HB3	2.16	0.45
1:A:159:ILE:HG23	1:A:161:TYR:CE2	2.52	0.45
1:A:460:SER:OG	1:A:481:ASN:ND2	2.45	0.45
1:A:291:LEU:HD12	1:A:291:LEU:O	2.16	0.45
1:A:310:ARG:O	1:A:313:SER:N	2.45	0.45
1:A:693:ASP:O	1:A:694:GLY:C	2.59	0.45
1:A:85:LEU:N	1:A:85:LEU:HD12	2.31	0.45
1:A:795:ARG:O	1:A:799:ARG:HG3	2.17	0.45
1:A:165:ILE:O	1:A:166:PHE:C	2.60	0.44
1:A:306:ASP:CG	1:A:309:ARG:HH21	2.25	0.44
1:A:488:PRO:O	1:A:492:LEU:HB3	2.18	0.44
1:A:498:GLY:HA3	3:A:1051:HOH:O	2.17	0.44
1:A:83:TYR:CE1	1:A:155:TYR:CD1	3.06	0.44
1:A:193:ARG:NH1	1:A:227:ASP:OD2	2.51	0.44
1:A:143:PHE:O	1:A:144:LEU:C	2.60	0.44
1:A:159:ILE:CG2	1:A:161:TYR:CZ	3.00	0.44
1:A:47:THR:O	1:A:48:PRO:C	2.58	0.43
1:A:351:ARG:O	1:A:352:VAL:C	2.61	0.43
1:A:764:MET:SD	1:A:764:MET:C	3.01	0.43
1:A:89:PHE:CD1	1:A:144:LEU:HD22	2.54	0.43
1:A:150:LEU:HD12	1:A:817:ILE:HG22	2.00	0.43
1:A:384:LEU:HD12	1:A:386:ARG:NH2	2.33	0.43
1:A:236:ASN:ND2	1:A:834:LEU:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:TRP:CH2	1:A:448:GLY:HA2	2.54	0.43
1:A:67:TRP:O	1:A:71:GLN:HG2	2.19	0.43
1:A:149:THR:O	1:A:831:ARG:HD2	2.19	0.43
1:A:159:ILE:HG23	1:A:161:TYR:CZ	2.54	0.42
1:A:338:ASN:O	1:A:339:ASP:CB	2.67	0.42
1:A:506:ARG:NH1	1:A:524:TYR:CE1	2.87	0.42
1:A:379:VAL:HG12	1:A:467:ILE:CD1	2.49	0.42
1:A:380:ILE:HG21	1:A:382:GLU:CD	2.45	0.42
1:A:515:LEU:HD12	1:A:515:LEU:HA	1.90	0.42
1:A:128:ASP:OD1	1:A:651:SER:HB3	2.19	0.42
1:A:511:TYR:HA	1:A:514:ASP:O	2.19	0.42
1:A:388:PRO:HB3	1:A:436:VAL:CG1	2.50	0.42
1:A:31:PHE:C	1:A:31:PHE:CD1	2.98	0.42
1:A:503:ILE:HG21	1:A:503:ILE:HD13	1.77	0.42
1:A:464:LYS:HB3	1:A:465:LYS:HE3	2.01	0.41
1:A:96:GLN:HA	1:A:99:MET:HE2	2.01	0.41
1:A:714:ARG:CD	1:A:714:ARG:N	2.83	0.41
1:A:105:GLU:O	1:A:119:MET:HE1	2.20	0.41
1:A:177:GLU:HG2	1:A:611:PRO:HG3	2.01	0.41
1:A:690:GLY:O	1:A:710:ILE:HA	2.21	0.41
1:A:455:VAL:HG22	1:A:459:HIS:CD2	2.54	0.41
1:A:227:ASP:CG	1:A:242:ARG:HH21	2.28	0.41
1:A:309:ARG:O	1:A:310:ARG:C	2.63	0.41
1:A:397:PRO:O	1:A:401:GLN:HG3	2.19	0.41
1:A:490:ARG:HD3	1:A:654:GLU:OE2	2.20	0.41
1:A:622:LEU:O	1:A:626:ILE:HG13	2.20	0.41
2:A:843:194:C2	2:A:843:194:C38	2.92	0.41
1:A:193:ARG:CG	1:A:193:ARG:HH11	2.32	0.41
1:A:291:LEU:HD12	1:A:291:LEU:C	2.46	0.41
1:A:582:HIS:HB2	1:A:780:TYR:CE2	2.56	0.40
1:A:267:LEU:O	1:A:270:ASN:ND2	2.55	0.40
1:A:734:ARG:C	1:A:735:ILE:HG13	2.46	0.40
1:A:351:ARG:O	1:A:355:ASP:N	2.53	0.40
1:A:498:GLY:N	3:A:1051:HOH:O	2.53	0.40
1:A:771:PHE:HB2	3:A:1088:HOH:O	2.21	0.40
1:A:169:LYS:HB2	1:A:176:MET:HB2	2.03	0.40
1:A:193:ARG:HD2	1:A:193:ARG:HA	1.89	0.40
1:A:343:SER:N	3:A:1048:HOH:O	2.54	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	A	806/842 (96%)	738 (92%)	61 (8%)	7 (1%)	14 22

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	ILE
1	A	339	ASP
1	A	325	ASN
1	A	406	ILE
1	A	342	PRO
1	A	354	VAL
1	A	100	VAL

5.3.2 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 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	A	704/730 (96%)	683 (97%)	21 (3%)	36 58

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	10	ARG
1	A	29	LYS
1	A	42	ASP

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Mol	Chain	Res	Type
1	A	47	THR
1	A	60	ARG
1	A	76	GLU
1	A	77	LYS
1	A	128	ASP
1	A	144	LEU
1	A	180	ASP
1	A	224	MET
1	A	235	ASN
1	A	250	ASN
1	A	313	SER
1	A	382	GLU
1	A	437	LYS
1	A	465	LYS
1	A	469	LYS
1	A	568	LYS
1	A	576	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	44	ASN
1	A	71	GLN
1	A	106	ASN
1	A	235	ASN
1	A	264	GLN
1	A	390	HIS
1	A	450	HIS
1	A	459	HIS
1	A	566	GLN
1	A	576	GLN
1	A	579	ASN
1	A	763	ASN
1	A	767	HIS
1	A	768	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is 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
1	LLP	A	680	1	23,24,25	4.89	10 (43%)	25,32,34	2.49	8 (32%)

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
1	LLP	A	680	1	-	0/16/17/19	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	680	LLP	C3-C2	15.95	1.57	1.41
1	A	680	LLP	C4-C3	8.45	1.55	1.41
1	A	680	LLP	C2-N1	7.37	1.46	1.33
1	A	680	LLP	C6-N1	6.27	1.47	1.34
1	A	680	LLP	C4-C5	6.20	1.50	1.42
1	A	680	LLP	C6-C5	6.04	1.49	1.37
1	A	680	LLP	C4'-NZ	4.80	1.43	1.27
1	A	680	LLP	P-OP1	2.68	1.58	1.50
1	A	680	LLP	C5'-C5	2.42	1.57	1.50
1	A	680	LLP	C4-C4'	2.23	1.51	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	680	LLP	C4-C3-C2	-6.38	116.55	120.14
1	A	680	LLP	C2'-C2-C3	5.43	127.16	120.80
1	A	680	LLP	C5-C4-C4'	-4.41	114.67	121.47
1	A	680	LLP	CD-CE-NZ	-3.91	100.49	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	680	LLP	C3-C4-C4'	2.87	125.58	120.40
1	A	680	LLP	C4-C4'-NZ	-2.76	111.29	124.04
1	A	680	LLP	C5-C6-N1	-2.08	120.45	123.83
1	A	680	LLP	C3-C2-N1	-2.05	118.37	120.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	194	A	843	-	33,33,33	1.67	7 (21%)	44,46,46	1.45	7 (15%)

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	194	A	843	-	-	10/22/24/24	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	843	194	O2-C10	4.72	1.36	1.22
2	A	843	194	O8-N2	3.81	1.29	1.22
2	A	843	194	O1-C10	-3.80	1.19	1.30
2	A	843	194	O7-N2	-2.57	1.18	1.35
2	A	843	194	O5-C20	2.25	1.37	1.30
2	A	843	194	C53-C54	2.23	1.42	1.39
2	A	843	194	C5-C20	-2.16	1.45	1.49

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	843	194	C56-C57-C51	3.83	124.13	120.36
2	A	843	194	C51-C44-N1	3.49	124.38	115.90
2	A	843	194	O1-C10-C6	2.56	122.55	115.28
2	A	843	194	C34-N1-C44	-2.49	119.97	126.90
2	A	843	194	O6-C44-N1	-2.36	117.76	123.75
2	A	843	194	C53-C54-N2	2.26	120.69	118.74
2	A	843	194	O2-C10-C6	-2.20	116.72	121.97

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	843	194	C31-C34-N1-C44
2	A	843	194	C35-C34-N1-C44
2	A	843	194	O5-C20-C5-C4
2	A	843	194	O4-C20-C5-C4
2	A	843	194	O2-C10-C6-C1
2	A	843	194	O1-C10-C6-C1
2	A	843	194	O5-C20-C5-C6
2	A	843	194	O4-C20-C5-C6
2	A	843	194	O6-C44-N1-C34
2	A	843	194	O2-C10-C6-C5

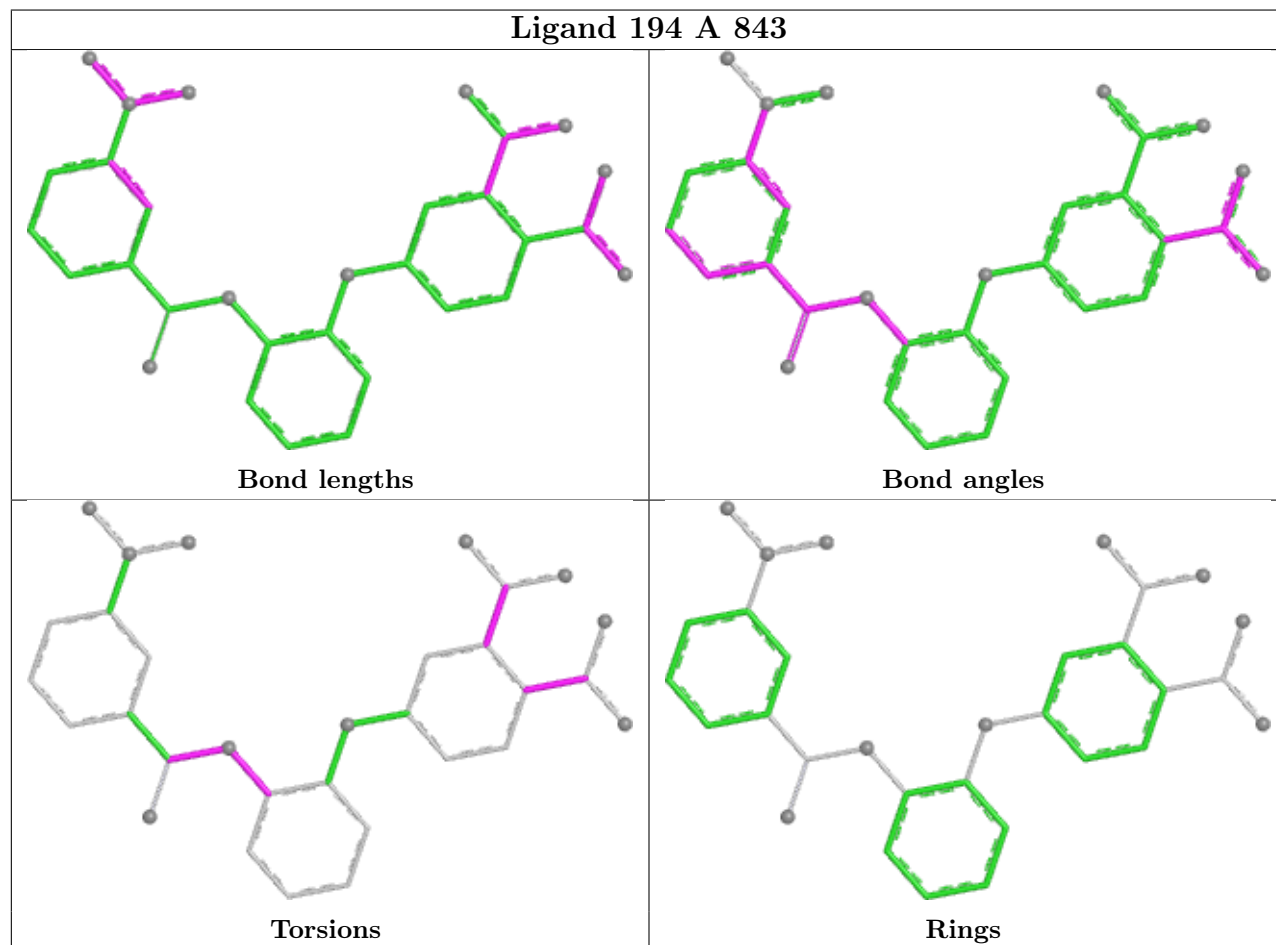
There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	843	194	5	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.