Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 12:32 AM EDT

PDB ID	:	1Z6Q
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 (i) 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 (1)) were used in the production of this report:

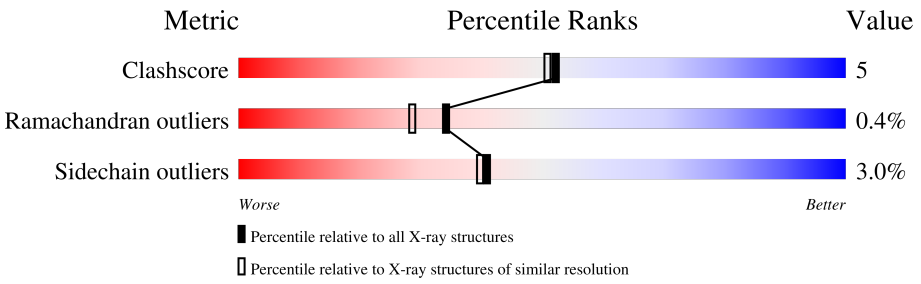
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)

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 <=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.

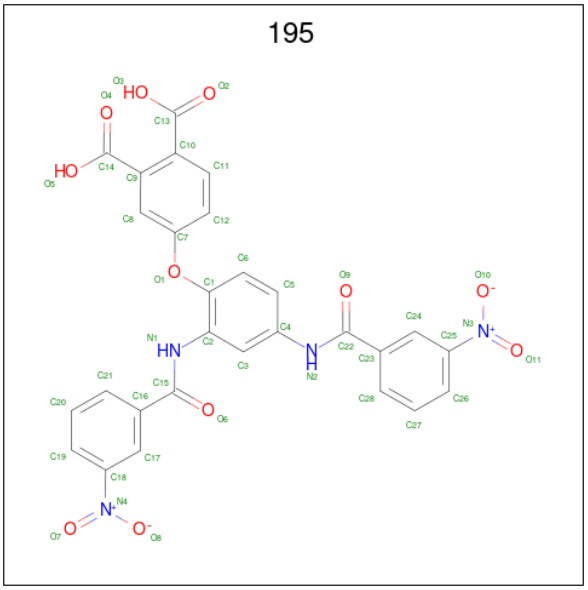
- Molecule 1 is a protein called Glycogen phosphorylase, muscle form.

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 (three-letter code: 195) (formula: $C_{28}H_{18}N_4O_{11}$).



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

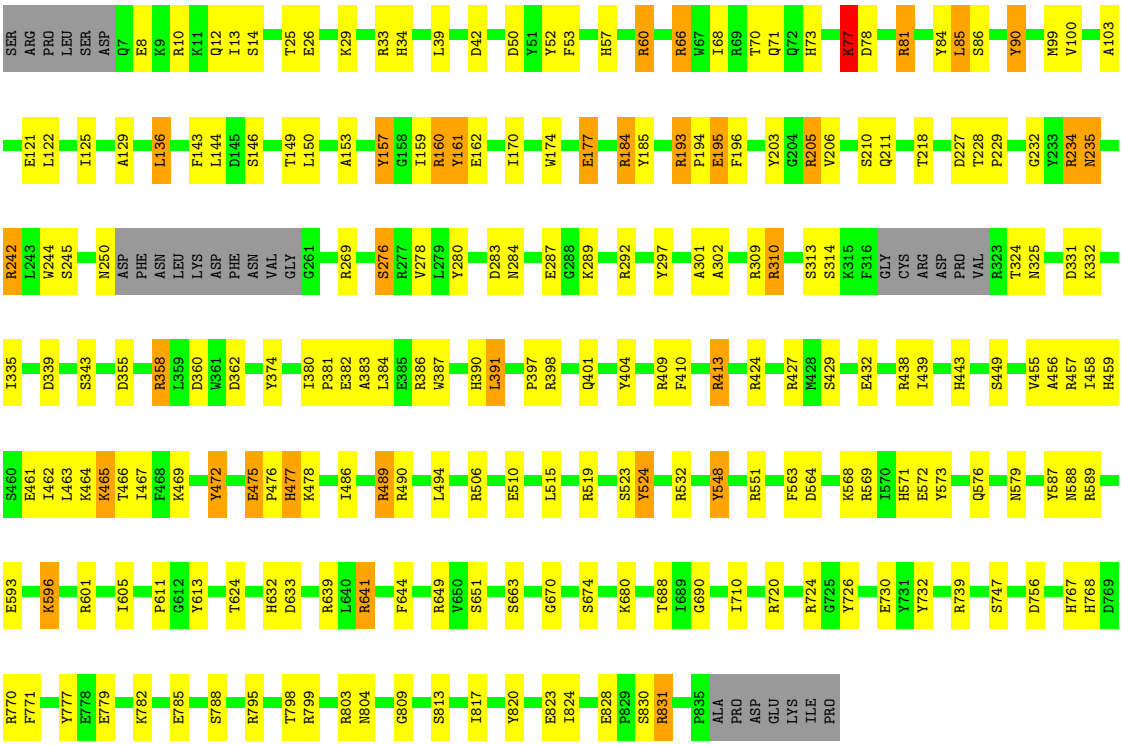
3 Residue-property plots (i)

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: 70% 22%



4 Data and refinement statistics (i)

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 (i)

5.1 Standard geometry (i)

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	1.43	34/6764 (0.5%)	1.80	132/9147 (1.4%)

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 (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	146	SER	CB-OG	8.79	1.53	1.42
1	A	195	GLU	CD-OE2	7.64	1.34	1.25
1	A	429	SER	CB-OG	7.48	1.51	1.42
1	A	193	ARG	CZ-NH1	-7.45	1.23	1.33
1	A	276	SER	CB-OG	7.45	1.51	1.42
1	A	747	SER	CB-OG	7.16	1.51	1.42
1	A	830	SER	CB-OG	6.67	1.50	1.42
1	A	828	GLU	CG-CD	6.57	1.61	1.51
1	A	674	SER	CB-OG	6.29	1.50	1.42
1	A	813	SER	CB-OG	6.15	1.50	1.42
1	A	177	GLU	CD-OE2	-6.06	1.19	1.25
1	A	510	GLU	CG-CD	6.05	1.61	1.51
1	A	210	SER	CB-OG	6.02	1.50	1.42
1	A	788	SER	CB-OG	5.91	1.50	1.42
1	A	14	SER	CB-OG	5.90	1.50	1.42
1	A	813	SER	CA-CB	5.83	1.61	1.52
1	A	432	GLU	CG-CD	5.77	1.60	1.51
1	A	663	SER	CB-OG	5.65	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	523	SER	CB-OG	5.58	1.49	1.42
1	A	449	SER	CB-OG	5.50	1.49	1.42
1	A	157	TYR	CE2-CZ	5.46	1.45	1.38
1	A	26	GLU	CG-CD	5.40	1.60	1.51
1	A	302	ALA	CA-C	5.28	1.66	1.52
1	A	475	GLU	CG-CD	5.22	1.59	1.51
1	A	313	SER	CB-OG	5.21	1.49	1.42
1	A	284	ASN	C-N	5.17	1.46	1.34
1	A	730	GLU	CD-OE1	-5.16	1.20	1.25
1	A	824	ILE	CA-C	5.15	1.66	1.52
1	A	86	SER	CB-OG	5.14	1.49	1.42
1	A	588	ASN	CA-C	5.14	1.66	1.52
1	A	244	TRP	NE1-CE2	5.10	1.44	1.37
1	A	777	TYR	CE1-CZ	5.07	1.45	1.38
1	A	651	SER	CB-OG	5.03	1.48	1.42
1	A	670	GLY	CA-C	5.00	1.59	1.51

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	424	ARG	NE-CZ-NH1	15.47	128.03	120.30
1	A	649	ARG	NE-CZ-NH1	14.47	127.53	120.30
1	A	193	ARG	NE-CZ-NH2	13.17	126.89	120.30
1	A	234	ARG	NE-CZ-NH1	13.02	126.81	120.30
1	A	409	ARG	NE-CZ-NH2	-11.65	114.47	120.30
1	A	269	ARG	NE-CZ-NH2	-11.46	114.57	120.30
1	A	519	ARG	NE-CZ-NH1	-11.08	114.76	120.30
1	A	569	ARG	NE-CZ-NH2	-10.36	115.12	120.30
1	A	424	ARG	NE-CZ-NH2	-10.01	115.30	120.30
1	A	10	ARG	NE-CZ-NH1	9.91	125.25	120.30
1	A	548	TYR	CB-CG-CD1	-9.63	115.22	121.00
1	A	404	TYR	CB-CG-CD1	9.58	126.75	121.00
1	A	280	TYR	CB-CG-CD2	-9.50	115.30	121.00
1	A	489	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	A	129	ALA	N-CA-CB	-9.08	97.39	110.10
1	A	33	ARG	NE-CZ-NH2	-9.05	115.77	120.30
1	A	770	ARG	NE-CZ-NH2	9.05	124.83	120.30
1	A	563	PHE	CB-CG-CD1	8.99	127.09	120.80
1	A	245	SER	N-CA-CB	-8.95	97.08	110.50
1	A	66	ARG	NE-CZ-NH1	8.88	124.74	120.30
1	A	427	ARG	NE-CZ-NH1	8.82	124.71	120.30
1	A	234	ARG	CD-NE-CZ	8.76	135.87	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	519	ARG	NE-CZ-NH2	8.46	124.53	120.30
1	A	569	ARG	NE-CZ-NH1	8.45	124.53	120.30
1	A	283	ASP	N-CA-CB	-8.42	95.45	110.60
1	A	242	ARG	NE-CZ-NH2	-8.21	116.20	120.30
1	A	355	ASP	CB-CG-OD1	8.16	125.64	118.30
1	A	688	THR	CA-CB-OG1	8.13	126.08	109.00
1	A	313	SER	N-CA-CB	-7.83	98.76	110.50
1	A	724	ARG	NE-CZ-NH1	-7.70	116.45	120.30
1	A	413	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	A	413	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	A	269	ARG	NE-CZ-NH1	7.59	124.10	120.30
1	A	563	PHE	CB-CG-CD2	-7.54	115.53	120.80
1	A	641	ARG	NE-CZ-NH1	-7.41	116.59	120.30
1	A	457	ARG	NE-CZ-NH2	-7.37	116.62	120.30
1	A	280	TYR	CB-CG-CD1	7.33	125.40	121.00
1	A	81	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	A	398	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	A	310	ARG	CB-CA-C	-7.11	96.18	110.40
1	A	358	ARG	NE-CZ-NH1	-7.01	116.79	120.30
1	A	81	ARG	CD-NE-CZ	-6.98	113.83	123.60
1	A	391	LEU	CB-CA-C	6.97	123.44	110.20
1	A	532	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	A	551	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	A	820	TYR	CB-CG-CD1	-6.55	117.07	121.00
1	A	161	TYR	CB-CG-CD1	-6.46	117.12	121.00
1	A	427	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	A	589	ARG	NE-CZ-NH1	-6.43	117.08	120.30
1	A	383	ALA	CB-CA-C	6.42	119.74	110.10
1	A	66	ARG	CD-NE-CZ	-6.38	114.67	123.60
1	A	60	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	A	205	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	A	724	ARG	NH1-CZ-NH2	6.29	126.32	119.40
1	A	60	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	A	639	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	A	195	GLU	CB-CA-C	6.16	122.71	110.40
1	A	724	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	823	GLU	OE1-CD-OE2	-6.12	115.95	123.30
1	A	84	TYR	CB-CG-CD2	-6.12	117.33	121.00
1	A	398	ARG	CG-CD-NE	-6.12	98.95	111.80
1	A	195	GLU	CA-CB-CG	6.11	126.83	113.40
1	A	302	ALA	CB-CA-C	6.11	119.26	110.10
1	A	81	ARG	O-C-N	6.08	132.43	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	803	ARG	NE-CZ-NH1	-6.08	117.26	120.30
1	A	771	PHE	CB-CG-CD1	6.02	125.01	120.80
1	A	362	ASP	CB-CA-C	5.99	122.37	110.40
1	A	77	LYS	N-CA-CB	-5.94	99.91	110.60
1	A	324	THR	CA-C-N	-5.92	104.17	117.20
1	A	475	GLU	OE1-CD-OE2	-5.91	116.21	123.30
1	A	624	THR	CA-CB-CG2	-5.90	104.14	112.40
1	A	153	ALA	CB-CA-C	5.86	118.89	110.10
1	A	343	SER	N-CA-CB	-5.79	101.81	110.50
1	A	184	ARG	CD-NE-CZ	5.79	131.70	123.60
1	A	302	ALA	N-CA-CB	-5.79	102.00	110.10
1	A	287	GLU	C-N-CA	-5.77	110.18	122.30
1	A	472	TYR	CB-CG-CD2	-5.77	117.54	121.00
1	A	157	TYR	CB-CG-CD1	-5.73	117.56	121.00
1	A	564	ASP	CB-CG-OD2	-5.73	113.15	118.30
1	A	633	ASP	CB-CG-OD1	5.67	123.41	118.30
1	A	383	ALA	N-CA-CB	-5.63	102.21	110.10
1	A	162	GLU	CA-CB-CG	-5.63	101.02	113.40
1	A	301	ALA	N-CA-CB	-5.62	102.23	110.10
1	A	25	THR	OG1-CB-CG2	-5.60	97.12	110.00
1	A	99	MET	CG-SD-CE	5.59	109.15	100.20
1	A	242	ARG	CG-CD-NE	-5.59	100.07	111.80
1	A	136	LEU	N-CA-CB	-5.58	99.23	110.40
1	A	551	ARG	CD-NE-CZ	5.56	131.38	123.60
1	A	234	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	798	THR	CA-CB-OG1	5.52	120.59	109.00
1	A	196	PHE	CG-CD1-CE1	-5.44	114.81	120.80
1	A	564	ASP	CB-CG-OD1	5.42	123.18	118.30
1	A	121	GLU	CB-CA-C	5.41	121.23	110.40
1	A	287	GLU	N-CA-CB	-5.41	100.86	110.60
1	A	427	ARG	CD-NE-CZ	5.40	131.16	123.60
1	A	564	ASP	N-CA-CB	-5.40	100.89	110.60
1	A	310	ARG	CG-CD-NE	-5.39	100.47	111.80
1	A	203	TYR	CZ-CE2-CD2	5.38	124.65	119.80
1	A	726	TYR	CB-CG-CD1	-5.37	117.78	121.00
1	A	218	THR	OG1-CB-CG2	-5.36	97.67	110.00
1	A	136	LEU	CA-CB-CG	5.35	127.61	115.30
1	A	194	PRO	C-N-CA	5.35	135.08	121.70
1	A	160	ARG	NE-CZ-NH1	-5.35	117.62	120.30
1	A	206	VAL	C-N-CA	5.35	135.07	121.70
1	A	331	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	A	632	HIS	CA-CB-CG	-5.32	104.56	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	587	TYR	CB-CG-CD2	5.31	124.19	121.00
1	A	205	ARG	CD-NE-CZ	5.30	131.03	123.60
1	A	85	LEU	CB-CG-CD1	-5.30	101.99	111.00
1	A	157	TYR	CD1-CE1-CZ	5.28	124.55	119.80
1	A	314	SER	N-CA-CB	-5.28	102.58	110.50
1	A	278	VAL	CA-CB-CG1	5.25	118.77	110.90
1	A	121	GLU	N-CA-CB	-5.24	101.17	110.60
1	A	804	ASN	CB-CA-C	5.23	120.86	110.40
1	A	548	TYR	CB-CG-CD2	5.22	124.13	121.00
1	A	81	ARG	CA-CB-CG	-5.21	101.94	113.40
1	A	297	TYR	CB-CG-CD2	5.19	124.12	121.00
1	A	177	GLU	OE1-CD-OE2	-5.18	117.08	123.30
1	A	404	TYR	CB-CG-CD2	-5.18	117.89	121.00
1	A	60	ARG	CD-NE-CZ	5.16	130.82	123.60
1	A	324	THR	CA-CB-OG1	5.14	119.79	109.00
1	A	309	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	477	HIS	CA-CB-CG	-5.13	104.87	113.60
1	A	143	PHE	CB-CG-CD2	-5.11	117.22	120.80
1	A	596	LYS	CD-CE-NZ	-5.07	100.03	111.70
1	A	443	HIS	CA-C-N	-5.07	106.04	117.20
1	A	813	SER	CB-CA-C	5.06	119.72	110.10
1	A	466	THR	CA-CB-OG1	5.06	119.62	109.00
1	A	205	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	53	PHE	N-CA-CB	-5.03	101.56	110.60
1	A	143	PHE	CB-CG-CD1	5.02	124.31	120.80
1	A	429	SER	N-CA-CB	5.01	118.01	110.50

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

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Mol	Chain	Res	Type	Group
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 (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	71	0
2	A	43	0	16	4	0
All	All	6685	0	6609	73	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 5.

All (73) 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: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:380:ILE:CG2	1:A:382:GLU:CD	2.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:380:ILE:HG23	1:A:382:GLU:CD	2.35	0.47
1:A:103:ALA:HB2	1:A:234:ARG:CD	2.45	0.47
1:A:593:GLU:OE1	1:A:596:LYS:NZ	2.45	0.47
1:A:227:ASP:CG	1:A:242:ARG:HH21	2.19	0.46
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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:170:ILE:HA	1:A:174:TRP:O	2.20	0.41
1:A:455:VAL:O	1:A:456:ALA:HB2	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: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: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%)	34 28

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%)	683 (97%)	21 (3%)	41 40

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

Mol	Chain	Res	Type
1	A	29	LYS
1	A	42	ASP
1	A	60	ARG
1	A	77	LYS
1	A	90	TYR
1	A	136	LEU
1	A	144	LEU
1	A	235	ASN
1	A	250	ASN
1	A	289	LYS
1	A	339	ASP
1	A	360	ASP
1	A	465	LYS
1	A	469	LYS
1	A	489	ARG
1	A	573	TYR
1	A	576	GLN
1	A	579	ASN
1	A	613	TYR
1	A	641	ARG
1	A	756	ASP

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	36	HIS
1	A	62	HIS
1	A	73	HIS

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Mol	Chain	Res	Type
1	A	106	ASN
1	A	235	ASN
1	A	264	GLN
1	A	390	HIS
1	A	459	HIS
1	A	477	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 (i)

There are no RNA molecules in this entry.

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

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(^{o})	Ideal(^{o})
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 monosaccharides 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(^{o})	Ideal(^{o})
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

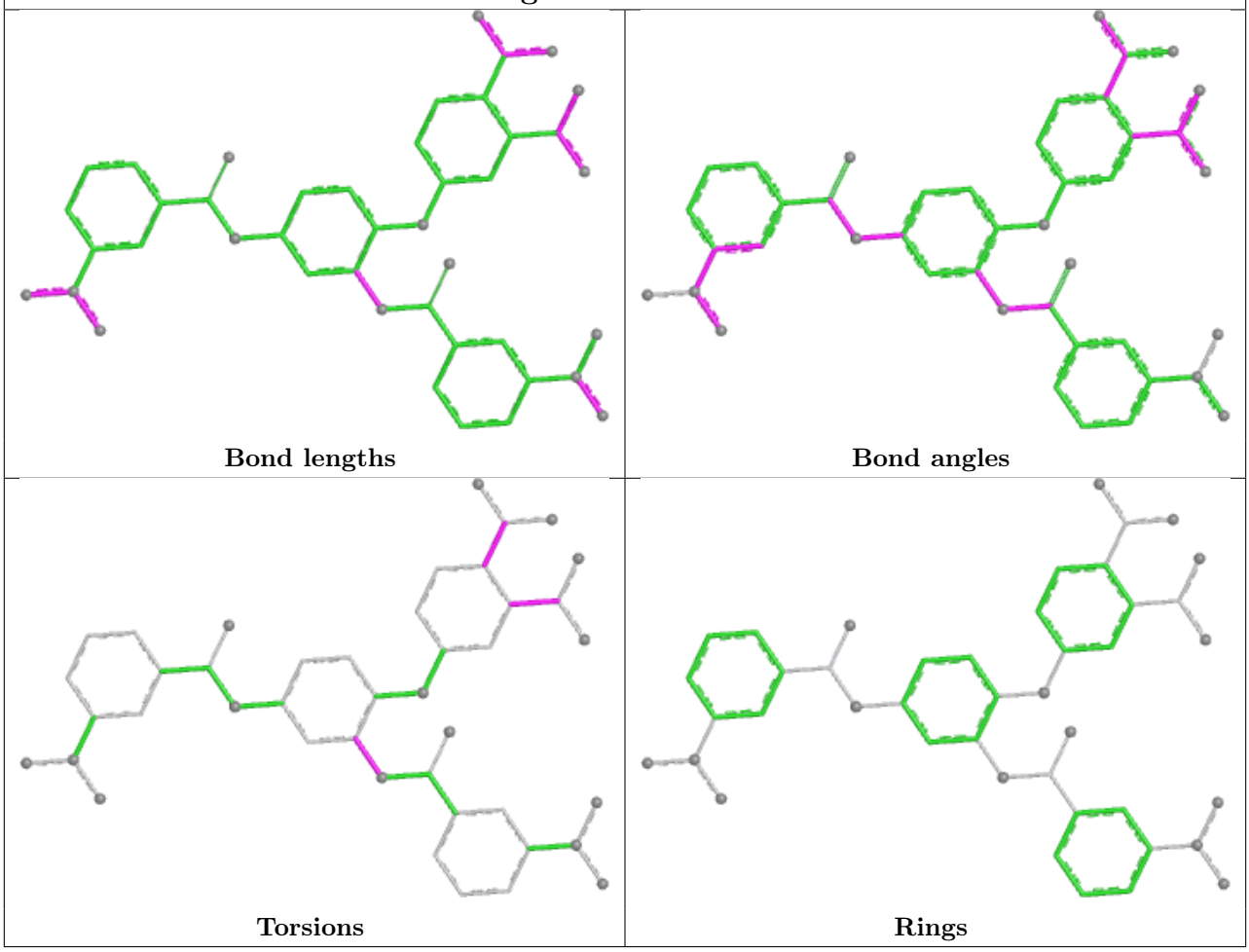
There are no ring outliers.

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 then 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.

Ligand 195 A 843



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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.