



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:07 AM UTC

PDB ID : 1Z6Q / pdb_00001z6q
Title : Glycogen phosphorylase with inhibitor in the AMP site
Authors : Kristiansen, M.; Andersen, B.; Iversen, L.F.; Westergaard, N.
Deposited on : 2005-03-23
Resolution : 2.03 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

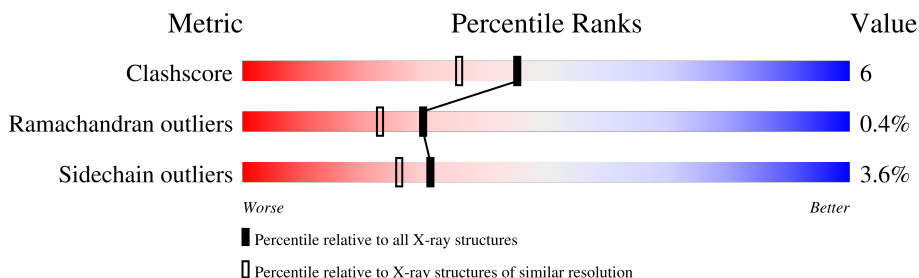
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)

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 2 unique types of molecules in this entry. The entry contains 6685 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.

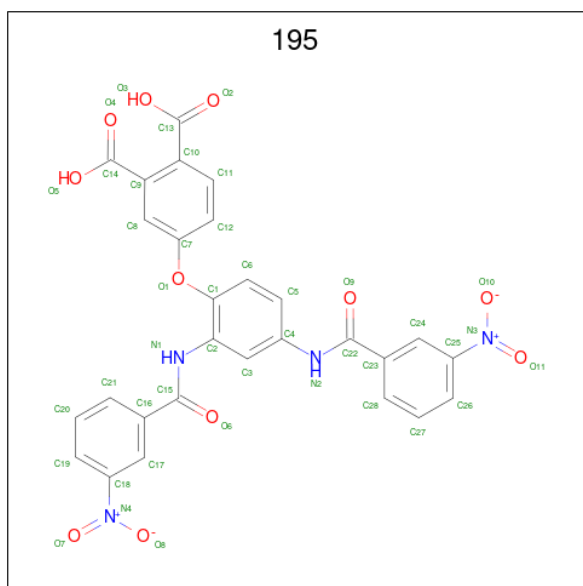
- Molecule 1 is a protein called Glycogen phosphorylase, muscle form.

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-{2,4-BIS[(3-NITROBENZOYL)AMINO]PHENOXY}PHTHALIC ACID (CCD ID: 195) (formula: C₂₈H₁₈N₄O₁₁).



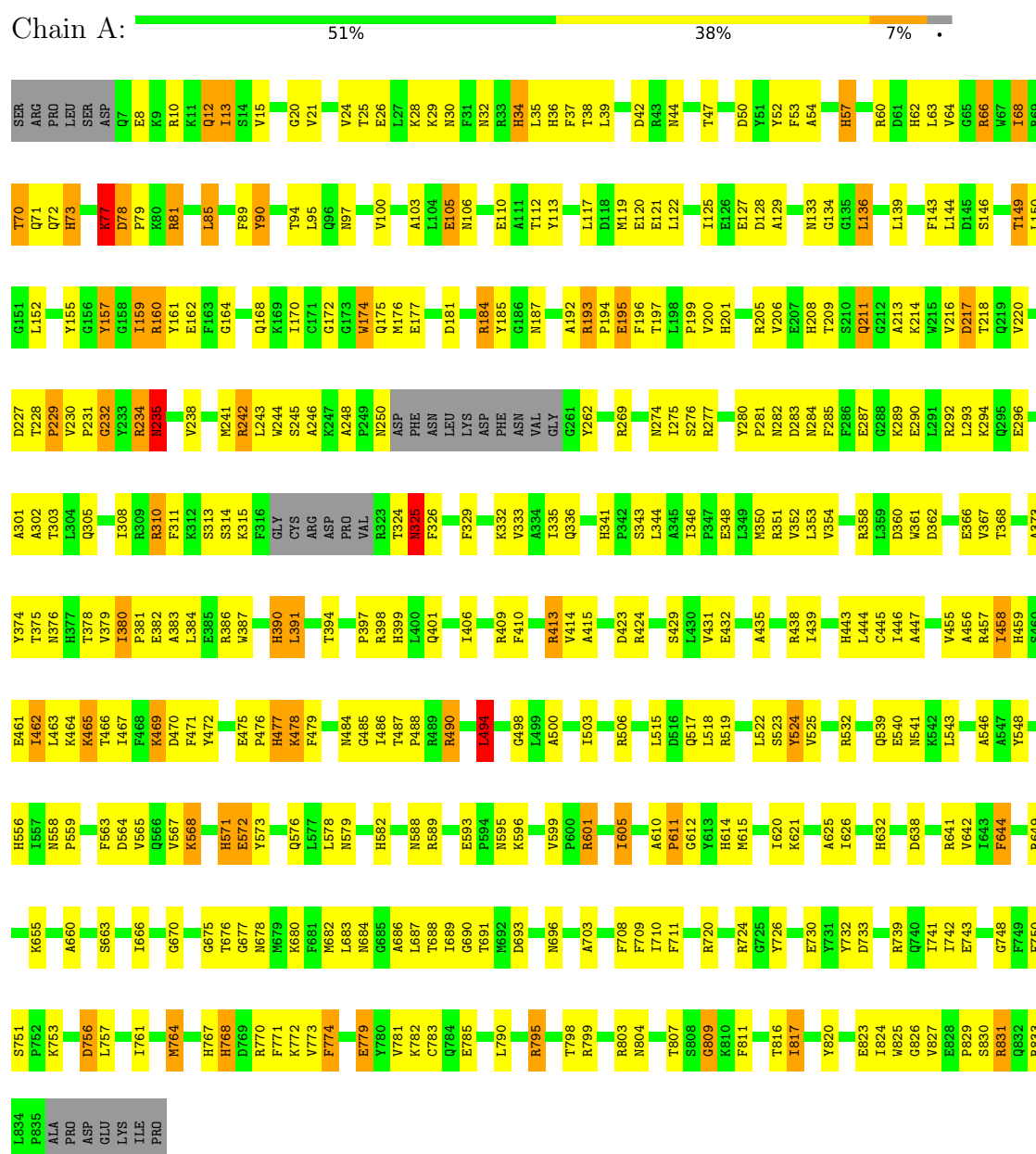
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	43	28	4	11	0	0

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	127.50Å 127.50Å 115.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.03	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.03)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.210 , 0.270	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6685	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: 195, 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	1.96	168/6764 (2.5%)	2.18	272/9147 (3.0%)

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	15

All (168) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	302	ALA	CA-C	10.48	1.66	1.52
1	A	588	ASN	CA-C	10.47	1.66	1.52
1	A	315	LYS	CA-C	10.23	1.59	1.53
1	A	567	VAL	CA-C	9.24	1.64	1.52
1	A	824	ILE	CA-C	9.07	1.66	1.53
1	A	314	SER	CA-C	8.95	1.64	1.52
1	A	773	VAL	CA-C	8.81	1.63	1.52
1	A	296	GLU	CA-C	8.75	1.64	1.52
1	A	284	ASN	C-N	8.74	1.46	1.33
1	A	280	TYR	CA-C	8.73	1.64	1.52
1	A	95	LEU	CA-C	8.69	1.64	1.52
1	A	284	ASN	CA-C	8.65	1.64	1.53
1	A	614	HIS	CA-C	8.26	1.63	1.52
1	A	380	ILE	CA-C	8.17	1.62	1.52
1	A	246	ALA	CA-C	8.16	1.63	1.52
1	A	406	ILE	CA-C	7.96	1.62	1.52
1	A	230	VAL	CA-C	7.69	1.60	1.52
1	A	341	HIS	CA-C	7.61	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	285	PHE	CA-C	7.52	1.62	1.52
1	A	443	HIS	CG-CD2	7.48	1.44	1.35
1	A	790	LEU	CA-C	7.37	1.62	1.52
1	A	675	GLY	N-CA	7.35	1.53	1.45
1	A	764	MET	CA-C	7.22	1.61	1.52
1	A	383	ALA	CA-C	7.21	1.62	1.52
1	A	479	PHE	CA-C	7.20	1.61	1.52
1	A	199	PRO	CA-C	7.16	1.60	1.52
1	A	571	HIS	CE1-NE2	7.11	1.39	1.32
1	A	761	ILE	CA-C	7.10	1.61	1.52
1	A	578	LEU	CA-C	7.02	1.61	1.52
1	A	532	ARG	CA-C	7.00	1.62	1.52
1	A	488	PRO	CA-C	6.98	1.61	1.52
1	A	28	LYS	CA-C	6.94	1.62	1.52
1	A	757	LEU	CA-C	6.94	1.62	1.52
1	A	398	ARG	CA-C	6.90	1.61	1.52
1	A	242	ARG	CA-C	6.90	1.61	1.52
1	A	81	ARG	CA-C	-6.84	1.44	1.52
1	A	152	LEU	CA-C	6.83	1.61	1.52
1	A	54	ALA	CA-C	6.82	1.61	1.52
1	A	346	ILE	CA-C	6.81	1.60	1.52
1	A	610	ALA	C-N	6.76	1.41	1.33
1	A	490	ARG	N-CA	6.74	1.54	1.46
1	A	543	LEU	CA-C	6.71	1.61	1.52
1	A	193	ARG	CZ-NH1	-6.71	1.23	1.32
1	A	655	LYS	CA-C	6.69	1.61	1.53
1	A	625	ALA	CA-C	6.60	1.61	1.52
1	A	350	MET	C-N	6.59	1.41	1.33
1	A	469	LYS	CA-C	6.56	1.61	1.52
1	A	15	VAL	CA-C	6.55	1.62	1.52
1	A	431	VAL	CA-C	6.51	1.61	1.52
1	A	399	HIS	CG-CD2	6.50	1.43	1.35
1	A	305	GLN	N-CA	6.49	1.54	1.46
1	A	329	PHE	CA-C	6.47	1.60	1.52
1	A	678	ASN	N-CA	6.45	1.53	1.46
1	A	193	ARG	N-CA	-6.37	1.39	1.46
1	A	211	GLN	CA-C	6.34	1.60	1.52
1	A	229	PRO	CA-C	6.33	1.60	1.52
1	A	176	MET	CA-C	6.30	1.59	1.52
1	A	175	GLN	CA-C	6.29	1.60	1.52
1	A	352	VAL	C-N	6.28	1.42	1.33
1	A	143	PHE	CA-C	6.27	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	293	LEU	CA-C	6.25	1.60	1.52
1	A	689	ILE	CA-C	6.21	1.60	1.52
1	A	678	ASN	CA-C	6.20	1.61	1.52
1	A	703	ALA	CA-C	6.18	1.61	1.52
1	A	558	ASN	CA-C	6.14	1.60	1.52
1	A	244	TRP	NE1-CE2	6.12	1.44	1.37
1	A	336	GLN	CA-C	6.10	1.60	1.52
1	A	589	ARG	C-N	6.10	1.41	1.33
1	A	670	GLY	CA-C	6.05	1.59	1.51
1	A	582	HIS	CG-CD2	6.04	1.42	1.35
1	A	68	ILE	CA-C	6.01	1.60	1.52
1	A	621	LYS	CA-C	6.01	1.60	1.52
1	A	708	PHE	CA-C	5.99	1.60	1.52
1	A	522	LEU	CA-C	5.98	1.60	1.52
1	A	477	HIS	CA-C	5.94	1.61	1.52
1	A	517	GLN	CA-C	5.93	1.61	1.52
1	A	487	THR	C-N	5.91	1.39	1.33
1	A	696	ASN	CA-C	5.91	1.60	1.52
1	A	379	VAL	CA-CB	5.90	1.61	1.54
1	A	688	THR	CA-CB	5.89	1.61	1.53
1	A	477	HIS	CG-CD2	5.86	1.42	1.35
1	A	772	LYS	CA-C	5.82	1.60	1.53
1	A	833	ARG	CA-C	5.82	1.60	1.52
1	A	432	GLU	CA-C	5.81	1.60	1.52
1	A	133	ASN	CA-C	5.81	1.60	1.52
1	A	352	VAL	CA-CB	-5.80	1.48	1.54
1	A	378	THR	CA-CB	5.80	1.63	1.53
1	A	21	VAL	CA-C	5.80	1.59	1.52
1	A	72	GLN	CA-C	5.76	1.60	1.52
1	A	146	SER	CB-OG	5.76	1.53	1.42
1	A	807	THR	CA-C	5.75	1.60	1.52
1	A	117	LEU	CA-C	5.74	1.59	1.52
1	A	262	TYR	CA-C	5.72	1.60	1.52
1	A	546	ALA	CA-C	5.71	1.60	1.52
1	A	38	THR	CA-C	-5.70	1.45	1.52
1	A	64	VAL	CA-CB	5.69	1.60	1.54
1	A	605	ILE	CA-CB	5.69	1.61	1.54
1	A	593	GLU	CA-C	5.67	1.59	1.52
1	A	571	HIS	CG-CD2	5.67	1.42	1.35
1	A	615	MET	CA-CB	5.65	1.62	1.53
1	A	95	LEU	C-N	5.64	1.41	1.33
1	A	478	LYS	CA-C	5.60	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	277	ARG	CA-C	5.60	1.60	1.52
1	A	691	THR	CB-OG1	5.59	1.52	1.43
1	A	820	TYR	N-CA	5.59	1.53	1.46
1	A	13	ILE	CA-C	5.57	1.59	1.52
1	A	457	ARG	CA-C	5.57	1.60	1.52
1	A	444	LEU	CA-CB	5.56	1.62	1.53
1	A	187	ASN	CA-CB	5.55	1.58	1.53
1	A	174	TRP	CA-C	5.54	1.59	1.52
1	A	164	GLY	N-CA	5.51	1.51	1.45
1	A	620	ILE	N-CA	5.50	1.53	1.46
1	A	413	ARG	CA-C	5.48	1.60	1.52
1	A	540	GLU	CA-C	5.47	1.59	1.52
1	A	24	VAL	CA-C	5.44	1.59	1.52
1	A	284	ASN	N-CA	5.44	1.54	1.46
1	A	79	PRO	CA-C	5.43	1.59	1.52
1	A	626	ILE	N-CA	5.43	1.52	1.46
1	A	134	GLY	C-N	5.43	1.41	1.33
1	A	768	HIS	CG-CD2	5.42	1.41	1.35
1	A	601	ARG	CA-C	5.42	1.59	1.52
1	A	756	ASP	CA-C	5.41	1.60	1.52
1	A	214	LYS	CA-C	5.40	1.58	1.52
1	A	248	ALA	CA-C	5.39	1.59	1.53
1	A	572	GLU	CA-C	5.39	1.59	1.52
1	A	168	GLN	CA-C	5.38	1.59	1.52
1	A	649	ARG	NE-CZ	5.37	1.39	1.33
1	A	181	ASP	CA-C	5.37	1.59	1.53
1	A	62	HIS	ND1-CE1	5.37	1.38	1.32
1	A	368	THR	N-CA	5.34	1.52	1.46
1	A	817	ILE	CA-CB	5.32	1.61	1.54
1	A	595	ASN	CA-C	-5.31	1.45	1.52
1	A	127	GLU	N-CA	5.31	1.52	1.46
1	A	128	ASP	N-CA	5.30	1.52	1.45
1	A	128	ASP	CA-C	5.26	1.59	1.52
1	A	36	HIS	CG-CD2	5.26	1.41	1.35
1	A	351	ARG	NE-CZ	5.25	1.38	1.33
1	A	578	LEU	C-N	5.21	1.40	1.33
1	A	565	VAL	CA-C	5.21	1.59	1.52
1	A	757	LEU	C-N	5.19	1.40	1.33
1	A	201	HIS	CG-CD2	5.18	1.41	1.35
1	A	172	GLY	CA-C	5.18	1.58	1.51
1	A	195	GLU	CA-CB	5.18	1.62	1.53
1	A	333	VAL	CA-C	5.17	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	373	ALA	CA-C	5.17	1.58	1.52
1	A	220	VAL	CA-CB	5.17	1.60	1.54
1	A	446	ILE	CA-CB	5.16	1.61	1.54
1	A	281	PRO	CA-C	5.16	1.59	1.52
1	A	146	SER	CA-C	-5.16	1.45	1.52
1	A	196	PHE	CA-CB	5.15	1.60	1.53
1	A	105	GLU	C-N	5.14	1.41	1.33
1	A	525	VAL	N-CA	5.14	1.52	1.46
1	A	136	LEU	N-CA	5.11	1.52	1.46
1	A	599	VAL	CA-C	5.11	1.58	1.52
1	A	447	ALA	CA-CB	5.11	1.61	1.53
1	A	596	LYS	CA-C	5.11	1.59	1.52
1	A	200	VAL	N-CA	5.10	1.52	1.46
1	A	471	PHE	CA-CB	5.09	1.61	1.53
1	A	294	LYS	CA-C	5.08	1.59	1.52
1	A	498	GLY	CA-C	5.08	1.59	1.51
1	A	157	TYR	N-CA	-5.07	1.40	1.46
1	A	620	ILE	CA-CB	5.07	1.60	1.54
1	A	612	GLY	N-CA	5.06	1.52	1.44
1	A	329	PHE	C-N	5.05	1.40	1.33
1	A	290	GLU	CA-C	5.04	1.59	1.52
1	A	361	TRP	CA-C	5.03	1.59	1.52
1	A	35	LEU	CA-C	5.03	1.59	1.52
1	A	435	ALA	CA-C	5.02	1.59	1.52

All (272) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	774	PHE	CA-CB-CG	11.58	125.38	113.80
1	A	688	THR	CA-CB-OG1	10.98	126.08	109.60
1	A	194	PRO	CA-C-N	10.07	135.08	120.38
1	A	194	PRO	C-N-CA	10.07	135.08	120.38
1	A	753	LYS	CA-C-N	-9.45	112.72	122.74
1	A	753	LYS	C-N-CA	-9.45	112.72	122.74
1	A	632	HIS	CA-CB-CG	-9.24	104.56	113.80
1	A	129	ALA	N-CA-CB	-9.16	97.39	110.58
1	A	283	ASP	N-CA-CB	-9.12	95.45	110.23
1	A	32	ASN	CA-CB-CG	-9.12	103.48	112.60
1	A	477	HIS	CA-CB-CG	-8.93	104.87	113.80
1	A	97	ASN	CA-CB-CG	-8.77	103.83	112.60
1	A	310	ARG	CB-CA-C	-8.77	96.18	110.74
1	A	644	PHE	CA-CB-CG	-8.74	105.06	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	676	THR	CA-C-N	8.71	129.83	119.99
1	A	676	THR	C-N-CA	8.71	129.83	119.99
1	A	193	ARG	NE-CZ-NH2	8.54	126.89	119.20
1	A	37	PHE	N-CA-C	8.51	120.64	111.36
1	A	206	VAL	CA-C-N	8.42	135.07	123.11
1	A	206	VAL	C-N-CA	8.42	135.07	123.11
1	A	34	HIS	CA-CB-CG	-8.26	105.54	113.80
1	A	234	ARG	CD-NE-CZ	8.19	135.87	124.40
1	A	750	PHE	CA-CB-CG	-8.14	105.66	113.80
1	A	391	LEU	CB-CA-C	8.10	123.44	110.96
1	A	564	ASP	CA-CB-CG	8.07	120.67	112.60
1	A	830	SER	N-CA-C	8.05	121.63	108.99
1	A	313	SER	N-CA-CB	-8.01	98.76	110.70
1	A	113	TYR	O-C-N	7.99	130.30	122.07
1	A	379	VAL	CA-C-O	7.98	125.92	118.90
1	A	62	HIS	CA-CB-CG	-7.71	106.09	113.80
1	A	245	SER	N-CA-CB	-7.69	97.08	111.00
1	A	781	VAL	N-CA-C	7.66	117.78	110.42
1	A	466	THR	CA-C-N	7.62	130.44	120.60
1	A	466	THR	C-N-CA	7.62	130.44	120.60
1	A	682	MET	N-CA-C	7.57	120.19	111.11
1	A	81	ARG	CD-NE-CZ	-7.55	113.83	124.40
1	A	290	GLU	N-CA-C	7.49	120.40	111.33
1	A	595	ASN	CA-CB-CG	-7.49	105.11	112.60
1	A	37	PHE	CA-CB-CG	-7.47	106.33	113.80
1	A	771	PHE	CA-CB-CG	-7.40	106.40	113.80
1	A	470	ASP	CA-CB-CG	7.35	119.95	112.60
1	A	518	LEU	CA-C-N	7.33	131.09	120.38
1	A	518	LEU	C-N-CA	7.33	131.09	120.38
1	A	798	THR	CA-CB-OG1	7.33	120.59	109.60
1	A	611	PRO	CA-C-N	-7.30	112.21	122.86
1	A	611	PRO	C-N-CA	-7.30	112.21	122.86
1	A	285	PHE	CA-CB-CG	-7.27	106.53	113.80
1	A	362	ASP	CB-CA-C	7.26	122.37	110.90
1	A	394	THR	N-CA-C	7.26	118.98	111.14
1	A	81	ARG	O-C-N	7.26	132.43	123.21
1	A	136	LEU	N-CA-CB	-7.22	99.23	110.06
1	A	324	THR	CA-C-O	7.18	128.59	120.90
1	A	485	GLY	CA-C-N	7.14	132.87	122.94
1	A	485	GLY	C-N-CA	7.14	132.87	122.94
1	A	315	LYS	CA-C-O	7.04	122.02	117.94
1	A	484	ASN	CA-CB-CG	7.00	119.60	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	556	HIS	CA-CB-CG	-6.96	106.84	113.80
1	A	66	ARG	CD-NE-CZ	-6.95	114.67	124.40
1	A	106	ASN	CA-CB-CG	6.90	119.50	112.60
1	A	30	ASN	CA-CB-CG	-6.88	105.72	112.60
1	A	208	HIS	CA-CB-CG	-6.88	106.92	113.80
1	A	567	VAL	N-CA-C	6.88	117.80	107.75
1	A	614	HIS	CA-CB-CG	-6.88	106.92	113.80
1	A	795	ARG	O-C-N	6.85	129.96	122.15
1	A	781	VAL	N-CA-CB	-6.82	102.57	110.55
1	A	443	HIS	CA-C-O	6.82	127.78	120.55
1	A	324	THR	CA-CB-OG1	6.79	119.79	109.60
1	A	663	SER	N-CA-C	6.76	119.75	108.73
1	A	380	ILE	N-CA-C	6.76	116.33	108.96
1	A	503	ILE	N-CA-C	6.75	117.54	110.72
1	A	519	ARG	NE-CZ-NH1	-6.74	114.76	121.50
1	A	77	LYS	N-CA-CB	-6.69	99.91	110.28
1	A	466	THR	CA-CB-OG1	6.68	119.62	109.60
1	A	572	GLU	N-CA-C	6.63	118.16	111.07
1	A	517	GLN	N-CA-C	6.60	120.92	112.34
1	A	232	GLY	CA-C-N	-6.59	112.17	121.72
1	A	232	GLY	C-N-CA	-6.59	112.17	121.72
1	A	197	THR	CA-CB-OG1	-6.57	99.74	109.60
1	A	469	LYS	N-CA-C	6.56	118.98	111.11
1	A	162	GLU	CA-CB-CG	-6.54	101.02	114.10
1	A	424	ARG	NE-CZ-NH1	6.53	128.03	121.50
1	A	462	ILE	N-CA-C	6.51	117.26	110.62
1	A	582	HIS	CA-CB-CG	-6.44	107.36	113.80
1	A	579	ASN	CA-CB-CG	6.44	119.04	112.60
1	A	726	TYR	CB-CA-C	6.43	119.91	110.26
1	A	687	LEU	CA-C-N	-6.42	114.06	123.05
1	A	687	LEU	C-N-CA	-6.42	114.06	123.05
1	A	366	GLU	CB-CG-CD	6.40	123.48	112.60
1	A	195	GLU	CA-CB-CG	6.37	126.83	114.10
1	A	773	VAL	N-CA-CB	-6.34	103.13	110.55
1	A	195	GLU	CB-CA-C	6.32	122.71	110.46
1	A	275	ILE	N-CA-C	6.31	117.05	110.62
1	A	121	GLU	CB-CA-C	6.29	121.23	110.79
1	A	770	ARG	NE-CZ-NH2	6.25	124.83	119.20
1	A	287	GLU	N-CA-CB	-6.19	100.86	110.57
1	A	494	LEU	CB-CA-C	-6.15	101.42	110.95
1	A	541	ASN	N-CA-C	6.14	117.97	111.28
1	A	211	GLN	CB-CG-CD	6.10	122.98	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	471	PHE	CA-C-O	6.10	126.98	120.70
1	A	25	THR	OG1-CB-CG2	-6.09	97.12	109.30
1	A	121	GLU	N-CA-CB	-6.09	101.17	110.12
1	A	81	ARG	CA-CB-CG	-6.08	101.94	114.10
1	A	112	THR	CA-CB-OG1	6.06	118.69	109.60
1	A	804	ASN	CB-CA-C	6.06	120.86	110.86
1	A	73	HIS	N-CA-C	6.05	118.37	111.11
1	A	649	ARG	NE-CZ-NH1	6.03	127.53	121.50
1	A	709	PHE	N-CA-CB	-6.01	103.61	110.35
1	A	376	ASN	OD1-CG-ND2	-6.01	116.59	122.60
1	A	296	GLU	N-CA-C	6.00	117.49	111.07
1	A	149	THR	CA-CB-OG1	-5.99	100.62	109.60
1	A	128	ASP	CA-CB-CG	5.96	118.56	112.60
1	A	398	ARG	CG-CD-NE	-5.93	98.95	112.00
1	A	519	ARG	NE-CZ-NH2	5.92	124.53	119.20
1	A	571	HIS	CA-CB-CG	-5.92	107.88	113.80
1	A	816	THR	OG1-CB-CG2	5.92	121.13	109.30
1	A	12	GLN	O-C-N	5.91	128.38	122.12
1	A	399	HIS	CA-CB-CG	-5.87	107.93	113.80
1	A	741	ILE	N-CA-C	5.84	116.02	110.53
1	A	391	LEU	N-CA-CB	-5.84	101.38	109.91
1	A	487	THR	CA-CB-OG1	5.84	118.36	109.60
1	A	97	ASN	N-CA-C	5.83	118.11	111.11
1	A	159	ILE	CA-CB-CG1	5.83	120.32	110.40
1	A	558	ASN	CA-C-O	5.83	124.89	119.24
1	A	26	GLU	CB-CG-CD	5.83	122.50	112.60
1	A	53	PHE	N-CA-CB	-5.83	101.56	110.12
1	A	378	THR	CA-CB-OG1	5.83	118.34	109.60
1	A	282	ASN	CB-CG-ND2	-5.82	107.67	116.40
1	A	218	THR	OG1-CB-CG2	-5.81	97.67	109.30
1	A	89	PHE	CA-CB-CG	-5.81	107.99	113.80
1	A	110	GLU	CA-C-O	5.78	126.66	120.70
1	A	184	ARG	CA-C-O	5.78	127.40	120.92
1	A	305	GLN	CB-CA-C	-5.78	101.19	110.79
1	A	213	ALA	O-C-N	5.77	129.55	123.03
1	A	564	ASP	N-CA-CB	-5.75	100.89	110.37
1	A	833	ARG	CB-CA-C	5.75	118.46	109.84
1	A	287	GLU	CA-C-N	-5.73	110.18	121.41
1	A	287	GLU	C-N-CA	-5.73	110.18	121.41
1	A	432	GLU	CA-C-O	5.71	127.06	120.60
1	A	168	GLN	CA-C-O	5.71	126.99	120.54
1	A	563	PHE	CA-C-N	5.70	130.25	122.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	563	PHE	C-N-CA	5.70	130.25	122.84
1	A	413	ARG	CA-C-N	5.70	127.83	120.70
1	A	413	ARG	C-N-CA	5.70	127.83	120.70
1	A	774	PHE	N-CA-CB	5.70	118.99	110.22
1	A	282	ASN	OD1-CG-ND2	5.68	128.28	122.60
1	A	85	LEU	CA-C-O	5.64	126.75	120.43
1	A	313	SER	N-CA-C	5.64	119.15	112.72
1	A	730	GLU	CA-C-O	5.62	126.72	120.82
1	A	803	ARG	CA-C-N	5.61	129.96	120.88
1	A	803	ARG	C-N-CA	5.61	129.96	120.88
1	A	743	GLU	CB-CA-C	5.58	120.34	110.85
1	A	344	LEU	CA-C-N	5.58	129.19	120.82
1	A	344	LEU	C-N-CA	5.58	129.19	120.82
1	A	500	ALA	N-CA-C	-5.58	105.20	111.28
1	A	311	PHE	CA-C-O	5.57	126.45	120.55
1	A	811	PHE	CA-CB-CG	-5.56	108.24	113.80
1	A	209	THR	CB-CA-C	-5.53	101.86	112.43
1	A	649	ARG	CA-C-O	-5.52	115.54	121.45
1	A	139	LEU	O-C-N	5.51	128.04	122.09
1	A	783	CYS	O-C-N	5.51	127.75	122.07
1	A	112	THR	CA-C-O	5.51	126.29	119.79
1	A	326	PHE	N-CA-CB	5.49	118.68	110.22
1	A	94	THR	N-CA-CB	-5.49	102.69	110.81
1	A	353	LEU	N-CA-CB	5.49	118.19	110.12
1	A	748	GLY	CA-C-O	5.48	123.92	118.77
1	A	216	VAL	CA-C-N	5.47	130.13	122.36
1	A	216	VAL	C-N-CA	5.47	130.13	122.36
1	A	282	ASN	CB-CA-C	-5.47	102.00	111.30
1	A	378	THR	CB-CA-C	-5.46	100.03	109.86
1	A	63	LEU	CB-CA-C	-5.46	101.57	110.85
1	A	70	THR	CA-CB-OG1	5.46	117.78	109.60
1	A	445	CYS	N-CA-C	5.45	117.92	111.33
1	A	238	VAL	CA-C-O	5.44	125.06	120.22
1	A	423	ASP	CA-CB-CG	-5.44	107.16	112.60
1	A	242	ARG	CG-CD-NE	-5.42	100.07	112.00
1	A	160	ARG	N-CA-CB	-5.41	102.78	110.46
1	A	206	VAL	O-C-N	5.41	129.10	123.26
1	A	301	ALA	N-CA-CB	-5.41	102.23	110.07
1	A	724	ARG	NH1-CZ-NH2	5.40	126.32	119.30
1	A	816	THR	N-CA-C	5.40	117.59	111.11
1	A	127	GLU	CB-CA-C	-5.39	100.43	109.65
1	A	211	GLN	OE1-CD-NE2	-5.38	117.22	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	390	HIS	CA-CB-CG	-5.38	108.42	113.80
1	A	368	THR	OG1-CB-CG2	-5.37	98.55	109.30
1	A	660	ALA	O-C-N	5.36	129.06	123.06
1	A	175	GLN	CA-C-N	5.36	130.55	123.00
1	A	175	GLN	C-N-CA	5.36	130.55	123.00
1	A	638	ASP	CB-CA-C	5.34	120.06	110.81
1	A	809	GLY	N-CA-C	5.34	120.38	113.27
1	A	689	ILE	CB-CA-C	5.34	117.54	110.91
1	A	375	THR	N-CA-C	5.34	117.67	109.07
1	A	302	ALA	N-CA-CB	-5.33	102.00	109.94
1	A	192	ALA	CA-C-N	-5.32	116.71	123.15
1	A	192	ALA	C-N-CA	-5.32	116.71	123.15
1	A	201	HIS	CA-CB-CG	-5.32	108.48	113.80
1	A	303	THR	O-C-N	5.32	127.55	122.07
1	A	478	LYS	N-CA-C	5.32	118.55	111.75
1	A	234	ARG	NE-CZ-NH1	5.31	126.81	121.50
1	A	678	ASN	CB-CA-C	5.31	119.65	110.84
1	A	677	GLY	N-CA-C	-5.31	106.22	112.64
1	A	539	GLN	CA-C-N	5.29	127.32	120.44
1	A	539	GLN	C-N-CA	5.29	127.32	120.44
1	A	779	GLU	N-CA-C	5.28	117.12	111.36
1	A	105	GLU	N-CA-C	5.28	117.45	111.11
1	A	302	ALA	CB-CA-C	5.28	119.26	110.81
1	A	683	LEU	CA-C-O	5.28	126.11	120.20
1	A	711	PHE	CA-CB-CG	-5.27	108.53	113.80
1	A	494	LEU	N-CA-CB	5.26	117.61	109.98
1	A	733	ASP	CA-CB-CG	-5.26	107.34	112.60
1	A	724	ARG	CD-NE-CZ	-5.26	117.04	124.40
1	A	409	ARG	NE-CZ-NH2	-5.25	114.47	119.20
1	A	399	HIS	ND1-CE1-NE2	5.25	113.65	108.40
1	A	751	SER	CA-C-O	5.24	127.34	120.16
1	A	310	ARG	CG-CD-NE	-5.24	100.47	112.00
1	A	429	SER	N-CA-CB	5.24	118.01	109.69
1	A	742	ILE	CA-CB-CG2	5.23	119.39	110.50
1	A	139	LEU	CA-C-N	5.22	128.65	120.82
1	A	139	LEU	C-N-CA	5.22	128.65	120.82
1	A	184	ARG	CD-NE-CZ	5.22	131.70	124.40
1	A	614	HIS	N-CA-C	5.21	117.38	111.02
1	A	567	VAL	O-C-N	-5.21	117.68	123.20
1	A	666	ILE	N-CA-C	5.21	117.19	111.77
1	A	231	PRO	O-C-N	5.20	128.92	123.10
1	A	352	VAL	CA-C-O	-5.19	116.01	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	367	VAL	N-CA-C	5.19	115.81	110.36
1	A	824	ILE	N-CA-C	5.19	116.36	111.48
1	A	688	THR	CA-C-N	-5.19	115.68	122.37
1	A	688	THR	C-N-CA	-5.19	115.68	122.37
1	A	235	ASN	CA-CB-CG	5.17	117.77	112.60
1	A	458	ILE	N-CA-C	5.17	115.90	110.62
1	A	445	CYS	CA-C-N	-5.17	113.08	120.42
1	A	445	CYS	C-N-CA	-5.17	113.08	120.42
1	A	518	LEU	O-C-N	5.17	128.09	122.20
1	A	783	CYS	CA-C-O	-5.16	115.40	120.82
1	A	32	ASN	CB-CG-ND2	-5.16	108.66	116.40
1	A	825	TRP	CA-C-O	5.16	125.70	119.31
1	A	57	HIS	CA-CB-CG	-5.16	108.64	113.80
1	A	20	GLY	CA-C-N	5.15	127.52	120.77
1	A	20	GLY	C-N-CA	5.15	127.52	120.77
1	A	10	ARG	CA-C-N	5.15	129.38	121.19
1	A	10	ARG	C-N-CA	5.15	129.38	121.19
1	A	269	ARG	NE-CZ-NH2	-5.15	114.57	119.20
1	A	686	ALA	N-CA-C	-5.14	101.78	109.95
1	A	120	GLU	CA-C-O	5.13	125.99	120.55
1	A	209	THR	N-CA-C	5.13	118.06	109.96
1	A	325	ASN	CA-CB-CG	5.13	117.73	112.60
1	A	47	THR	OG1-CB-CG2	5.12	119.55	109.30
1	A	675	GLY	CA-C-O	-5.12	118.14	122.29
1	A	409	ARG	N-CA-CB	-5.12	102.59	110.16
1	A	523	SER	CA-CB-OG	-5.11	100.88	111.10
1	A	78	ASP	CA-CB-CG	5.10	117.70	112.60
1	A	798	THR	N-CA-C	5.10	116.92	111.36
1	A	642	VAL	CA-C-N	-5.10	115.86	122.94
1	A	642	VAL	C-N-CA	-5.10	115.86	122.94
1	A	285	PHE	CA-C-N	5.09	129.20	122.42
1	A	285	PHE	C-N-CA	5.09	129.20	122.42
1	A	684	ASN	N-CA-CB	-5.09	102.85	110.73
1	A	826	GLY	O-C-N	5.09	127.73	122.54
1	A	443	HIS	CE1-NE2-CD2	-5.08	103.92	109.00
1	A	155	TYR	CB-CA-C	-5.07	102.03	110.14
1	A	354	VAL	CB-CA-C	5.06	118.62	111.94
1	A	559	PRO	N-CA-C	-5.06	107.14	114.18
1	A	217	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	348	GLU	N-CA-C	5.05	116.60	111.14
1	A	724	ARG	NE-CZ-NH1	-5.05	116.45	121.50
1	A	274	ASN	CB-CG-ND2	-5.04	108.84	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	823	GLU	CA-C-N	5.04	127.91	122.97
1	A	823	GLU	C-N-CA	5.04	127.91	122.97
1	A	383	ALA	N-CA-CB	-5.02	102.21	110.40
1	A	693	ASP	CA-CB-CG	5.02	117.62	112.60
1	A	829	PRO	N-CA-C	5.00	118.49	111.33
1	A	343	SER	N-CA-CB	-5.00	101.81	110.32

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	157	TYR	Sidechain
1	A	160	ARG	Sidechain
1	A	205	ARG	Sidechain
1	A	292	ARG	Sidechain
1	A	310	ARG	Sidechain
1	A	374	TYR	Sidechain
1	A	52	TYR	Sidechain
1	A	524	TYR	Sidechain
1	A	548	TYR	Sidechain
1	A	601	ARG	Sidechain
1	A	66	ARG	Sidechain
1	A	720	ARG	Sidechain
1	A	81	ARG	Sidechain
1	A	831	ARG	Sidechain
1	A	90	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	76	0
2	A	43	0	16	4	0
All	All	6685	0	6609	78	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 6.

All (78) 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:100:VAL:HG21	1:A:494:LEU:HD22	1.48	0.95
1:A:100:VAL:HG21	1:A:494:LEU:CD2	1.97	0.94
1:A:235:ASN:H	1:A:235:ASN:HD22	1.31	0.79
2:A:843:195:O9	2:A:843:195:H5	1.87	0.74
1:A:211:GLN:HB3	1:A:358:ARG:HH12	1.56	0.71
1:A:85:LEU:HD13	1:A:335:ILE:HG23	1.81	0.62
1:A:100:VAL:CG2	1:A:494:LEU:CD2	2.76	0.62
1:A:384:LEU:HD12	1:A:386:ARG:NH2	2.15	0.61
2:A:843:195:O9	2:A:843:195:C5	2.49	0.59
1:A:380:ILE:CG2	1:A:382:GLU:CD	2.77	0.57
1:A:105:GLU:O	1:A:119:MET:HE1	2.06	0.56
1:A:193:ARG:NH1	1:A:195:GLU:OE2	2.38	0.55
1:A:506:ARG:NH1	1:A:524:TYR:CE1	2.76	0.54
1:A:150:LEU:HD12	1:A:817:ILE:HG22	1.89	0.54
1:A:34:HIS:CD2	1:A:57:HIS:HB3	2.44	0.53
1:A:461:GLU:OE1	1:A:465:LYS:NZ	2.42	0.53
1:A:159:ILE:HD11	1:A:276:SER:HA	1.90	0.52
1:A:381:PRO:HD2	1:A:382:GLU:OE1	2.10	0.52
1:A:380:ILE:HG23	1:A:382:GLU:CD	2.35	0.51
1:A:235:ASN:H	1:A:235:ASN:ND2	2.03	0.51
1:A:100:VAL:HG21	1:A:494:LEU:HD23	1.89	0.51
1:A:455:VAL:H	1:A:459:HIS:HD2	1.59	0.51
1:A:227:ASP:CG	1:A:242:ARG:HH21	2.19	0.51
1:A:78:ASP:O	1:A:332:LYS:NZ	2.43	0.50
1:A:100:VAL:CG2	1:A:494:LEU:HD22	2.30	0.50
1:A:71:GLN:HB2	2:A:843:195:H21	1.95	0.49
1:A:463:LEU:HD23	1:A:467:ILE:HD12	1.95	0.48
1:A:779:GLU:OE2	1:A:782:LYS:NZ	2.38	0.48
1:A:782:LYS:O	1:A:785:GLU:HB2	2.14	0.48
1:A:211:GLN:CB	1:A:358:ARG:HH12	2.25	0.47
1:A:73:HIS:O	1:A:77:LYS:HB2	2.14	0.47
1:A:397:PRO:O	1:A:401:GLN:HG3	2.14	0.47
1:A:490:ARG:HA	1:A:494:LEU:HG	1.95	0.47
1:A:159:ILE:CG2	1:A:161:TYR:CZ	2.98	0.47
1:A:103:ALA:HB2	1:A:234:ARG:CD	2.45	0.47
1:A:486:ILE:O	1:A:486:ILE:HG13	2.16	0.46
1:A:384:LEU:HB2	1:A:386:ARG:NH1	2.32	0.45
1:A:232:GLY:HA3	1:A:235:ASN:HD21	1.82	0.45
1:A:73:HIS:CE1	1:A:77:LYS:HG3	2.52	0.45
1:A:410:PHE:O	1:A:413:ARG:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:LEU:CG	1:A:809:GLY:HA2	2.47	0.45
1:A:184:ARG:NE	1:A:185:TYR:CZ	2.85	0.45
1:A:39:LEU:HD13	1:A:50:ASP:HA	1.99	0.45
1:A:795:ARG:O	1:A:799:ARG:HG3	2.17	0.44
1:A:515:LEU:HD23	1:A:809:GLY:HA2	2.00	0.44
1:A:228:THR:HG23	1:A:229:PRO:HD2	2.00	0.44
1:A:70:THR:O	1:A:73:HIS:HB3	2.18	0.44
1:A:690:GLY:O	1:A:710:ILE:HA	2.18	0.44
1:A:464:LYS:HD2	1:A:472:TYR:CE1	2.53	0.43
1:A:767:HIS:C	1:A:768:HIS:CG	2.96	0.43
1:A:68:ILE:HA	2:A:843:195:C21	2.48	0.43
1:A:732:TYR:CZ	1:A:739:ARG:HG3	2.53	0.43
1:A:159:ILE:HG23	1:A:161:TYR:CE2	2.54	0.43
1:A:387:TRP:O	1:A:438:ARG:HA	2.19	0.43
1:A:515:LEU:HG	1:A:809:GLY:HA2	2.00	0.43
1:A:764:MET:SD	1:A:764:MET:C	3.02	0.43
1:A:475:GLU:N	1:A:476:PRO:CD	2.82	0.42
1:A:477:HIS:CD2	1:A:478:LYS:N	2.87	0.42
1:A:332:LYS:HD3	1:A:332:LYS:HA	1.82	0.42
1:A:8:GLU:O	1:A:12:GLN:HG3	2.20	0.42
1:A:159:ILE:HG21	1:A:161:TYR:CZ	2.53	0.42
1:A:462:ILE:HD12	1:A:462:ILE:HA	1.96	0.42
1:A:477:HIS:CD2	1:A:477:HIS:C	2.97	0.42
1:A:241:MET:HE3	1:A:243:LEU:HD11	2.02	0.42
1:A:170:ILE:HA	1:A:174:TRP:O	2.20	0.41
1:A:177:GLU:HG2	1:A:611:PRO:HG3	2.02	0.41
1:A:380:ILE:HA	1:A:381:PRO:HD3	1.85	0.41
1:A:455:VAL:O	1:A:456:ALA:HB2	2.20	0.41
1:A:571:HIS:ND1	1:A:572:GLU:N	2.69	0.41
1:A:390:HIS:CD2	1:A:391:LEU:N	2.89	0.40
1:A:414:VAL:O	1:A:415:ALA:C	2.63	0.40
1:A:467:ILE:H	1:A:467:ILE:HG13	1.53	0.40
1:A:122:LEU:O	1:A:125:ILE:HG12	2.22	0.40
1:A:458:ILE:HG23	1:A:459:HIS:N	2.36	0.40
1:A:767:HIS:HB2	1:A:768:HIS:CE1	2.56	0.40
1:A:386:ARG:HA	1:A:439:ILE:O	2.20	0.40
1:A:605:ILE:O	1:A:644:PHE:HA	2.21	0.40
1:A:149:THR:O	1:A:831:ARG:HD2	2.22	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%)	744 (92%)	59 (7%)	3 (0%)	30	22

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	325	ASN
1	A	568	LYS
1	A	13	ILE

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%)	679 (96%)	25 (4%)	31	26

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	42	ASP
1	A	44	ASN
1	A	60	ARG
1	A	77	LYS
1	A	90	TYR
1	A	136	LEU
1	A	144	LEU

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Mol	Chain	Res	Type
1	A	217	ASP
1	A	235	ASN
1	A	250	ASN
1	A	289	LYS
1	A	308	ILE
1	A	325	ASN
1	A	360	ASP
1	A	465	LYS
1	A	469	LYS
1	A	494	LEU
1	A	568	LYS
1	A	573	TYR
1	A	576	GLN
1	A	641	ARG
1	A	756	ASP
1	A	774	PHE
1	A	827	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	62	HIS
1	A	71	GLN
1	A	73	HIS
1	A	106	ASN
1	A	219	GLN
1	A	235	ASN
1	A	390	HIS
1	A	450	HIS
1	A	459	HIS
1	A	477	HIS
1	A	481	ASN
1	A	560	ASN
1	A	566	GLN
1	A	576	GLN
1	A	579	ASN
1	A	614	HIS
1	A	768	HIS
1	A	804	ASN

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	4.37	10 (43%)	25,32,34	2.11	12 (48%)

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	-	2/16/17/19	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	14.41	1.55	1.41
1	A	680	LLP	C4-C3	6.72	1.52	1.41
1	A	680	LLP	C6-C5	6.64	1.50	1.37
1	A	680	LLP	C6-N1	5.97	1.46	1.34
1	A	680	LLP	C2-N1	5.91	1.44	1.33
1	A	680	LLP	C4-C5	5.04	1.49	1.42
1	A	680	LLP	C4'-NZ	4.33	1.41	1.27
1	A	680	LLP	C5'-C5	2.66	1.57	1.50
1	A	680	LLP	C4-C4'	2.39	1.51	1.46
1	A	680	LLP	C2'-C2	2.20	1.53	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	680	LLP	CD-CE-NZ	-4.37	99.27	110.83
1	A	680	LLP	C5-C4-C4'	-3.52	116.04	121.47
1	A	680	LLP	OP4-P-OP1	-3.32	97.47	106.44
1	A	680	LLP	OP4-C5'-C5	3.16	115.28	109.36
1	A	680	LLP	OP3-P-OP4	2.91	114.25	106.67
1	A	680	LLP	C5-C6-N1	-2.60	119.61	123.83
1	A	680	LLP	C3-C2-N1	-2.57	117.72	120.96
1	A	680	LLP	OP2-P-OP4	2.45	113.05	106.67
1	A	680	LLP	C6-N1-C2	2.34	123.44	119.20
1	A	680	LLP	C3-C4-C4'	2.31	124.57	120.40
1	A	680	LLP	C4-C4'-NZ	-2.28	113.53	124.04
1	A	680	LLP	C2'-C2-C3	2.06	123.21	120.80

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	680	LLP	C4-C5-C5'-OP4
1	A	680	LLP	C6-C5-C5'-OP4

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	195	A	843	-	46,46,46	1.87	8 (17%)	61,65,65	1.15	7 (11%)

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	195	A	843	-	-	8/32/36/36	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	843	195	O11-N3	7.77	1.36	1.22
2	A	843	195	O4-C14	4.69	1.36	1.22
2	A	843	195	O2-C13	4.27	1.35	1.22
2	A	843	195	O5-C14	-3.65	1.19	1.30
2	A	843	195	O3-C13	-3.58	1.19	1.30
2	A	843	195	C2-N1	-2.62	1.36	1.41
2	A	843	195	O10-N3	-2.35	1.19	1.35
2	A	843	195	O7-N4	-2.01	1.19	1.22

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	843	195	C2-N1-C15	-3.25	117.87	126.90
2	A	843	195	O4-C14-C9	-2.97	114.87	121.97
2	A	843	195	O11-N3-C25	-2.83	114.92	118.82
2	A	843	195	O2-C13-C10	-2.68	115.58	121.97
2	A	843	195	C24-C25-N3	2.40	120.80	118.74
2	A	843	195	C4-N2-C22	-2.35	120.41	126.61
2	A	843	195	O5-C14-C9	2.11	121.28	115.28

There are no chirality outliers.

All (8) torsion outliers are listed below:

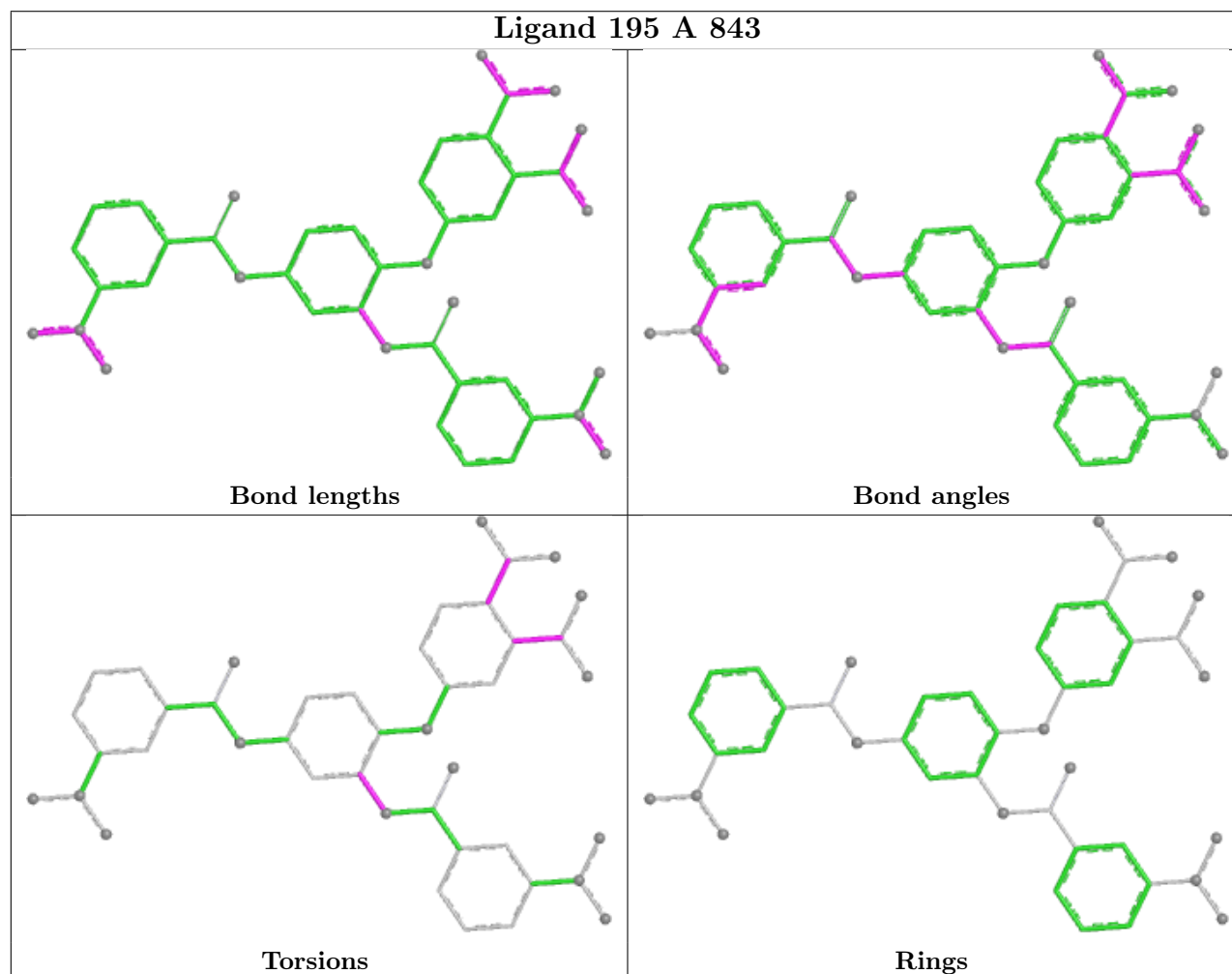
Mol	Chain	Res	Type	Atoms
2	A	843	195	C1-C2-N1-C15
2	A	843	195	O5-C14-C9-C8
2	A	843	195	O4-C14-C9-C8
2	A	843	195	O5-C14-C9-C10
2	A	843	195	O4-C14-C9-C10
2	A	843	195	C11-C10-C13-O3
2	A	843	195	C11-C10-C13-O2
2	A	843	195	C3-C2-N1-C15

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	843	195	4	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.