



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2025 – 03:44 PM EDT

PDB ID : 1Z6P
Title : Glycogen phosphorylase AMP site inhibitor complex
Authors : Kristiansen, M.; Andersen, B.; Iversen, L.F.; Westergaard, N.
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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

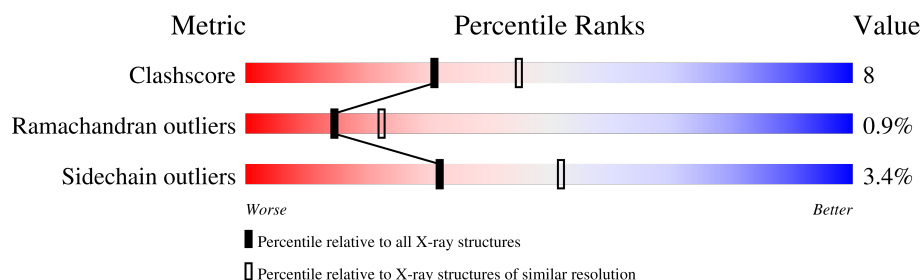
1 Overall quality at a glance

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	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (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.

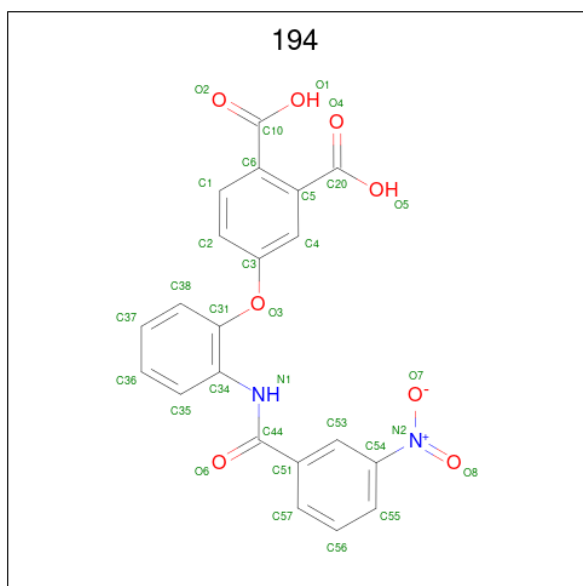
- Molecule 1 is a protein called Glycogen phosphorylase, muscle form.

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 (three-letter code: 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.

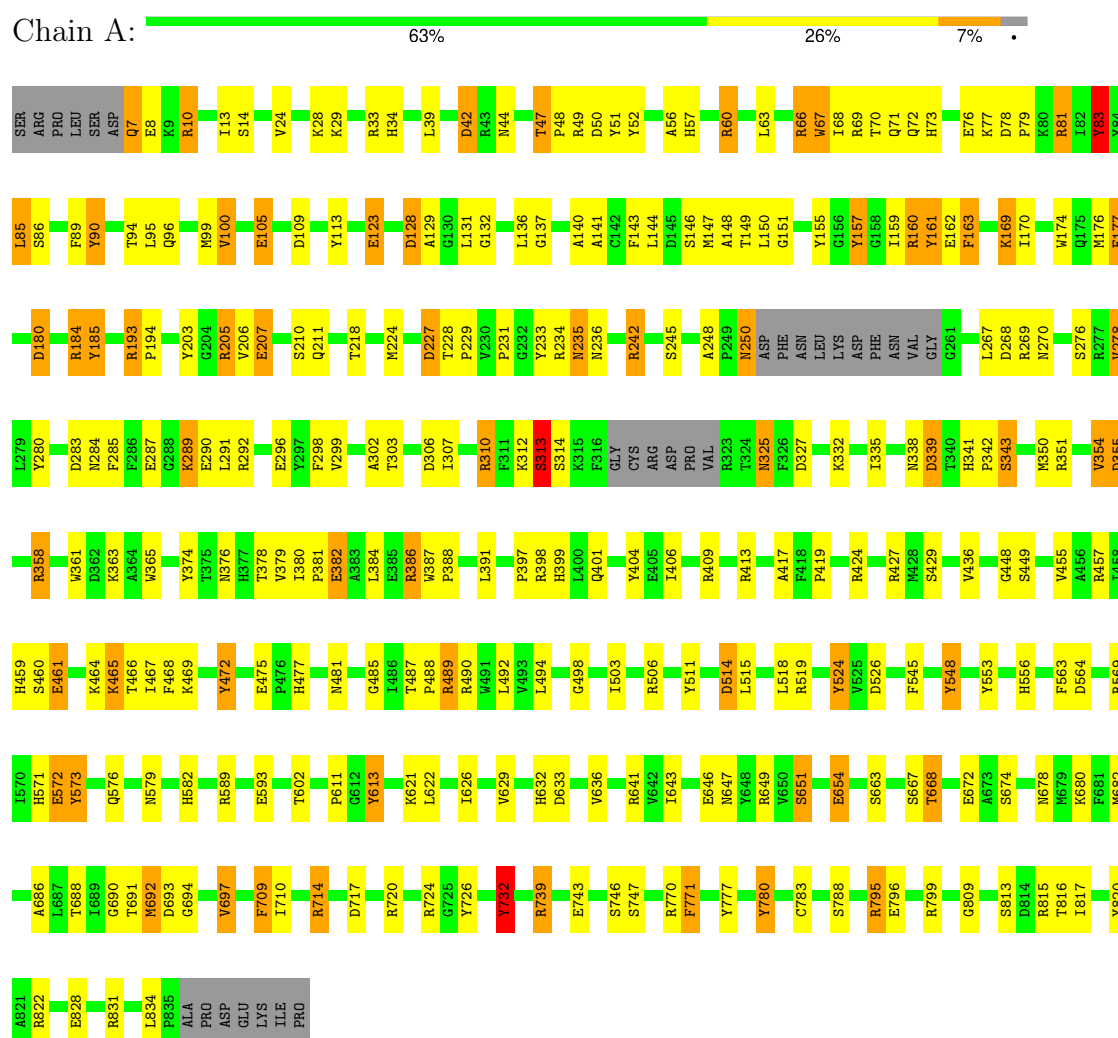
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	121	Total 121	O 121	0	0

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



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	1.50	46/6764 (0.7%)	2.00	172/9147 (1.9%)

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 outliers	#Planarity outliers
1	A	0	18

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	674	SER	CB-OG	8.96	1.53	1.42
1	A	284	ASN	C-N	8.17	1.52	1.34
1	A	747	SER	CB-OG	7.56	1.52	1.42
1	A	651	SER	CB-OG	7.40	1.51	1.42
1	A	146	SER	CB-OG	7.15	1.51	1.42
1	A	788	SER	CB-OG	7.00	1.51	1.42
1	A	461	GLU	CG-CD	6.93	1.62	1.51
1	A	654	GLU	CD-OE1	-6.71	1.18	1.25
1	A	813	SER	CB-OG	6.61	1.50	1.42
1	A	284	ASN	N-CA	6.51	1.59	1.46
1	A	14	SER	CB-OG	6.47	1.50	1.42
1	A	123	GLU	CD-OE1	-6.34	1.18	1.25
1	A	796	GLU	CG-CD	6.34	1.61	1.51
1	A	296	GLU	CD-OE1	-6.28	1.18	1.25
1	A	67	TRP	CG-CD1	6.17	1.45	1.36
1	A	284	ASN	CA-C	6.15	1.69	1.52
1	A	672	GLU	CG-CD	6.06	1.61	1.51
1	A	667	SER	CB-OG	6.01	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	151	GLY	CA-C	-5.89	1.42	1.51
1	A	449	SER	CB-OG	5.88	1.49	1.42
1	A	343	SER	CB-OG	5.86	1.49	1.42
1	A	663	SER	CB-OG	5.85	1.49	1.42
1	A	743	GLU	CG-CD	5.79	1.60	1.51
1	A	210	SER	CB-OG	5.78	1.49	1.42
1	A	86	SER	CB-OG	5.75	1.49	1.42
1	A	341	HIS	CA-C	5.67	1.67	1.52
1	A	14	SER	CA-CB	5.64	1.61	1.52
1	A	276	SER	CB-OG	5.63	1.49	1.42
1	A	123	GLU	CD-OE2	-5.58	1.19	1.25
1	A	161	TYR	CE2-CZ	5.58	1.45	1.38
1	A	746	SER	CB-OG	5.46	1.49	1.42
1	A	429	SER	CB-OG	5.42	1.49	1.42
1	A	828	GLU	CG-CD	5.37	1.59	1.51
1	A	290	GLU	CD-OE1	-5.33	1.19	1.25
1	A	160	ARG	CZ-NH1	-5.29	1.26	1.33
1	A	477	HIS	CG-CD2	5.28	1.44	1.35
1	A	83	TYR	CG-CD1	-5.27	1.32	1.39
1	A	132	GLY	CA-C	5.21	1.60	1.51
1	A	672	GLU	CB-CG	5.20	1.62	1.52
1	A	203	TYR	CZ-OH	5.18	1.46	1.37
1	A	79	PRO	CA-C	5.08	1.63	1.52
1	A	822	ARG	CZ-NH1	-5.07	1.26	1.33
1	A	105	GLU	CD-OE2	-5.07	1.20	1.25
1	A	809	GLY	CA-C	5.04	1.59	1.51
1	A	250	ASN	CA-C	5.03	1.66	1.52
1	A	489	ARG	CZ-NH2	-5.02	1.26	1.33

All (172) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	ARG	NE-CZ-NH2	21.81	131.21	120.30
1	A	649	ARG	NE-CZ-NH1	20.73	130.67	120.30
1	A	424	ARG	NE-CZ-NH1	19.24	129.92	120.30
1	A	770	ARG	NE-CZ-NH2	16.12	128.36	120.30
1	A	185	TYR	CB-CG-CD1	-14.10	112.54	121.00
1	A	269	ARG	NE-CZ-NH2	-13.79	113.40	120.30
1	A	519	ARG	NE-CZ-NH1	-12.59	114.01	120.30
1	A	569	ARG	NE-CZ-NH2	-12.57	114.02	120.30
1	A	489	ARG	NE-CZ-NH1	12.32	126.46	120.30
1	A	185	TYR	CB-CG-CD2	11.66	128.00	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	424	ARG	NE-CZ-NH2	-11.65	114.47	120.30
1	A	457	ARG	NE-CZ-NH2	-11.47	114.56	120.30
1	A	409	ARG	NE-CZ-NH2	-11.38	114.61	120.30
1	A	33	ARG	NE-CZ-NH2	-10.94	114.83	120.30
1	A	283	ASP	N-CA-CB	-10.69	91.36	110.60
1	A	280	TYR	CB-CG-CD2	-10.55	114.67	121.00
1	A	795	ARG	NE-CZ-NH1	10.43	125.52	120.30
1	A	815	ARG	NE-CZ-NH2	10.13	125.36	120.30
1	A	519	ARG	NE-CZ-NH2	9.94	125.27	120.30
1	A	398	ARG	NE-CZ-NH2	-9.87	115.36	120.30
1	A	69	ARG	NE-CZ-NH2	-9.39	115.60	120.30
1	A	413	ARG	NE-CZ-NH1	9.39	125.00	120.30
1	A	720	ARG	NE-CZ-NH2	-9.11	115.75	120.30
1	A	269	ARG	NE-CZ-NH1	9.10	124.85	120.30
1	A	569	ARG	NE-CZ-NH1	8.97	124.78	120.30
1	A	649	ARG	NE-CZ-NH2	-8.96	115.82	120.30
1	A	732	TYR	CB-CG-CD1	-8.66	115.80	121.00
1	A	160	ARG	NE-CZ-NH1	-8.59	116.01	120.30
1	A	487	THR	CA-CB-CG2	8.58	124.41	112.40
1	A	10	ARG	NE-CZ-NH1	8.47	124.54	120.30
1	A	280	TYR	CB-CG-CD1	8.36	126.02	121.00
1	A	193	ARG	NH1-CZ-NH2	-8.03	110.56	119.40
1	A	475	GLU	OE1-CD-OE2	-8.02	113.67	123.30
1	A	391	LEU	CB-CA-C	7.93	125.26	110.20
1	A	161	TYR	CB-CG-CD1	-7.89	116.27	121.00
1	A	245	SER	N-CA-CB	-7.88	98.67	110.50
1	A	358	ARG	NE-CZ-NH1	-7.84	116.38	120.30
1	A	641	ARG	NE-CZ-NH1	-7.84	116.38	120.30
1	A	234	ARG	CD-NE-CZ	7.78	134.50	123.60
1	A	688	THR	CA-CB-OG1	7.76	125.29	109.00
1	A	49	ARG	NE-CZ-NH1	7.71	124.15	120.30
1	A	355	ASP	CB-CG-OD1	7.69	125.22	118.30
1	A	193	ARG	CD-NE-CZ	-7.63	112.92	123.60
1	A	33	ARG	CD-NE-CZ	7.51	134.11	123.60
1	A	563	PHE	CB-CG-CD1	7.51	126.06	120.80
1	A	90	TYR	CB-CG-CD1	-7.50	116.50	121.00
1	A	692	MET	CG-SD-CE	-7.49	88.21	100.20
1	A	203	TYR	CB-CG-CD2	7.45	125.47	121.00
1	A	160	ARG	NE-CZ-NH2	7.42	124.01	120.30
1	A	302	ALA	CB-CA-C	7.41	121.21	110.10
1	A	518	LEU	CB-CG-CD2	7.40	123.57	111.00
1	A	771	PHE	CB-CG-CD1	7.32	125.92	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157	TYR	CB-CG-CD1	-7.29	116.63	121.00
1	A	24	VAL	CA-CB-CG1	7.26	121.80	110.90
1	A	206	VAL	C-N-CA	7.26	139.86	121.70
1	A	564	ASP	CB-CG-OD1	7.25	124.82	118.30
1	A	404	TYR	CB-CG-CD1	7.15	125.29	121.00
1	A	545	PHE	CB-CG-CD1	7.15	125.80	120.80
1	A	427	ARG	CD-NE-CZ	7.03	133.44	123.60
1	A	90	TYR	CB-CG-CD2	7.01	125.21	121.00
1	A	668	THR	OG1-CB-CG2	-7.00	93.89	110.00
1	A	143	PHE	CB-CG-CD2	-7.00	115.90	120.80
1	A	573	TYR	CB-CG-CD2	6.98	125.19	121.00
1	A	732	TYR	CB-CG-CD2	6.94	125.17	121.00
1	A	177	GLU	OE1-CD-OE2	-6.86	115.07	123.30
1	A	312	LYS	O-C-N	-6.80	111.83	122.70
1	A	726	TYR	CB-CG-CD2	-6.79	116.92	121.00
1	A	42	ASP	CB-CA-C	6.77	123.94	110.40
1	A	548	TYR	CB-CG-CD1	-6.76	116.94	121.00
1	A	726	TYR	CG-CD2-CE2	-6.75	115.90	121.30
1	A	160	ARG	CD-NE-CZ	6.69	132.96	123.60
1	A	94	THR	N-CA-CB	-6.62	97.72	110.30
1	A	242	ARG	NE-CZ-NH1	-6.61	117.00	120.30
1	A	81	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	A	69	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	A	563	PHE	CB-CG-CD2	-6.41	116.31	120.80
1	A	724	ARG	NE-CZ-NH1	-6.39	117.11	120.30
1	A	413	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	A	398	ARG	CG-CD-NE	-6.33	98.51	111.80
1	A	815	ARG	NH1-CZ-NH2	-6.31	112.46	119.40
1	A	66	ARG	CD-NE-CZ	-6.30	114.78	123.60
1	A	654	GLU	OE1-CD-OE2	-6.21	115.84	123.30
1	A	739	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	A	314	SER	N-CA-CB	-6.20	101.20	110.50
1	A	248	ALA	CB-CA-C	6.19	119.39	110.10
1	A	820	TYR	CB-CG-CD1	-6.18	117.29	121.00
1	A	129	ALA	N-CA-CB	-6.13	101.52	110.10
1	A	129	ALA	C-N-CA	6.09	135.09	122.30
1	A	33	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	A	278	VAL	CA-CB-CG1	6.08	120.02	110.90
1	A	306	ASP	CB-CG-OD1	6.06	123.75	118.30
1	A	60	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	A	60	ARG	CD-NE-CZ	6.04	132.05	123.60
1	A	131	LEU	CB-CG-CD2	6.03	121.26	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	777	TYR	CB-CG-CD1	-6.01	117.39	121.00
1	A	413	ARG	CD-NE-CZ	6.01	132.01	123.60
1	A	686	ALA	O-C-N	5.99	132.29	122.70
1	A	613	TYR	CB-CG-CD2	-5.99	117.41	121.00
1	A	148	ALA	N-CA-CB	-5.97	101.74	110.10
1	A	203	TYR	CB-CG-CD1	-5.94	117.44	121.00
1	A	378	THR	OG1-CB-CG2	-5.92	96.38	110.00
1	A	788	SER	N-CA-CB	-5.88	101.68	110.50
1	A	632	HIS	CA-CB-CG	-5.87	103.61	113.60
1	A	234	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	A	399	HIS	CA-CB-CG	-5.87	103.62	113.60
1	A	248	ALA	N-CA-CB	-5.86	101.90	110.10
1	A	310	ARG	CD-NE-CZ	-5.85	115.41	123.60
1	A	180	ASP	N-CA-CB	-5.84	100.08	110.60
1	A	633	ASP	CB-CG-OD1	5.84	123.56	118.30
1	A	136	LEU	N-CA-CB	-5.81	98.78	110.40
1	A	292	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	688	THR	OG1-CB-CG2	-5.79	96.67	110.00
1	A	289	LYS	N-CA-CB	-5.78	100.19	110.60
1	A	724	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	A	593	GLU	CB-CG-CD	-5.75	98.67	114.20
1	A	381	PRO	CA-C-N	-5.75	104.55	117.20
1	A	667	SER	N-CA-CB	-5.72	101.92	110.50
1	A	526	ASP	CB-CG-OD1	-5.72	113.16	118.30
1	A	28	LYS	N-CA-CB	-5.71	100.33	110.60
1	A	468	PHE	CB-CG-CD1	-5.70	116.81	120.80
1	A	553	TYR	CZ-CE2-CD2	5.70	124.93	119.80
1	A	81	ARG	O-C-N	5.64	131.73	122.70
1	A	227	ASP	CB-CG-OD1	5.60	123.34	118.30
1	A	285	PHE	CB-CG-CD2	-5.56	116.91	120.80
1	A	280	TYR	N-CA-CB	-5.56	100.60	110.60
1	A	472	TYR	N-CA-CB	-5.54	100.62	110.60
1	A	724	ARG	NH1-CZ-NH2	5.53	125.48	119.40
1	A	378	THR	CA-CB-OG1	5.52	120.59	109.00
1	A	387	TRP	CH2-CZ2-CE2	5.51	122.92	117.40
1	A	285	PHE	N-CA-C	5.51	125.88	111.00
1	A	56	ALA	CB-CA-C	5.50	118.36	110.10
1	A	218	THR	OG1-CB-CG2	-5.46	97.43	110.00
1	A	325	ASN	CB-CA-C	5.46	121.33	110.40
1	A	485	GLY	C-N-CA	5.46	135.35	121.70
1	A	636	VAL	CA-C-N	-5.45	105.29	116.20
1	A	572	GLU	OE1-CD-OE2	5.40	129.78	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	162	GLU	CA-CB-CG	-5.39	101.53	113.40
1	A	386	ARG	CG-CD-NE	-5.39	100.47	111.80
1	A	51	TYR	CB-CG-CD2	-5.38	117.77	121.00
1	A	649	ARG	NH1-CZ-NH2	-5.38	113.48	119.40
1	A	691	THR	N-CA-CB	-5.36	100.11	110.30
1	A	207	GLU	CB-CA-C	-5.36	99.68	110.40
1	A	457	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	A	85	LEU	CB-CG-CD1	-5.34	101.92	111.00
1	A	313	SER	N-CA-CB	-5.34	102.49	110.50
1	A	245	SER	CB-CA-C	5.33	120.22	110.10
1	A	299	VAL	CG1-CB-CG2	-5.32	102.39	110.90
1	A	697	VAL	CA-CB-CG2	5.31	118.87	110.90
1	A	387	TRP	CB-CG-CD1	-5.31	120.10	127.00
1	A	629	VAL	CA-C-N	-5.31	105.52	117.20
1	A	514	ASP	N-CA-CB	-5.29	101.08	110.60
1	A	602	THR	OG1-CB-CG2	-5.27	97.88	110.00
1	A	682	MET	CA-CB-CG	-5.21	104.44	113.30
1	A	163	PHE	CB-CG-CD1	5.20	124.44	120.80
1	A	298	PHE	N-CA-CB	-5.19	101.25	110.60
1	A	184	ARG	CD-NE-CZ	5.18	130.86	123.60
1	A	79	PRO	CB-CA-C	5.18	124.94	112.00
1	A	816	THR	CA-CB-OG1	5.17	119.87	109.00
1	A	387	TRP	CG-CD2-CE3	5.17	138.55	133.90
1	A	717	ASP	CB-CG-OD1	5.17	122.95	118.30
1	A	51	TYR	CB-CA-C	5.15	120.71	110.40
1	A	771	PHE	CB-CG-CD2	-5.12	117.22	120.80
1	A	770	ARG	NH1-CZ-NH2	-5.12	113.77	119.40
1	A	714	ARG	CG-CD-NE	-5.11	101.06	111.80
1	A	268	ASP	CB-CG-OD1	5.11	122.90	118.30
1	A	180	ASP	CB-CA-C	5.10	120.60	110.40
1	A	83	TYR	CB-CG-CD1	-5.08	117.95	121.00
1	A	709	PHE	CB-CG-CD2	-5.08	117.25	120.80
1	A	90	TYR	CB-CA-C	5.08	120.55	110.40
1	A	564	ASP	CB-CG-OD2	-5.05	113.75	118.30
1	A	466	THR	CA-CB-OG1	5.03	119.57	109.00
1	A	602	THR	CA-CB-CG2	-5.03	105.36	112.40

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	TYR	Sidechain

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Mol	Chain	Res	Type	Group
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 ⓘ

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	107	0
2	A	31	0	13	5	0
3	A	121	0	0	15	0
All	All	6794	0	6606	108	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 8.

All (108) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:380:ILE:CG2	1:A:382:GLU:CD	2.82	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
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:376:ASN:OD1	1:A:459:HIS:CE1	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:159:ILE:CG2	1:A:161:TYR:CZ	3.00	0.44
1:A:646:GLU:O	1:A:647:ASN:C	2.55	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:96:GLN:HA	1:A:99:MET:HE2	2.00	0.43
1:A:236:ASN:ND2	1:A:834:LEU:O	2.51	0.43
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:361:TRP:CD1	1:A:361:TRP:C	2.91	0.42
1:A:379:VAL:HG12	1:A:467:ILE:CD1	2.49	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:503:ILE:HG21	1:A:503:ILE:HD13	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:LYS:HB3	1:A:465:LYS:HE3	2.01	0.41
1:A:714:ARG:CD	1:A:714:ARG:N	2.83	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:692:MET:HE3	1:A:697:VAL:HG13	2.02	0.41
1:A:47:THR:O	1:A:48:PRO:C	2.58	0.41
1:A:193:ARG:O	1:A:194:PRO:C	2.57	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:417:ALA:C	1:A:419:PRO:HD3	2.42	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: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:693:ASP:O	1:A:694:GLY:C	2.59	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 ⓘ

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%)	680 (97%)	24 (3%)	32 52

All (24) 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
1	A	47	THR
1	A	60	ARG
1	A	76	GLU
1	A	77	LYS
1	A	90	TYR
1	A	128	ASP
1	A	169	LYS
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	465	LYS
1	A	469	LYS
1	A	489	ARG

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Mol	Chain	Res	Type
1	A	573	TYR
1	A	576	GLN
1	A	579	ASN
1	A	613	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	44	ASN
1	A	235	ASN
1	A	264	GLN
1	A	390	HIS
1	A	459	HIS
1	A	481	ASN
1	A	566	GLN
1	A	576	GLN
1	A	579	ASN
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
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

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:

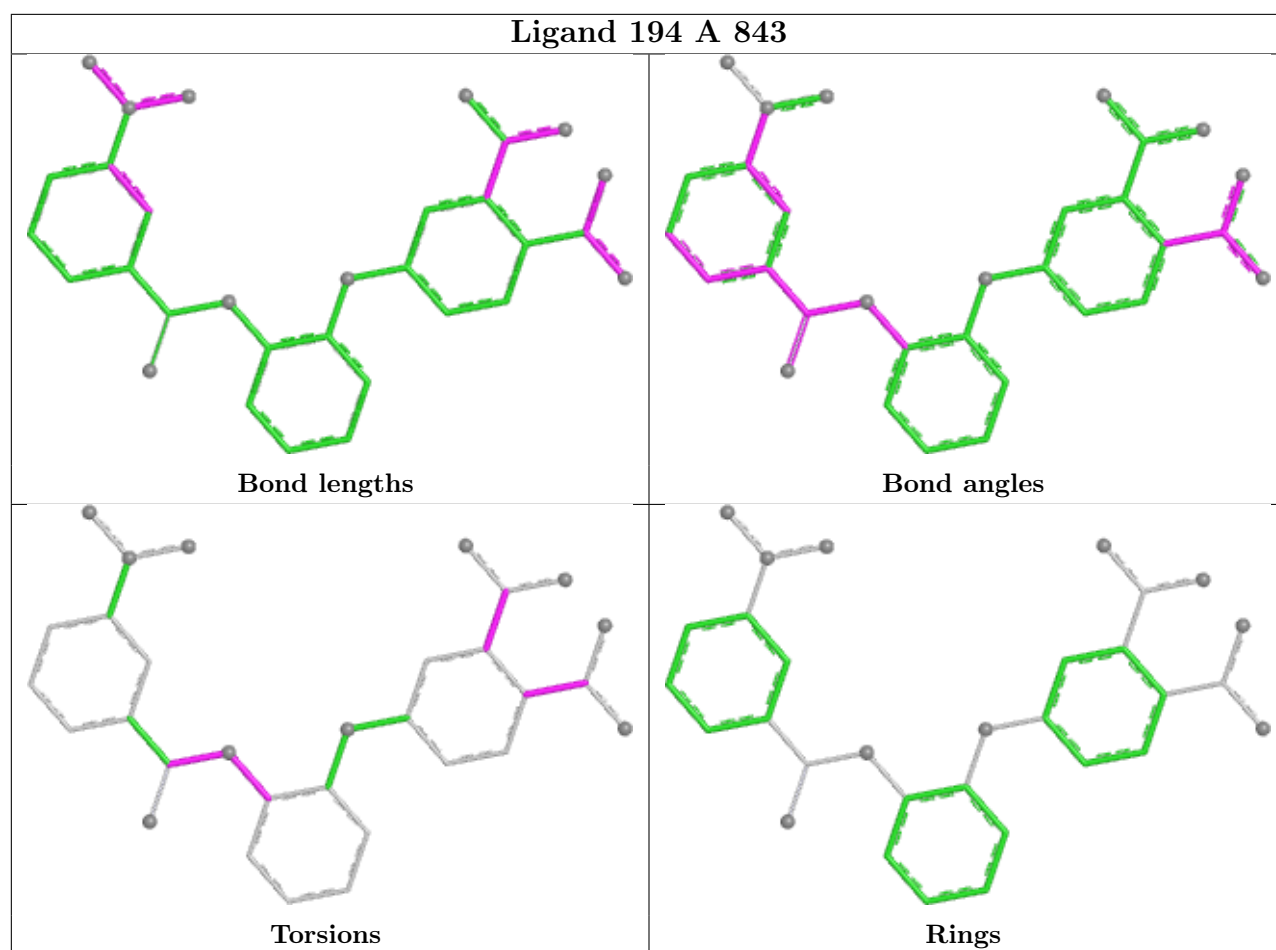
Mol	Chain	Res	Type	Atoms
2	A	843	194	C31-C34-N1-C44
2	A	843	194	C35-C34-N1-C44
2	A	843	194	O5-C20-C5-C4
2	A	843	194	O4-C20-C5-C4
2	A	843	194	O2-C10-C6-C1
2	A	843	194	O1-C10-C6-C1
2	A	843	194	O5-C20-C5-C6
2	A	843	194	O4-C20-C5-C6
2	A	843	194	O6-C44-N1-C34
2	A	843	194	O2-C10-C6-C5

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.