



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 06:27 am BST

PDB ID : 8GPB
Title : STRUCTURAL MECHANISM FOR GLYCOGEN PHOSPHORYLASE
CONTROL BY PHOSPHORYLATION AND AMP
Authors : Barford, D.; Hu, S.-H.; Johnson, L.N.
Deposited on : 1990-11-13
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (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) : 2.11

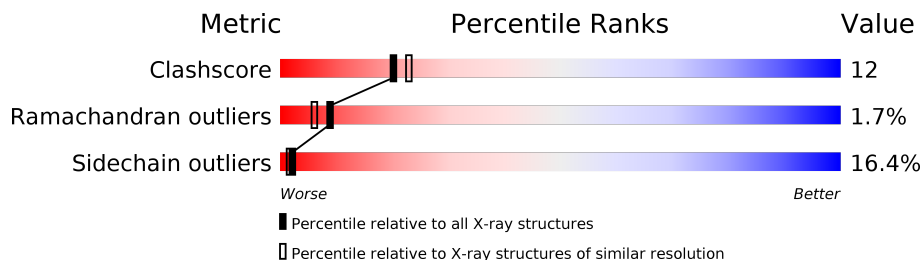
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	58% 29% 9% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7462 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.

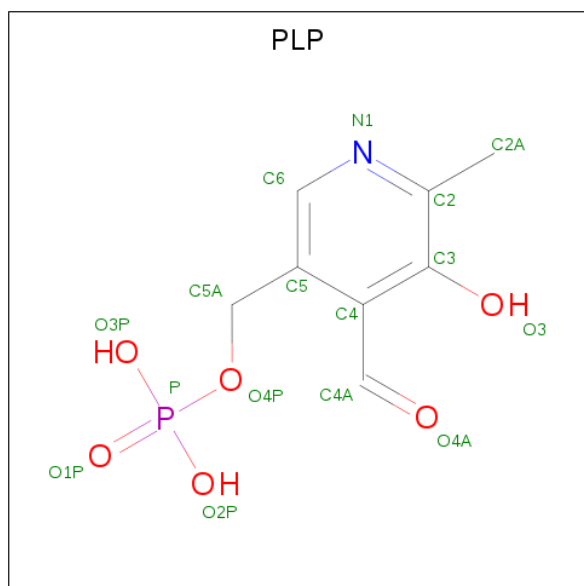
- Molecule 1 is a protein called GLYCOGEN PHOSPHORYLASE B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	832	6761	4308	1192	1231	30	0	0	0

There is a discrepancy between the modelled and reference sequences:

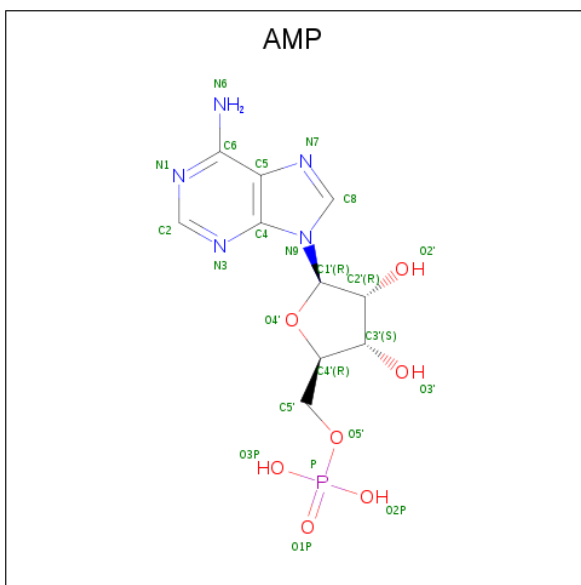
Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	CONFLICT	UNP P00489

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	15	8	1	5	1	0	0

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C₁₀H₁₄N₅O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 4 is water.

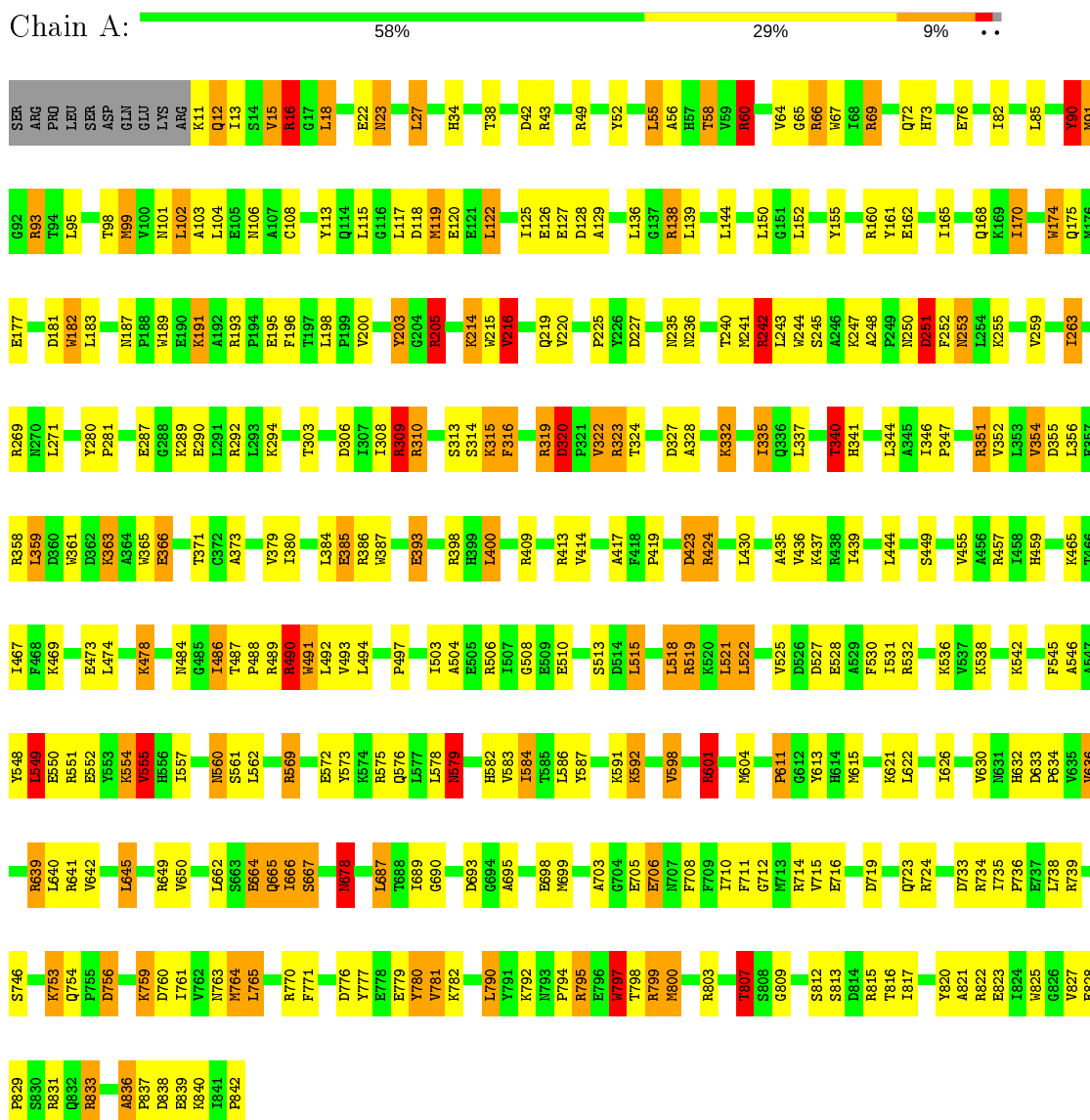
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	640	Total	O	0	0
			640	640		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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 B



4 Data and refinement statistics

Xtrriage (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	128.50Å 128.50Å 116.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.206 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	7462	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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: AMP, PLP

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	0.98	2/6915 (0.0%)	1.87	170/9359 (1.8%)

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	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	842	PRO	N-CD	5.63	1.55	1.47
1	A	664	GLU	CD-OE2	-5.05	1.20	1.25

All (170) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	490	ARG	NE-CZ-NH2	-21.00	109.80	120.30
1	A	309	ARG	NE-CZ-NH2	-18.13	111.23	120.30
1	A	424	ARG	NE-CZ-NH2	-15.37	112.62	120.30
1	A	490	ARG	NE-CZ-NH1	14.32	127.46	120.30
1	A	800	MET	CA-CB-CG	12.26	134.14	113.30
1	A	60	ARG	NE-CZ-NH2	-11.90	114.35	120.30
1	A	309	ARG	NE-CZ-NH1	11.69	126.14	120.30
1	A	138	ARG	NE-CZ-NH1	11.61	126.11	120.30
1	A	138	ARG	NE-CZ-NH2	-11.27	114.67	120.30
1	A	575	ARG	NE-CZ-NH2	-11.03	114.79	120.30
1	A	99	MET	CG-SD-CE	-10.79	82.93	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	242	ARG	NE-CZ-NH2	-10.78	114.91	120.30
1	A	93	ARG	NE-CZ-NH1	10.35	125.47	120.30
1	A	519	ARG	NE-CZ-NH2	-10.26	115.17	120.30
1	A	90	TYR	CB-CG-CD2	-9.61	115.23	121.00
1	A	15	VAL	CA-C-N	-9.45	96.42	117.20
1	A	799	ARG	NE-CZ-NH2	-9.24	115.68	120.30
1	A	770	ARG	NE-CZ-NH2	-9.22	115.69	120.30
1	A	457	ARG	NE-CZ-NH1	9.03	124.82	120.30
1	A	244	TRP	CD1-CG-CD2	8.84	113.37	106.30
1	A	457	ARG	NE-CZ-NH2	-8.77	115.91	120.30
1	A	351	ARG	NE-CZ-NH2	-8.76	115.92	120.30
1	A	43	ARG	NE-CZ-NH1	8.50	124.55	120.30
1	A	807	THR	N-CA-CB	-8.44	94.27	110.30
1	A	409	ARG	NE-CZ-NH2	-8.41	116.09	120.30
1	A	365	TRP	CG-CD2-CE3	8.39	141.45	133.90
1	A	119	MET	CG-SD-CE	-8.32	86.88	100.20
1	A	15	VAL	CA-CB-CG1	-8.27	98.50	110.90
1	A	560	ASN	CA-CB-CG	-8.09	95.60	113.40
1	A	205	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	A	67	TRP	CD1-CG-CD2	7.95	112.66	106.30
1	A	16	ARG	NE-CZ-NH1	7.83	124.21	120.30
1	A	189	TRP	CD1-CG-CD2	7.82	112.56	106.30
1	A	601	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	A	117	LEU	N-CA-C	7.75	131.93	111.00
1	A	601	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	A	365	TRP	CD1-CG-CD2	7.63	112.40	106.30
1	A	387	TRP	CG-CD2-CE3	7.60	140.74	133.90
1	A	575	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	A	380	ILE	CG1-CB-CG2	-7.57	94.75	111.40
1	A	263	ILE	CG1-CB-CG2	-7.56	94.76	111.40
1	A	242	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	A	244	TRP	CE2-CD2-CG	-7.52	101.29	107.30
1	A	825	TRP	CD1-CG-CD2	7.51	112.31	106.30
1	A	280	TYR	CB-CG-CD2	-7.51	116.50	121.00
1	A	770	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	A	203	TYR	CB-CG-CD2	-7.45	116.53	121.00
1	A	198	LEU	CA-CB-CG	7.43	132.39	115.30
1	A	205	ARG	NE-CZ-NH2	-7.37	116.61	120.30
1	A	575	ARG	CB-CG-CD	-7.35	92.48	111.60
1	A	215	TRP	CG-CD2-CE3	7.35	140.51	133.90
1	A	340	THR	N-CA-CB	-7.33	96.36	110.30
1	A	365	TRP	CE2-CD2-CG	-7.29	101.47	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	TRP	CE2-CD2-CG	-7.28	101.48	107.30
1	A	424	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	A	491	TRP	CD1-CG-CD2	7.12	111.99	106.30
1	A	15	VAL	CA-C-O	7.12	135.04	120.10
1	A	780	TYR	CB-CG-CD2	-7.07	116.76	121.00
1	A	555	VAL	N-CA-C	7.05	130.03	111.00
1	A	365	TRP	CB-CG-CD1	-7.04	117.85	127.00
1	A	387	TRP	CE2-CD2-CG	-7.04	101.67	107.30
1	A	664	GLU	N-CA-CB	-7.03	97.94	110.60
1	A	189	TRP	CE2-CD2-CG	-7.03	101.68	107.30
1	A	214	LYS	N-CA-CB	-6.99	98.02	110.60
1	A	174	TRP	CE2-CD2-CG	-6.98	101.72	107.30
1	A	491	TRP	CE2-CD2-CG	-6.96	101.73	107.30
1	A	155	TYR	CB-CG-CD1	-6.94	116.83	121.00
1	A	215	TRP	CE2-CD2-CG	-6.93	101.76	107.30
1	A	650	VAL	CG1-CB-CG2	-6.86	99.92	110.90
1	A	825	TRP	CE2-CD2-CG	-6.82	101.85	107.30
1	A	842	PRO	CA-N-CD	-6.80	101.98	111.50
1	A	387	TRP	CB-CG-CD1	-6.78	118.19	127.00
1	A	639	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	A	506	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	A	666	ILE	CG1-CB-CG2	-6.55	96.99	111.40
1	A	174	TRP	CD1-CG-CD2	6.55	111.54	106.30
1	A	292	ARG	CA-CB-CG	-6.51	99.07	113.40
1	A	215	TRP	CD1-CG-CD2	6.46	111.47	106.30
1	A	244	TRP	CG-CD2-CE3	6.46	139.71	133.90
1	A	161	TYR	CB-CG-CD2	-6.44	117.14	121.00
1	A	181	ASP	CB-CG-OD1	6.43	124.09	118.30
1	A	797	TRP	CE2-CD2-CG	-6.43	102.16	107.30
1	A	319	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	A	555	VAL	CG1-CB-CG2	6.36	121.08	110.90
1	A	244	TRP	CB-CG-CD1	-6.32	118.78	127.00
1	A	777	TYR	CB-CG-CD2	-6.28	117.23	121.00
1	A	214	LYS	CA-CB-CG	6.27	127.20	113.40
1	A	361	TRP	CE2-CD2-CG	-6.27	102.29	107.30
1	A	398	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	A	182	TRP	CD1-CG-CD2	6.22	111.27	106.30
1	A	220	VAL	CG1-CB-CG2	-6.18	101.01	110.90
1	A	579	ASN	CB-CG-ND2	6.15	131.46	116.70
1	A	803	ARG	CA-CB-CG	-6.12	99.94	113.40
1	A	361	TRP	CD1-CG-CD2	6.11	111.19	106.30
1	A	319	ARG	NE-CZ-NH2	-6.10	117.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	781	VAL	CA-CB-CG2	-6.10	101.74	110.90
1	A	387	TRP	CD1-CG-CD2	6.09	111.17	106.30
1	A	797	TRP	NE1-CE2-CZ2	-6.06	123.73	130.40
1	A	555	VAL	N-CA-CB	-6.05	98.20	111.50
1	A	113	TYR	CB-CG-CD1	-6.04	117.37	121.00
1	A	491	TRP	CG-CD2-CE3	6.04	139.34	133.90
1	A	244	TRP	CG-CD1-NE1	-5.99	104.11	110.10
1	A	323	ARG	CA-CB-CG	5.94	126.47	113.40
1	A	636	VAL	CA-C-N	5.91	128.02	116.20
1	A	800	MET	CB-CG-SD	-5.90	94.69	112.40
1	A	776	ASP	CB-CG-OD1	5.86	123.57	118.30
1	A	598	VAL	CA-CB-CG2	-5.85	102.13	110.90
1	A	797	TRP	CB-CG-CD1	-5.84	119.41	127.00
1	A	573	TYR	CB-CG-CD2	-5.83	117.50	121.00
1	A	66	ARG	NE-CZ-NH2	5.82	123.21	120.30
1	A	136	LEU	CA-CB-CG	5.78	128.58	115.30
1	A	160	ARG	CB-CG-CD	-5.76	96.63	111.60
1	A	310	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	A	43	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	A	216	VAL	N-CA-CB	-5.74	98.88	111.50
1	A	15	VAL	CA-CB-CG2	5.73	119.49	110.90
1	A	251	ASP	CA-C-N	5.69	129.73	117.20
1	A	678	ASN	N-CA-CB	-5.68	100.37	110.60
1	A	91	MET	CG-SD-CE	5.67	109.28	100.20
1	A	292	ARG	CB-CG-CD	5.67	126.34	111.60
1	A	324	THR	N-CA-C	-5.67	95.71	111.00
1	A	678	ASN	CA-CB-CG	5.66	125.84	113.40
1	A	393	GLU	CA-CB-CG	5.64	125.82	113.40
1	A	795	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	A	815	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	A	764	MET	CG-SD-CE	-5.58	91.27	100.20
1	A	200	VAL	CG1-CB-CG2	-5.55	102.03	110.90
1	A	823	GLU	OE1-CD-OE2	-5.51	116.69	123.30
1	A	182	TRP	CE2-CD2-CG	-5.50	102.90	107.30
1	A	413	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	155	TYR	CG-CD2-CE2	-5.49	116.91	121.30
1	A	354	VAL	CG1-CB-CG2	-5.48	102.13	110.90
1	A	724	ARG	CA-CB-CG	5.46	125.42	113.40
1	A	67	TRP	CG-CD1-NE1	-5.42	104.68	110.10
1	A	586	LEU	N-CA-CB	-5.41	99.57	110.40
1	A	532	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	A	632	HIS	CA-CB-CG	-5.39	104.44	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	TRP	CG-CD2-CE3	5.37	138.73	133.90
1	A	122	LEU	CB-CG-CD2	-5.37	101.88	111.00
1	A	385	GLU	N-CA-CB	-5.36	100.95	110.60
1	A	803	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	A	247	LYS	CA-CB-CG	5.35	125.17	113.40
1	A	478	LYS	CA-CB-CG	-5.35	101.64	113.40
1	A	491	TRP	CG-CD1-NE1	-5.35	104.75	110.10
1	A	822	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	A	549	LEU	CA-CB-CG	5.31	127.52	115.30
1	A	699	MET	CG-SD-CE	5.30	108.69	100.20
1	A	611	PRO	CA-C-N	5.30	126.81	116.20
1	A	366	GLU	CA-CB-CG	5.29	125.04	113.40
1	A	569	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	491	TRP	CB-CG-CD1	-5.26	120.16	127.00
1	A	58	THR	CA-CB-CG2	-5.26	105.04	112.40
1	A	490	ARG	CG-CD-NE	-5.25	100.79	111.80
1	A	562	LEU	CA-CB-CG	5.23	127.32	115.30
1	A	734	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	313	SER	N-CA-CB	-5.21	102.68	110.50
1	A	101	ASN	CB-CG-ND2	5.21	129.21	116.70
1	A	584	ILE	CA-CB-CG2	-5.21	100.48	110.90
1	A	310	ARG	CA-C-N	5.18	128.60	117.20
1	A	387	TRP	NE1-CE2-CZ2	-5.18	124.71	130.40
1	A	120	GLU	CA-CB-CG	5.17	124.77	113.40
1	A	384	LEU	CA-CB-CG	5.12	127.08	115.30
1	A	698	GLU	CA-CB-CG	-5.11	102.16	113.40
1	A	435	ALA	C-N-CA	5.10	134.44	121.70
1	A	251	ASP	N-CA-CB	-5.08	101.46	110.60
1	A	251	ASP	O-C-N	-5.05	114.62	122.70
1	A	833	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	A	519	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	A	320	ASP	CA-CB-CG	5.01	124.41	113.40
1	A	423	ASP	CA-CB-CG	-5.01	102.39	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	320	ASP	Peptide

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	6761	0	6696	167	0
2	A	15	0	6	0	0
3	A	46	0	24	3	0
4	A	640	0	0	22	0
All	All	7462	0	6726	169	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 12.

All (169) 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:346:ILE:HB	1:A:347:PRO:HD3	1.71	0.72
1:A:393:GLU:HB3	1:A:400:LEU:HD12	1.71	0.72
1:A:549:LEU:HB2	1:A:555:VAL:HG11	1.72	0.71
1:A:546:ALA:HA	1:A:557:ILE:HD11	1.72	0.71
1:A:756:ASP:HB2	1:A:759:LYS:HE3	1.71	0.71
1:A:12:GLN:OE1	1:A:16:ARG:HD2	1.94	0.68
1:A:236:ASN:HB3	1:A:836:ALA:HB3	1.76	0.67
1:A:582:HIS:HB2	1:A:780:TYR:HE2	1.60	0.66
1:A:93:ARG:HD3	1:A:126:GLU:O	1.96	0.65
1:A:424:ARG:HH22	1:A:473:GLU:HG3	1.61	0.65
1:A:424:ARG:NH2	1:A:473:GLU:HG3	2.12	0.65
1:A:548:TYR:HD2	1:A:549:LEU:HD13	1.63	0.64
1:A:93:ARG:HD2	1:A:126:GLU:HB3	1.79	0.63
1:A:582:HIS:HB2	1:A:780:TYR:CE2	2.34	0.62
1:A:551:ARG:HG3	1:A:552:GLU:H	1.62	0.62
1:A:248:ALA:HB1	1:A:253:ASN:OD1	1.99	0.61
1:A:763:ASN:HB3	4:A:1070:HOH:O	2.01	0.60
1:A:314:SER:HB2	4:A:1554:HOH:O	2.01	0.60
1:A:455:VAL:H	1:A:459:HIS:HD2	1.50	0.60
1:A:510:GLU:HG3	1:A:831:ARG:NH2	2.17	0.59
1:A:108:CYS:HB3	1:A:119:MET:HE1	1.83	0.59
1:A:191:LYS:HG2	1:A:193:ARG:CZ	2.33	0.59
1:A:756:ASP:HA	1:A:759:LYS:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:HIS:HD2	1:A:38:THR:OG1	1.86	0.58
1:A:551:ARG:HG3	1:A:552:GLU:N	2.18	0.58
1:A:719:ASP:O	1:A:723:GLN:HG2	2.03	0.57
1:A:98:THR:O	1:A:102:LEU:HB2	2.05	0.57
1:A:310:ARG:O	1:A:314:SER:HB3	2.04	0.57
1:A:340:THR:HG21	4:A:1241:HOH:O	2.05	0.57
1:A:465:LYS:O	1:A:469:LYS:HD3	2.05	0.57
1:A:548:TYR:CD2	1:A:549:LEU:HD13	2.40	0.57
1:A:795:ARG:O	1:A:799:ARG:HG3	2.05	0.55
1:A:703:ALA:HA	1:A:807:THR:HG21	1.88	0.55
1:A:250:ASN:HA	1:A:269:ARG:HH12	1.72	0.55
1:A:790:LEU:HG	1:A:797:TRP:CD1	2.42	0.55
1:A:626:ILE:HG22	1:A:642:VAL:HG21	1.89	0.54
1:A:227:ASP:OD1	1:A:242:ARG:HD3	2.08	0.54
1:A:52:TYR:HE1	1:A:95:LEU:HD22	1.73	0.54
1:A:636:VAL:O	1:A:639:ARG:HD3	2.09	0.53
1:A:56:ALA:O	1:A:60:ARG:HB2	2.07	0.53
1:A:469:LYS:HD2	4:A:1152:HOH:O	2.09	0.53
1:A:379:VAL:HG22	4:A:1638:HOH:O	2.09	0.52
1:A:572:GLU:HB3	4:A:1318:HOH:O	2.09	0.52
1:A:52:TYR:CE1	1:A:95:LEU:HD22	2.44	0.52
1:A:792:LYS:O	1:A:794:PRO:HD3	2.10	0.51
1:A:373:ALA:HA	1:A:449:SER:HB3	1.92	0.51
1:A:65:GLY:O	1:A:69:ARG:HB2	2.10	0.51
1:A:515:LEU:HB3	1:A:809:GLY:HA2	1.92	0.51
1:A:604:MET:HB3	1:A:645:LEU:HD22	1.90	0.51
1:A:665:GLN:N	1:A:666:ILE:HD12	2.25	0.51
3:A:940:AMP:H3'	3:A:940:AMP:O2P	2.10	0.51
1:A:150:LEU:HD12	1:A:817:ILE:HG22	1.93	0.51
1:A:753:LYS:H	1:A:753:LYS:HE2	1.75	0.50
1:A:487:THR:O	1:A:491:TRP:HB2	2.11	0.50
1:A:666:ILE:HG22	1:A:666:ILE:O	2.12	0.50
1:A:665:GLN:NE2	1:A:678:ASN:HA	2.27	0.50
1:A:225:PRO:HB2	1:A:242:ARG:HD2	1.93	0.50
1:A:351:ARG:O	1:A:355:ASP:HB2	2.12	0.50
1:A:55:LEU:HD11	1:A:119:MET:HE2	1.94	0.50
1:A:12:GLN:NE2	1:A:497:PRO:HB2	2.27	0.49
1:A:666:ILE:HG23	1:A:711:PHE:HZ	1.77	0.49
1:A:241:MET:HG2	1:A:243:LEU:HD13	1.94	0.49
1:A:525:VAL:O	1:A:799:ARG:HD2	2.12	0.49
1:A:85:LEU:HD11	1:A:303:THR:HG21	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:703:ALA:CA	1:A:807:THR:HG21	2.41	0.49
1:A:490:ARG:NH2	4:A:1400:HOH:O	2.46	0.49
1:A:55:LEU:HD11	1:A:119:MET:CE	2.42	0.49
1:A:790:LEU:HG	1:A:797:TRP:HD1	1.77	0.49
1:A:753:LYS:HB2	4:A:1082:HOH:O	2.12	0.49
1:A:754:GLN:HB2	4:A:1562:HOH:O	2.13	0.49
1:A:527:ASP:O	1:A:531:ILE:HG12	2.13	0.48
1:A:515:LEU:HD22	1:A:518:LEU:HD22	1.94	0.48
1:A:108:CYS:CB	1:A:119:MET:HE1	2.43	0.48
1:A:379:VAL:HG12	1:A:467:ILE:HD11	1.95	0.48
1:A:538:LYS:O	1:A:542:LYS:HG3	2.13	0.48
1:A:168:GLN:HG3	1:A:175:GLN:HG3	1.95	0.48
1:A:667:SER:HB2	4:A:1491:HOH:O	2.12	0.48
1:A:103:ALA:HA	4:A:1557:HOH:O	2.12	0.48
1:A:66:ARG:HG3	1:A:836:ALA:HB1	1.94	0.48
1:A:518:LEU:O	1:A:521:LEU:HB2	2.13	0.48
1:A:545:PHE:O	1:A:549:LEU:HD22	2.14	0.48
1:A:561:SER:HB2	1:A:601:ARG:HA	1.95	0.48
1:A:542:LYS:NZ	1:A:561:SER:O	2.47	0.48
1:A:322:VAL:O	1:A:323:ARG:HD2	2.15	0.47
1:A:587:TYR:CD1	1:A:630:VAL:HG22	2.49	0.47
1:A:710:ILE:H	1:A:710:ILE:HD12	1.79	0.47
1:A:82:ILE:HD11	1:A:827:VAL:HG11	1.97	0.47
1:A:821:ALA:HB1	1:A:827:VAL:HG12	1.97	0.47
1:A:183:LEU:HB2	4:A:1534:HOH:O	2.15	0.47
1:A:203:TYR:OH	1:A:294:LYS:NZ	2.47	0.47
1:A:490:ARG:HD2	4:A:1375:HOH:O	2.14	0.47
1:A:494:LEU:HA	4:A:1407:HOH:O	2.15	0.47
1:A:170:ILE:HA	1:A:174:TRP:O	2.15	0.47
1:A:816:THR:O	1:A:820:TYR:HD1	1.98	0.47
1:A:359:LEU:HD23	1:A:363:LYS:HG3	1.96	0.47
1:A:490:ARG:HA	1:A:494:LEU:HB3	1.97	0.46
1:A:504:ALA:HA	1:A:508:GLY:O	2.14	0.46
1:A:309:ARG:HH22	3:A:930:AMP:P	2.38	0.46
1:A:386:ARG:HA	1:A:439:ILE:O	2.15	0.46
1:A:424:ARG:HH22	1:A:473:GLU:CG	2.28	0.46
1:A:91:MET:HB2	1:A:129:ALA:HB3	1.97	0.46
1:A:455:VAL:HB	1:A:484:ASN:ND2	2.31	0.45
1:A:252:PHE:HA	1:A:255:LYS:HB3	1.97	0.45
1:A:706:GLU:HG3	1:A:706:GLU:H	1.46	0.45
1:A:16:ARG:HB2	1:A:106:ASN:ND2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:ILE:HG12	1:A:521:LEU:HD21	1.98	0.45
1:A:314:SER:C	1:A:316:PHE:H	2.20	0.45
1:A:515:LEU:HD12	1:A:812:SER:HB2	1.99	0.45
1:A:486:ILE:HD13	4:A:1571:HOH:O	2.16	0.45
1:A:314:SER:OG	1:A:332:LYS:NZ	2.50	0.45
1:A:16:ARG:NH2	1:A:493:VAL:O	2.49	0.44
1:A:592:LYS:O	1:A:592:LYS:HD3	2.16	0.44
1:A:666:ILE:HD11	1:A:689:ILE:HG23	1.99	0.44
1:A:790:LEU:HD12	1:A:790:LEU:O	2.18	0.44
1:A:252:PHE:HE1	1:A:255:LYS:HZ2	1.63	0.44
1:A:678:ASN:OD1	1:A:695:ALA:HB3	2.17	0.44
1:A:69:ARG:O	1:A:73:HIS:HB2	2.17	0.44
1:A:615:MET:HB2	4:A:1123:HOH:O	2.17	0.44
1:A:23:ASN:O	1:A:27:LEU:HD22	2.18	0.43
1:A:335:ILE:HG23	1:A:371:THR:HG22	2.00	0.43
1:A:621:LYS:NZ	4:A:1322:HOH:O	2.48	0.43
1:A:667:SER:HB3	1:A:693:ASP:OD2	2.18	0.43
1:A:449:SER:O	1:A:478:LYS:HE2	2.18	0.43
1:A:716:GLU:HB2	4:A:1101:HOH:O	2.18	0.43
1:A:90:TYR:HE1	4:A:1569:HOH:O	2.01	0.43
1:A:488:PRO:O	1:A:492:LEU:HB3	2.19	0.43
1:A:549:LEU:HB3	1:A:555:VAL:HG21	2.00	0.43
1:A:735:ILE:HA	1:A:736:PRO:HD2	1.88	0.43
3:A:940:AMP:H8	3:A:940:AMP:O5'	2.01	0.43
1:A:687:LEU:HD21	1:A:800:MET:HG3	2.01	0.43
1:A:690:GLY:O	1:A:710:ILE:HA	2.18	0.43
1:A:127:GLU:HG2	1:A:182:TRP:HA	1.99	0.43
1:A:18:LEU:HD22	1:A:18:LEU:HA	1.87	0.42
1:A:177:GLU:HG2	1:A:611:PRO:HG3	2.01	0.42
1:A:316:PHE:HD1	1:A:316:PHE:HA	1.66	0.42
1:A:828:GLU:HA	1:A:829:PRO:HD3	1.76	0.42
1:A:354:VAL:O	1:A:358:ARG:HA	2.19	0.42
1:A:664:GLU:OE2	1:A:666:ILE:HD13	2.20	0.42
1:A:582:HIS:HD2	1:A:781:VAL:HG22	1.84	0.42
1:A:205:ARG:HH11	1:A:216:VAL:HG11	1.83	0.42
1:A:550:GLU:HA	1:A:555:VAL:H	1.83	0.42
1:A:550:GLU:HA	1:A:555:VAL:N	2.35	0.42
1:A:633:ASP:HA	1:A:634:PRO:HD2	1.92	0.42
1:A:225:PRO:CB	1:A:242:ARG:HD2	2.50	0.42
1:A:352:VAL:O	1:A:356:LEU:HB2	2.20	0.42
1:A:756:ASP:CA	1:A:759:LYS:HG3	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:761:ILE:HG22	1:A:765:LEU:HD22	2.02	0.42
1:A:99:MET:CE	1:A:108:CYS:HB2	2.50	0.41
1:A:76:GLU:HB3	4:A:1343:HOH:O	2.20	0.41
1:A:205:ARG:NH1	1:A:216:VAL:HG11	2.36	0.41
1:A:519:ARG:O	1:A:522:LEU:HB2	2.20	0.41
1:A:578:LEU:HD23	1:A:666:ILE:CG2	2.50	0.41
1:A:779:GLU:HG2	4:A:1564:HOH:O	2.20	0.41
1:A:139:LEU:HD12	1:A:139:LEU:HA	1.90	0.41
1:A:417:ALA:C	1:A:419:PRO:HD3	2.40	0.41
1:A:733:ASP:O	1:A:739:ARG:NH1	2.54	0.41
1:A:227:ASP:HB3	1:A:240:THR:HG23	2.03	0.41
1:A:352:VAL:HG22	1:A:356:LEU:HD22	2.03	0.40
1:A:340:THR:HG23	1:A:385:GLU:OE1	2.21	0.40
1:A:531:ILE:HG23	1:A:798:THR:CG2	2.51	0.40
1:A:290:GLU:O	1:A:294:LYS:HG3	2.21	0.40
1:A:251:ASP:CG	1:A:252:PHE:N	2.75	0.40
1:A:579:ASN:O	1:A:583:VAL:HG23	2.21	0.40
1:A:712:GLY:O	1:A:714:ARG:NH1	2.51	0.40
1:A:414:VAL:HG22	1:A:474:LEU:HD22	2.03	0.40
1:A:49:ARG:HA	1:A:125:ILE:HG21	2.03	0.40
1:A:771:PHE:HD2	4:A:1318:HOH:O	2.03	0.40
1:A:193:ARG:HB3	1:A:196:PHE:HD2	1.87	0.40
1:A:341:HIS:CD2	1:A:341:HIS:N	2.90	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	830/842 (99%)	763 (92%)	53 (6%)	14 (2%)	9 6

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	436	VAL
1	A	554	LYS
1	A	678	ASN
1	A	840	LYS
1	A	322	VAL
1	A	328	ALA
1	A	837	PRO
1	A	838	ASP
1	A	315	LYS
1	A	836	ALA
1	A	118	ASP
1	A	320	ASP
1	A	259	VAL
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	719/731 (98%)	601 (84%)	118 (16%)	2 2

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	12	GLN
1	A	15	VAL
1	A	16	ARG
1	A	18	LEU
1	A	22	GLU
1	A	23	ASN
1	A	27	LEU
1	A	42	ASP
1	A	55	LEU
1	A	58	THR
1	A	60	ARG
1	A	64	VAL

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Mol	Chain	Res	Type
1	A	69	ARG
1	A	72	GLN
1	A	90	TYR
1	A	102	LEU
1	A	104	LEU
1	A	115	LEU
1	A	122	LEU
1	A	128	ASP
1	A	138	ARG
1	A	144	LEU
1	A	152	LEU
1	A	162	GLU
1	A	165	ILE
1	A	170	ILE
1	A	187	ASN
1	A	191	LYS
1	A	195	GLU
1	A	205	ARG
1	A	214	LYS
1	A	216	VAL
1	A	219	GLN
1	A	235	ASN
1	A	242	ARG
1	A	245	SER
1	A	251	ASP
1	A	253	ASN
1	A	263	ILE
1	A	271	LEU
1	A	281	PRO
1	A	287	GLU
1	A	289	LYS
1	A	306	ASP
1	A	308	ILE
1	A	309	ARG
1	A	315	LYS
1	A	316	PHE
1	A	319	ARG
1	A	320	ASP
1	A	327	ASP
1	A	332	LYS
1	A	335	ILE
1	A	337	LEU

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Mol	Chain	Res	Type
1	A	340	THR
1	A	344	LEU
1	A	359	LEU
1	A	363	LYS
1	A	366	GLU
1	A	400	LEU
1	A	423	ASP
1	A	430	LEU
1	A	437	LYS
1	A	444	LEU
1	A	486	ILE
1	A	489	ARG
1	A	490	ARG
1	A	513	SER
1	A	515	LEU
1	A	518	LEU
1	A	521	LEU
1	A	522	LEU
1	A	528	GLU
1	A	530	PHE
1	A	536	LYS
1	A	549	LEU
1	A	554	LYS
1	A	555	VAL
1	A	560	ASN
1	A	569	ARG
1	A	576	GLN
1	A	579	ASN
1	A	584	ILE
1	A	591	LYS
1	A	592	LYS
1	A	598	VAL
1	A	601	ARG
1	A	613	TYR
1	A	622	LEU
1	A	640	LEU
1	A	641	ARG
1	A	645	LEU
1	A	649	ARG
1	A	662	LEU
1	A	665	GLN
1	A	667	SER

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Mol	Chain	Res	Type
1	A	678	ASN
1	A	687	LEU
1	A	705	GLU
1	A	706	GLU
1	A	708	PHE
1	A	715	VAL
1	A	738	LEU
1	A	746	SER
1	A	753	LYS
1	A	756	ASP
1	A	759	LYS
1	A	760	ASP
1	A	764	MET
1	A	765	LEU
1	A	782	LYS
1	A	790	LEU
1	A	797	TRP
1	A	807	THR
1	A	813	SER
1	A	833	ARG
1	A	839	GLU

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

Mol	Chain	Res	Type
1	A	23	ASN
1	A	34	HIS
1	A	36	HIS
1	A	97	ASN
1	A	167	ASN
1	A	187	ASN
1	A	235	ASN
1	A	376	ASN
1	A	459	HIS
1	A	481	ASN
1	A	484	ASN
1	A	539	GLN
1	A	566	GLN
1	A	576	GLN
1	A	579	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AMP	A	940	-	22,25,25	1.39	4 (18%)	25,38,38	1.40	2 (8%)
2	PLP	A	999	1	15,15,16	2.23	4 (26%)	20,22,23	1.42	3 (15%)
3	AMP	A	930	-	22,25,25	1.35	4 (18%)	25,38,38	1.67	6 (24%)

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
3	AMP	A	940	-	-	2/6/26/26	0/3/3/3
2	PLP	A	999	1	-	1/6/6/8	0/1/1/1
3	AMP	A	930	-	-	3/6/26/26	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	999	PLP	C3-C2	-7.04	1.33	1.40
3	A	940	AMP	O4'-C1'	3.28	1.45	1.41
2	A	999	PLP	C5-C4	-2.93	1.37	1.40
3	A	930	AMP	C5'-C4'	2.87	1.60	1.51
3	A	930	AMP	C8-N7	-2.63	1.30	1.34
3	A	940	AMP	P-O5'	2.36	1.67	1.60
3	A	940	AMP	C5'-C4'	2.34	1.58	1.51
3	A	930	AMP	C2'-C1'	-2.33	1.50	1.53
3	A	930	AMP	O4'-C1'	2.09	1.44	1.41
3	A	940	AMP	C8-N7	-2.05	1.31	1.34
2	A	999	PLP	P-O3P	-2.02	1.47	1.54
2	A	999	PLP	C6-N1	2.02	1.38	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	930	AMP	C4-C5-N7	4.03	113.60	109.40
3	A	940	AMP	P-O5'-C5'	3.84	128.88	118.30
2	A	999	PLP	C2A-C2-C3	-3.37	116.72	120.89
3	A	930	AMP	N6-C6-N1	3.18	125.18	118.57
3	A	930	AMP	O4'-C1'-C2'	-3.12	102.37	106.93
2	A	999	PLP	C5-C6-N1	-2.54	119.59	123.82
3	A	940	AMP	C4-C5-N7	2.50	112.01	109.40
2	A	999	PLP	C6-C5-C4	2.46	120.09	118.16
3	A	930	AMP	C5-C6-N6	-2.22	116.98	120.35
3	A	930	AMP	O5'-C5'-C4'	2.17	116.47	108.99
3	A	930	AMP	O2'-C2'-C1'	-2.12	103.04	110.85

There are no chirality outliers.

All (6) torsion outliers are listed below:

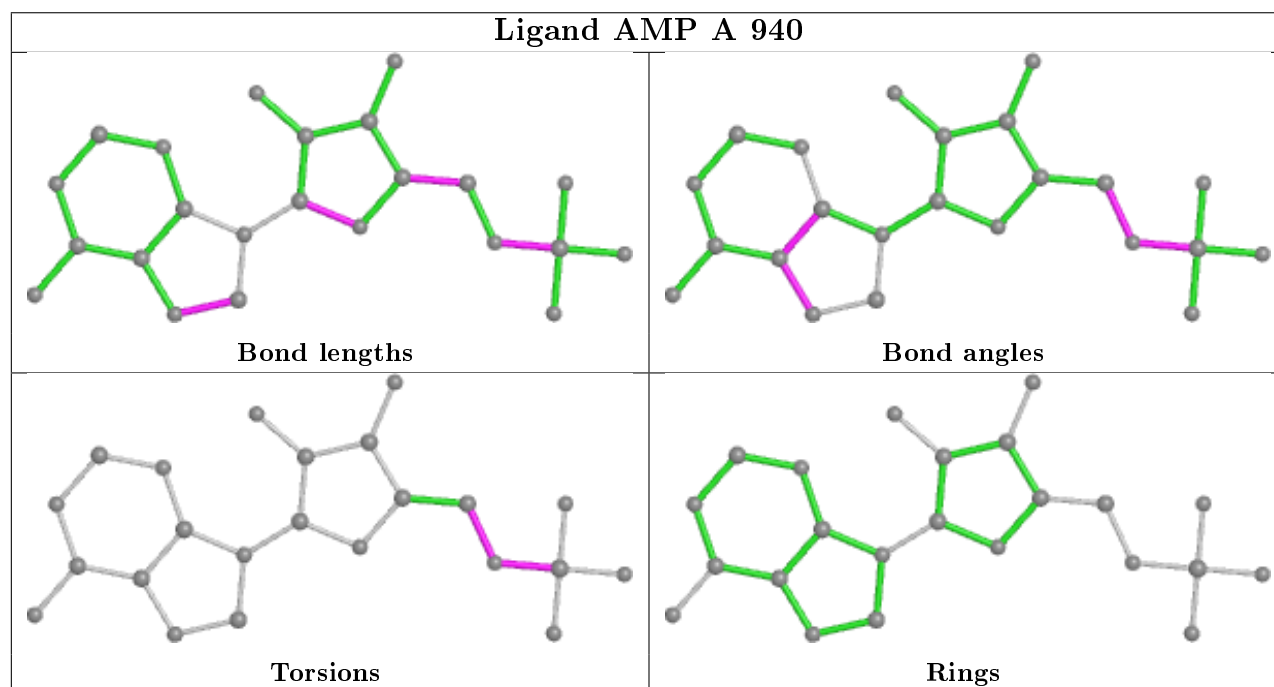
Mol	Chain	Res	Type	Atoms
3	A	940	AMP	C5'-O5'-P-O3P
2	A	999	PLP	C4-C5-C5A-O4P
3	A	930	AMP	O4'-C4'-C5'-O5'
3	A	930	AMP	C3'-C4'-C5'-O5'
3	A	940	AMP	C4'-C5'-O5'-P
3	A	930	AMP	C5'-O5'-P-O1P

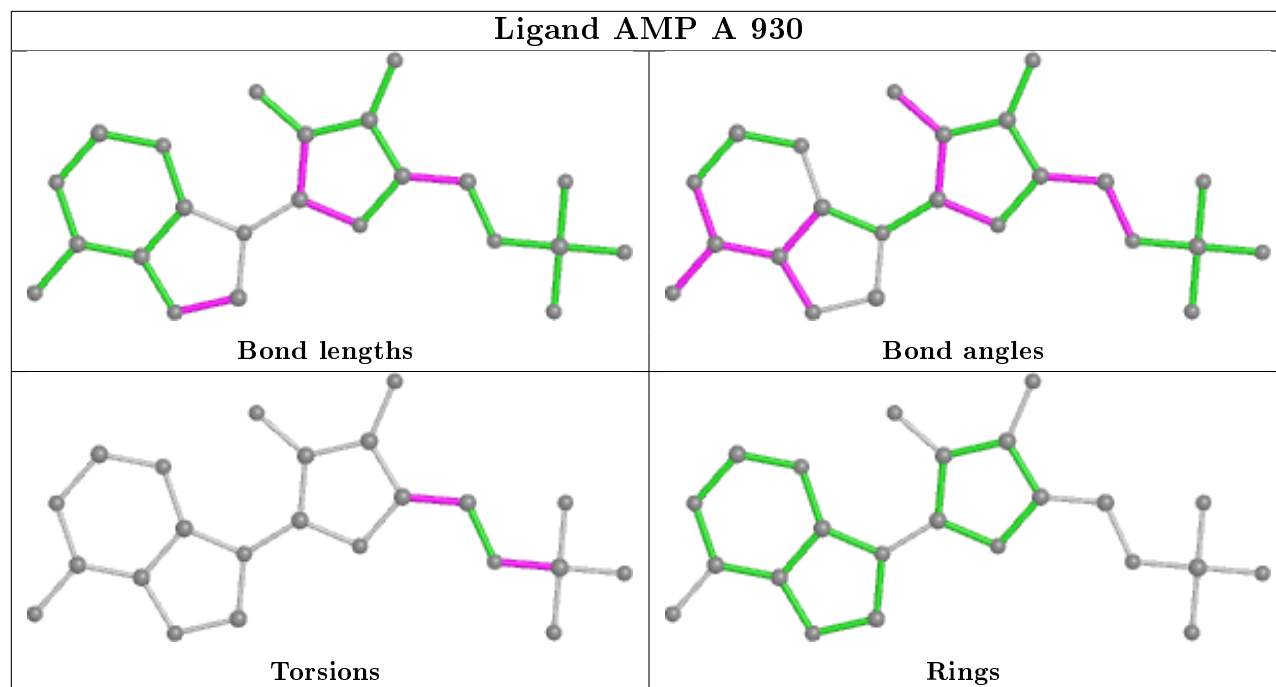
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	940	AMP	2	0
3	A	930	AMP	1	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.