



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:54 PM UTC

PDB ID : 8GPB / pdb_00008gpb
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 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

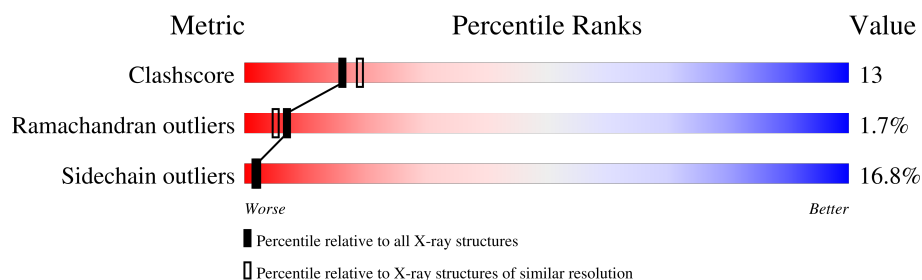
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (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 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 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 (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



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 (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



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.

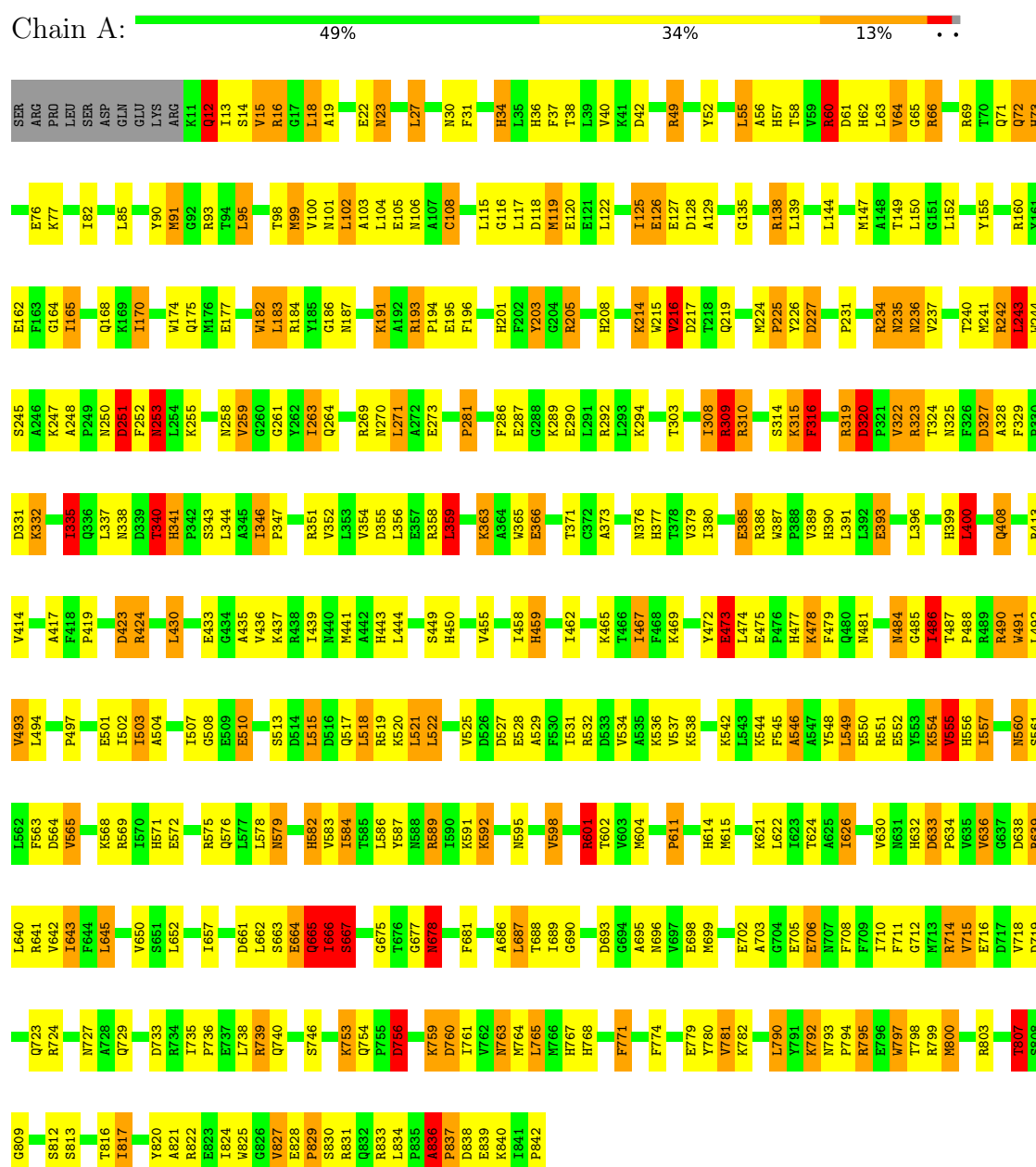
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	640	Total	O	0	0
			640	640		

3 Residue-property plots

These plots are drawn for all protein, RNA, 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 B



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	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.	Xtriage
Total number of atoms	7462	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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: PLP, AMP

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	1.26	44/6915 (0.6%)	2.19	267/9359 (2.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	335	ILE	CA-CB	8.39	1.64	1.54
1	A	571	HIS	CD2-NE2	-7.88	1.29	1.37
1	A	459	HIS	CD2-NE2	-7.43	1.29	1.37
1	A	443	HIS	CD2-NE2	-7.40	1.29	1.37
1	A	208	HIS	CD2-NE2	-7.28	1.29	1.37
1	A	399	HIS	CD2-NE2	-7.16	1.29	1.37
1	A	263	ILE	CA-CB	7.09	1.62	1.54
1	A	57	HIS	CD2-NE2	-7.09	1.30	1.37
1	A	632	HIS	CD2-NE2	-6.93	1.30	1.37
1	A	450	HIS	CD2-NE2	-6.80	1.30	1.37
1	A	34	HIS	CD2-NE2	-6.57	1.30	1.37
1	A	62	HIS	CD2-NE2	-6.56	1.30	1.37
1	A	346	ILE	CA-CB	6.48	1.62	1.54
1	A	424	ARG	CA-CB	-6.43	1.43	1.53
1	A	36	HIS	CD2-NE2	-6.33	1.30	1.37
1	A	556	HIS	CD2-NE2	-6.27	1.30	1.37
1	A	767	HIS	CD2-NE2	-6.25	1.30	1.37
1	A	377	HIS	CD2-NE2	-6.15	1.31	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	HIS	CD2-NE2	-6.12	1.31	1.37
1	A	390	HIS	CD2-NE2	-6.12	1.31	1.37
1	A	450	HIS	CG-ND1	-6.12	1.31	1.38
1	A	201	HIS	CD2-NE2	-5.95	1.31	1.37
1	A	582	HIS	CD2-NE2	-5.94	1.31	1.37
1	A	477	HIS	CD2-NE2	-5.83	1.31	1.37
1	A	715	VAL	CA-CB	5.78	1.61	1.54
1	A	237	VAL	CA-CB	5.72	1.61	1.54
1	A	842	PRO	N-CD	5.70	1.55	1.47
1	A	632	HIS	CG-ND1	-5.66	1.32	1.38
1	A	341	HIS	CD2-NE2	-5.66	1.31	1.37
1	A	208	HIS	CG-ND1	-5.61	1.32	1.38
1	A	261	GLY	CA-C	5.52	1.55	1.52
1	A	458	ILE	CA-CB	5.44	1.61	1.54
1	A	34	HIS	CG-ND1	-5.42	1.32	1.38
1	A	341	HIS	CG-ND1	-5.41	1.32	1.38
1	A	389	VAL	CA-CB	5.41	1.61	1.54
1	A	36	HIS	CG-ND1	-5.36	1.32	1.38
1	A	614	HIS	CD2-NE2	-5.35	1.31	1.37
1	A	507	ILE	CA-CB	5.29	1.60	1.54
1	A	767	HIS	CG-ND1	-5.28	1.32	1.38
1	A	40	VAL	CA-CB	5.26	1.61	1.54
1	A	740	GLN	CA-CB	-5.19	1.45	1.53
1	A	663	SER	CA-CB	-5.16	1.46	1.53
1	A	100	VAL	CA-CB	5.05	1.60	1.54
1	A	768	HIS	CD2-NE2	-5.04	1.32	1.37

All (267) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	560	ASN	CA-CB-CG	-17.00	95.60	112.60
1	A	117	LEU	N-CA-C	14.43	131.93	114.04
1	A	15	VAL	CA-C-O	14.27	135.04	122.63
1	A	678	ASN	CA-CB-CG	13.24	125.84	112.60
1	A	320	ASP	CA-CB-CG	11.81	124.41	112.60
1	A	327	ASP	CA-CB-CG	11.06	123.66	112.60
1	A	579	ASN	OD1-CG-ND2	-10.94	111.66	122.60
1	A	638	ASP	CA-CB-CG	10.92	123.52	112.60
1	A	101	ASN	OD1-CG-ND2	-10.64	111.96	122.60
1	A	490	ARG	NE-CZ-NH2	-10.45	109.80	119.20
1	A	187	ASN	OD1-CG-ND2	-10.34	112.26	122.60
1	A	423	ASP	CA-CB-CG	-10.21	102.39	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	807	THR	N-CA-CB	-10.13	94.27	110.98
1	A	579	ASN	CB-CG-ND2	10.04	131.46	116.40
1	A	800	MET	CA-CB-CG	10.02	134.14	114.10
1	A	555	VAL	N-CA-C	9.95	130.03	109.34
1	A	793	ASN	CA-CB-CG	9.79	122.39	112.60
1	A	727	ASN	OD1-CG-ND2	-9.74	112.86	122.60
1	A	340	THR	N-CA-CB	-9.72	96.36	110.56
1	A	632	HIS	CA-CB-CG	-9.36	104.44	113.80
1	A	316	PHE	N-CA-C	-9.04	102.38	113.41
1	A	309	ARG	NE-CZ-NH2	-8.85	111.23	119.20
1	A	91	MET	N-CA-C	8.79	120.95	111.36
1	A	760	ASP	CA-CB-CG	-8.77	103.83	112.60
1	A	325	ASN	CA-CB-CG	-8.65	103.95	112.60
1	A	264	GLN	OE1-CD-NE2	-8.65	113.95	122.60
1	A	101	ASN	CB-CG-ND2	8.54	129.21	116.40
1	A	235	ASN	OD1-CG-ND2	-8.43	114.17	122.60
1	A	324	THR	N-CA-C	-8.36	95.71	108.67
1	A	484	ASN	OD1-CG-ND2	-8.30	114.30	122.60
1	A	253	ASN	OD1-CG-ND2	-8.25	114.35	122.60
1	A	575	ARG	CB-CG-CD	-8.18	92.48	111.30
1	A	99	MET	CG-SD-CE	-8.17	82.93	100.90
1	A	57	HIS	CB-CG-CD2	-8.16	120.59	131.20
1	A	253	ASN	CB-CG-ND2	8.16	128.63	116.40
1	A	501	GLU	CA-C-O	-8.12	112.48	121.00
1	A	72	GLN	OE1-CD-NE2	-8.06	114.54	122.60
1	A	763	ASN	OD1-CG-ND2	-8.02	114.58	122.60
1	A	16	ARG	N-CA-C	-8.01	103.07	112.92
1	A	319	ARG	N-CA-C	7.94	120.98	108.67
1	A	135	GLY	N-CA-C	7.94	121.71	112.50
1	A	236	ASN	OD1-CG-ND2	-7.92	114.69	122.60
1	A	555	VAL	N-CA-CB	-7.90	98.20	111.23
1	A	95	LEU	N-CA-C	7.72	119.33	111.07
1	A	214	LYS	N-CA-CB	-7.61	98.02	110.81
1	A	807	THR	CB-CA-C	7.57	123.66	110.64
1	A	365	TRP	CG-CD2-CE3	7.55	141.45	133.90
1	A	664	GLU	N-CA-CB	-7.55	97.94	110.47
1	A	258	ASN	OD1-CG-ND2	-7.53	115.07	122.60
1	A	292	ARG	CA-CB-CG	-7.51	99.07	114.10
1	A	15	VAL	O-C-N	7.47	128.23	121.96
1	A	128	ASP	CA-CB-CG	7.43	120.03	112.60
1	A	727	ASN	CB-CG-ND2	7.38	127.46	116.40
1	A	216	VAL	N-CA-CB	-7.36	98.88	112.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	424	ARG	NE-CZ-NH2	-7.32	112.62	119.20
1	A	595	ASN	CA-CB-CG	-7.28	105.32	112.60
1	A	340	THR	CB-CA-C	7.27	122.85	110.56
1	A	270	ASN	CA-CB-CG	-7.24	105.36	112.60
1	A	529	ALA	N-CA-C	-7.19	103.37	111.07
1	A	842	PRO	CA-N-CD	-7.16	101.98	112.00
1	A	718	VAL	N-CA-C	-7.14	103.82	110.53
1	A	15	VAL	N-CA-C	7.13	113.84	106.21
1	A	803	ARG	CA-CB-CG	-7.08	99.94	114.10
1	A	774	PHE	CA-CB-CG	7.07	120.87	113.80
1	A	771	PHE	CA-CB-CG	-7.06	106.74	113.80
1	A	15	VAL	CA-CB-CG1	-7.00	98.50	110.40
1	A	586	LEU	N-CA-CB	-6.96	99.57	109.94
1	A	264	GLN	CG-CD-NE2	6.95	126.83	116.40
1	A	435	ALA	CA-C-N	6.93	134.44	121.97
1	A	435	ALA	C-N-CA	6.93	134.44	121.97
1	A	822	ARG	N-CA-C	6.91	118.89	111.36
1	A	329	PHE	CA-C-O	-6.90	112.28	118.63
1	A	399	HIS	CB-CG-CD2	-6.89	122.24	131.20
1	A	387	TRP	CG-CD2-CE3	6.84	140.74	133.90
1	A	677	GLY	N-CA-C	-6.83	104.57	112.50
1	A	49	ARG	CA-C-O	-6.82	113.32	120.55
1	A	215	TRP	CG-CD2-CE3	6.62	140.51	133.90
1	A	331	ASP	CA-CB-CG	-6.61	105.99	112.60
1	A	214	LYS	CA-CB-CG	6.55	127.20	114.10
1	A	71	GLN	OE1-CD-NE2	-6.54	116.06	122.60
1	A	292	ARG	CB-CG-CD	6.54	126.34	111.30
1	A	601	ARG	N-CA-C	6.45	119.12	108.99
1	A	376	ASN	OD1-CG-ND2	-6.44	116.16	122.60
1	A	459	HIS	CB-CG-CD2	-6.43	122.84	131.20
1	A	225	PRO	N-CA-C	6.43	121.28	111.19
1	A	510	GLU	CB-CG-CD	6.43	123.53	112.60
1	A	391	LEU	N-CA-C	-6.42	103.79	111.69
1	A	201	HIS	CB-CG-CD2	-6.42	122.86	131.20
1	A	165	ILE	CB-CA-C	6.38	120.40	111.34
1	A	575	ARG	N-CA-C	6.38	120.04	111.24
1	A	160	ARG	CB-CG-CD	-6.38	96.63	111.30
1	A	119	MET	CG-SD-CE	-6.37	86.88	100.90
1	A	602	THR	N-CA-C	-6.37	98.14	108.52
1	A	589	ARG	N-CA-C	-6.34	104.06	110.97
1	A	346	ILE	CA-C-N	6.33	125.95	119.56
1	A	346	ILE	C-N-CA	6.33	125.95	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	PRO	O-C-N	-6.28	115.93	123.03
1	A	696	ASN	CB-CA-C	-6.26	100.40	110.79
1	A	611	PRO	O-C-N	-6.26	115.22	122.85
1	A	478	LYS	CA-CB-CG	-6.23	101.64	114.10
1	A	338	ASN	OD1-CG-ND2	-6.23	116.37	122.60
1	A	194	PRO	CA-C-O	6.22	128.49	119.34
1	A	565	VAL	N-CA-C	6.22	117.08	108.12
1	A	624	THR	N-CA-C	-6.19	104.61	111.36
1	A	473	GLU	CB-CG-CD	6.19	123.12	112.60
1	A	323	ARG	CA-CB-CG	6.18	126.47	114.10
1	A	836	ALA	N-CA-C	6.15	123.41	109.81
1	A	61	ASP	CA-CB-CG	6.15	118.75	112.60
1	A	564	ASP	CA-CB-CG	6.12	118.72	112.60
1	A	399	HIS	CB-CG-ND1	6.12	131.88	122.70
1	A	652	LEU	N-CA-C	-6.08	104.21	111.69
1	A	633	ASP	CA-C-N	6.06	125.95	119.28
1	A	633	ASP	C-N-CA	6.06	125.95	119.28
1	A	365	TRP	CB-CG-CD1	-6.03	117.85	126.90
1	A	165	ILE	N-CA-CB	-6.03	102.00	110.26
1	A	756	ASP	CA-CB-CG	6.01	118.61	112.60
1	A	800	MET	CB-CG-SD	-6.00	94.69	112.70
1	A	108	CYS	CA-C-O	-5.99	112.72	119.79
1	A	251	ASP	O-C-N	-5.99	114.62	122.59
1	A	678	ASN	N-CA-CB	-5.99	100.37	110.49
1	A	208	HIS	CB-CG-CD2	-5.98	123.43	131.20
1	A	698	GLU	CA-CB-CG	-5.97	102.16	114.10
1	A	203	TYR	CB-CA-C	-5.96	109.71	116.63
1	A	490	ARG	NE-CZ-NH1	5.96	127.46	121.50
1	A	217	ASP	N-CA-C	5.94	119.38	111.30
1	A	557	ILE	N-CA-C	-5.93	101.20	109.45
1	A	186	GLY	CA-C-O	-5.93	117.84	122.52
1	A	560	ASN	N-CA-C	5.92	120.50	113.16
1	A	817	ILE	CA-C-O	-5.91	113.93	120.96
1	A	64	VAL	N-CA-C	5.90	119.34	111.44
1	A	187	ASN	CB-CG-ND2	5.89	125.24	116.40
1	A	584	ILE	CA-CB-CG2	-5.89	100.48	110.50
1	A	430	LEU	N-CA-C	-5.87	105.61	112.89
1	A	377	HIS	CB-CG-CD2	-5.86	123.58	131.20
1	A	393	GLU	CA-CB-CG	5.86	125.82	114.10
1	A	517	GLN	CA-CB-CG	-5.85	102.41	114.10
1	A	234	ARG	N-CA-CB	-5.83	103.27	112.08
1	A	571	HIS	CB-CG-CD2	-5.83	123.62	131.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	MET	CA-C-N	5.83	125.59	119.76
1	A	224	MET	C-N-CA	5.83	125.59	119.76
1	A	664	GLU	CB-CA-C	5.83	120.29	110.79
1	A	234	ARG	N-CA-C	5.82	119.58	111.90
1	A	244	TRP	CG-CD2-CE3	5.81	139.71	133.90
1	A	387	TRP	CB-CG-CD1	-5.81	118.19	126.90
1	A	666	ILE	N-CA-CB	-5.80	101.66	111.23
1	A	556	HIS	N-CA-C	5.77	123.10	110.80
1	A	214	LYS	CB-CA-C	5.77	119.74	109.65
1	A	31	PHE	N-CA-C	-5.75	104.65	111.03
1	A	270	ASN	N-CA-C	5.75	119.10	111.75
1	A	486	ILE	N-CA-CB	-5.74	101.30	111.93
1	A	385	GLU	N-CA-CB	-5.71	100.95	110.37
1	A	393	GLU	CB-CG-CD	-5.70	102.91	112.60
1	A	57	HIS	CB-CG-ND1	5.69	131.24	122.70
1	A	472	TYR	O-C-N	-5.69	116.09	122.12
1	A	546	ALA	CA-C-O	5.67	126.77	120.82
1	A	724	ARG	CA-CB-CG	5.66	125.42	114.10
1	A	643	ILE	N-CA-CB	-5.66	102.17	111.44
1	A	650	VAL	O-C-N	-5.65	116.39	121.87
1	A	396	LEU	CA-C-N	5.64	125.48	119.28
1	A	396	LEU	C-N-CA	5.64	125.48	119.28
1	A	126	GLU	CA-C-O	5.63	127.29	120.81
1	A	308	ILE	N-CA-CB	-5.62	102.90	110.54
1	A	479	PHE	N-CA-C	5.62	118.69	109.76
1	A	149	THR	CA-CB-OG1	-5.62	101.18	109.60
1	A	639	ARG	N-CA-C	5.58	117.36	111.28
1	A	286	PHE	CA-CB-CG	5.58	119.38	113.80
1	A	485	GLY	CA-C-N	5.56	131.53	122.69
1	A	485	GLY	C-N-CA	5.56	131.53	122.69
1	A	12	GLN	OE1-CD-NE2	-5.56	117.04	122.60
1	A	390	HIS	CB-CG-CD2	-5.55	123.98	131.20
1	A	359	LEU	N-CA-C	-5.54	103.38	110.53
1	A	247	LYS	CA-CB-CG	5.53	125.17	114.10
1	A	30	ASN	OD1-CG-ND2	-5.53	117.07	122.60
1	A	714	ARG	O-C-N	-5.51	116.23	122.68
1	A	829	PRO	N-CA-C	5.50	119.50	111.03
1	A	626	ILE	N-CA-C	-5.48	105.03	111.00
1	A	216	VAL	CB-CA-C	5.47	119.01	111.19
1	A	366	GLU	CA-CB-CG	5.47	125.04	114.10
1	A	116	GLY	CA-C-O	-5.47	113.48	119.88
1	A	49	ARG	O-C-N	5.44	127.89	122.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	491	TRP	CG-CD2-CE3	5.44	139.34	133.90
1	A	661	ASP	N-CA-C	-5.44	105.45	112.68
1	A	408	GLN	OE1-CD-NE2	-5.43	117.17	122.60
1	A	829	PRO	CA-C-O	-5.43	115.42	121.23
1	A	571	HIS	CA-CB-CG	5.42	119.22	113.80
1	A	686	ALA	N-CA-C	-5.42	102.17	110.14
1	A	236	ASN	CB-CG-ND2	5.42	124.53	116.40
1	A	287	GLU	CA-C-O	5.42	125.98	120.24
1	A	338	ASN	CB-CG-ND2	5.42	124.52	116.40
1	A	244	TRP	CB-CG-CD1	-5.41	118.78	126.90
1	A	739	ARG	N-CA-CB	-5.40	101.90	109.94
1	A	19	ALA	N-CA-C	-5.40	102.10	109.71
1	A	60	ARG	NE-CZ-NH2	-5.39	114.35	119.20
1	A	834	LEU	N-CA-C	-5.37	103.01	109.83
1	A	767	HIS	CB-CG-CD2	-5.35	124.24	131.20
1	A	37	PHE	N-CA-C	5.35	117.11	111.28
1	A	273	GLU	CB-CG-CD	5.35	121.69	112.60
1	A	15	VAL	CA-CB-CG2	5.35	119.49	110.40
1	A	251	ASP	N-CA-CB	-5.34	101.46	110.49
1	A	380	ILE	CA-C-N	5.34	124.98	119.05
1	A	380	ILE	C-N-CA	5.34	124.98	119.05
1	A	503	ILE	N-CA-C	-5.34	105.51	110.53
1	A	657	ILE	O-C-N	-5.34	115.01	121.10
1	A	678	ASN	CA-C-O	5.34	128.14	120.51
1	A	73	HIS	CA-CB-CG	-5.33	108.47	113.80
1	A	120	GLU	CA-CB-CG	5.33	124.77	114.10
1	A	193	ARG	O-C-N	-5.33	116.59	121.34
1	A	310	ARG	CA-C-O	-5.33	114.90	120.55
1	A	182	TRP	CE2-CD2-CE3	5.32	124.12	118.80
1	A	481	ASN	CA-CB-CG	-5.32	107.28	112.60
1	A	380	ILE	CG1-CB-CG2	-5.32	94.75	110.70
1	A	263	ILE	CG1-CB-CG2	-5.31	94.76	110.70
1	A	310	ARG	O-C-N	-5.31	116.50	122.12
1	A	63	LEU	N-CA-CB	-5.31	102.13	110.30
1	A	793	ASN	CA-C-N	5.29	126.45	119.84
1	A	793	ASN	C-N-CA	5.29	126.45	119.84
1	A	598	VAL	N-CA-CB	-5.28	102.70	111.36
1	A	601	ARG	CA-C-O	5.28	126.91	120.99
1	A	681	PHE	CA-CB-CG	5.27	119.07	113.80
1	A	184	ARG	N-CA-C	5.27	120.01	111.37
1	A	817	ILE	N-CA-C	-5.26	105.71	110.82
1	A	164	GLY	N-CA-C	-5.25	103.63	112.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	675	GLY	N-CA-C	-5.24	105.17	112.18
1	A	235	ASN	CB-CG-ND2	5.23	124.25	116.40
1	A	484	ASN	CA-CB-CG	5.23	117.83	112.60
1	A	399	HIS	N-CA-C	-5.23	105.76	111.82
1	A	556	HIS	CB-CG-CD2	-5.22	124.41	131.20
1	A	125	ILE	N-CA-C	-5.22	105.38	113.16
1	A	688	THR	CA-C-O	-5.21	114.78	120.36
1	A	665	GLN	OE1-CD-NE2	-5.21	117.39	122.60
1	A	636	VAL	O-C-N	-5.19	116.50	121.90
1	A	117	LEU	N-CA-CB	-5.18	103.14	110.81
1	A	183	LEU	N-CA-C	5.18	119.60	113.28
1	A	226	TYR	CA-C-O	-5.18	114.75	120.24
1	A	537	VAL	CB-CA-C	-5.17	105.35	111.97
1	A	244	TRP	N-CA-C	5.17	117.98	109.76
1	A	824	ILE	O-C-N	-5.16	116.12	122.57
1	A	729	GLN	CA-C-N	5.13	127.41	120.38
1	A	729	GLN	C-N-CA	5.13	127.41	120.38
1	A	837	PRO	N-CA-C	-5.13	101.90	112.47
1	A	243	LEU	N-CA-CB	-5.13	101.96	110.47
1	A	281	PRO	O-C-N	-5.11	115.74	122.64
1	A	310	ARG	CB-CG-CD	-5.11	99.56	111.30
1	A	490	ARG	CG-CD-NE	-5.10	100.79	112.00
1	A	795	ARG	CA-CB-CG	-5.09	103.91	114.10
1	A	62	HIS	CB-CG-CD2	-5.09	124.58	131.20
1	A	781	VAL	CA-CB-CG2	-5.09	101.74	110.40
1	A	271	LEU	CA-C-O	-5.08	115.14	120.63
1	A	37	PHE	CA-CB-CG	-5.08	108.72	113.80
1	A	534	VAL	CA-C-O	-5.08	115.78	121.17
1	A	650	VAL	CA-C-O	-5.08	115.67	120.95
1	A	486	ILE	CB-CA-C	5.07	118.80	110.69
1	A	400	LEU	CA-C-O	-5.06	114.15	119.97
1	A	77	LYS	CA-CB-CG	5.06	124.22	114.10
1	A	227	ASP	CB-CA-C	-5.06	100.97	109.72
1	A	636	VAL	CA-C-O	-5.05	115.44	121.05
1	A	105	GLU	CA-CB-CG	-5.05	104.00	114.10
1	A	502	ILE	CB-CA-C	-5.04	104.34	112.16
1	A	138	ARG	NE-CZ-NH2	-5.04	114.67	119.20
1	A	14	SER	O-C-N	-5.03	115.89	122.59
1	A	433	GLU	N-CA-C	-5.03	102.41	109.96
1	A	667	SER	O-C-N	-5.03	116.83	122.97
1	A	259	VAL	N-CA-CB	-5.03	102.93	111.23
1	A	479	PHE	CA-CB-CG	-5.02	108.78	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	424	ARG	CB-CG-CD	-5.01	99.78	111.30
1	A	702	GLU	O-C-N	-5.00	116.69	122.09
1	A	155	TYR	N-CA-C	5.00	116.92	108.02

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 ⓘ

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	175	0
2	A	15	0	6	0	0
3	A	46	0	24	3	0
4	A	640	0	0	23	0
All	All	7462	0	6726	177	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 13.

All (177) 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:55:LEU:HD11	1:A:119:MET:HE2	1.68	0.74
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:99:MET:HE1	1:A:108:CYS:HB2	1.88	0.56
1:A:703:ALA:HA	1:A:807:THR:HG21	1.88	0.55
1:A:795:ARG:O	1:A:799:ARG:HG3	2.05	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:615:MET:HE3	1:A:764:MET:HG3	1.89	0.55
1:A:99:MET:HE3	1:A:108:CYS:SG	2.47	0.54
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:52:TYR:CE1	1:A:95:LEU:HD22	2.44	0.52
1:A:572:GLU:HB3	4:A:1318:HOH:O	2.09	0.52
1:A:792:LYS:O	1:A:794:PRO:HD3	2.10	0.51
1:A:65:GLY:O	1:A:69:ARG:HB2	2.10	0.51
1:A:373:ALA:HA	1:A:449:SER:HB3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HE2	1:A:753:LYS:H	1.75	0.50
1:A:699:MET:HE2	1:A:708:PHE:HZ	1.74	0.50
1:A:487:THR:O	1:A:491:TRP:HB2	2.11	0.50
1:A:665:GLN:NE2	1:A:678:ASN:HA	2.27	0.50
1:A:666:ILE:HG22	1:A:666:ILE:O	2.12	0.50
1:A:225:PRO:HB2	1:A:242:ARG:HD2	1.93	0.50
1:A:108:CYS:HB3	1:A:119:MET:HE1	1.94	0.50
1:A:351:ARG:O	1:A:355:ASP:HB2	2.12	0.50
1:A:314:SER:C	1:A:316:PHE:H	2.20	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
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: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: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:66:ARG:HG3	1:A:836:ALA:HB1	1.94	0.48
1:A:103:ALA:HA	4:A:1557:HOH:O	2.12	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:82:ILE:HD11	1:A:827:VAL:HG11	1.97	0.47
1:A:710:ILE:HD12	1:A:710:ILE:H	1.79	0.47
1:A:821:ALA:HB1	1:A:827:VAL:HG12	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:CYS:CB	1:A:119:MET:HE1	2.45	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:309:ARG:HH22	3:A:930:AMP:P	2.38	0.46
1:A:504:ALA:HA	1:A:508:GLY:O	2.14	0.46
1:A:386:ARG:HA	1:A:439:ILE:O	2.15	0.46
1:A:417:ALA:C	1:A:419:PRO:HD3	2.40	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:343:SER:OG	1:A:441:MET:HE3	2.17	0.46
1:A:455:VAL:HB	1:A:484:ASN:ND2	2.31	0.45
1:A:764:MET:HE1	4:A:1318:HOH:O	2.16	0.45
1:A:252:PHE:HA	1:A:255:LYS:HB3	1.97	0.45
1:A:706:GLU:H	1:A:706:GLU:HG3	1.46	0.45
1:A:16:ARG:HB2	1:A:106:ASN:ND2	2.32	0.45
1:A:503:ILE:HG12	1:A:521:LEU:HD21	1.98	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:55:LEU:HD11	1:A:119:MET:CE	2.42	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:O	1:A:790:LEU:HD12	2.18	0.44
1:A:413:ARG:HH22	1:A:475:GLU:CD	2.25	0.44
1:A:563:PHE:CD2	1:A:604:MET:HE1	2.53	0.44
1:A:69:ARG:O	1:A:73:HIS:HB2	2.17	0.44
1:A:678:ASN:OD1	1:A:695:ALA:HB3	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:90:TYR:HE1	4:A:1569:HOH:O	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:ASP:CG	1:A:252:PHE:N	2.75	0.43
1:A:716:GLU:HB2	4:A:1101:HOH:O	2.18	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:147:MET:HE3	1:A:825:TRP:CH2	2.55	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:99:MET:HE1	1:A:119:MET:HE1	2.00	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
1:A:761:ILE:HG22	1:A:765:LEU:HD22	2.02	0.42
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:HA	1:A:139:LEU:HD12	1.90	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:340:THR:HG23	1:A:385:GLU:OE1	2.21	0.40
1:A:352:VAL:HG22	1:A:356:LEU:HD22	2.03	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: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:49:ARG:HA	1:A:125:ILE:HG21	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:VAL:HG22	1:A:474:LEU:HD22	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%)	7 5

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 ⓘ

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%)	598 (83%)	121 (17%)	2 2

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	15	VAL
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
1	A	66	ARG
1	A	72	GLN
1	A	102	LEU
1	A	104	LEU
1	A	115	LEU
1	A	122	LEU
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	191	LYS
1	A	195	GLU
1	A	205	ARG
1	A	214	LYS
1	A	216	VAL
1	A	219	GLN
1	A	234	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	235	ASN
1	A	242	ARG
1	A	243	LEU
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	289	LYS
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
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	408	GLN
1	A	423	ASP
1	A	430	LEU
1	A	437	LYS
1	A	444	LEU
1	A	462	ILE
1	A	467	ILE
1	A	473	GLU
1	A	486	ILE
1	A	493	VAL
1	A	513	SER
1	A	515	LEU
1	A	518	LEU
1	A	520	LYS
1	A	521	LEU
1	A	522	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	528	GLU
1	A	532	ARG
1	A	536	LYS
1	A	544	LYS
1	A	549	LEU
1	A	554	LYS
1	A	555	VAL
1	A	560	ASN
1	A	565	VAL
1	A	568	LYS
1	A	569	ARG
1	A	576	GLN
1	A	584	ILE
1	A	589	ARG
1	A	591	LYS
1	A	592	LYS
1	A	598	VAL
1	A	601	ARG
1	A	622	LEU
1	A	640	LEU
1	A	641	ARG
1	A	643	ILE
1	A	645	LEU
1	A	662	LEU
1	A	665	GLN
1	A	666	ILE
1	A	667	SER
1	A	678	ASN
1	A	687	LEU
1	A	705	GLU
1	A	706	GLU
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	765	LEU
1	A	782	LYS
1	A	790	LEU
1	A	792	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	797	TRP
1	A	807	THR
1	A	813	SER
1	A	827	VAL
1	A	830	SER
1	A	833	ARG
1	A	839	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	34	HIS
1	A	36	HIS
1	A	208	HIS
1	A	235	ASN
1	A	258	ASN
1	A	459	HIS
1	A	484	ASN
1	A	539	GLN
1	A	576	GLN
1	A	665	GLN
1	A	678	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 oligosaccharides 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	$\# Z > 2$
2	PLP	A	999	1	15,15,16	2.21	4 (26%)	21,22,23	1.40	4 (19%)
3	AMP	A	940	-	25,25,25	1.07	2 (8%)	37,38,38	1.35	3 (8%)
3	AMP	A	930	-	25,25,25	1.07	1 (4%)	37,38,38	1.46	8 (21%)

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	PLP	A	999	1	-	1/6/6/8	0/1/1/1
3	AMP	A	940	-	-	2/10/26/26	0/3/3/3
3	AMP	A	930	-	-	3/10/26/26	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	999	PLP	C3-C2	-6.85	1.33	1.41
3	A	930	AMP	C5'-C4'	2.99	1.60	1.51
2	A	999	PLP	C5-C4	-2.91	1.37	1.40
3	A	940	AMP	C5'-C4'	2.44	1.58	1.51
3	A	940	AMP	P-O5'	2.38	1.67	1.60
2	A	999	PLP	C6-N1	2.10	1.38	1.34
2	A	999	PLP	P-O3P	-2.09	1.47	1.54

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	940	AMP	O4'-C1'-N9	-4.06	100.30	108.09
2	A	999	PLP	C2A-C2-C3	-3.48	116.72	120.80
3	A	940	AMP	C2'-C1'-N9	3.33	121.58	113.30
3	A	930	AMP	N6-C6-N1	3.06	125.18	118.38
3	A	930	AMP	N9-C8-N7	2.91	118.07	113.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	930	AMP	C4-C5-N7	2.64	113.60	110.58
2	A	999	PLP	C5-C6-N1	-2.61	119.59	123.83
3	A	930	AMP	C5-N7-C8	-2.58	99.40	103.45
3	A	930	AMP	C5-C6-N6	-2.55	116.98	123.29
2	A	999	PLP	C6-C5-C4	2.43	120.09	118.10
3	A	940	AMP	C4-N9-C8	-2.27	103.35	105.74
3	A	930	AMP	O5'-C5'-C4'	2.20	116.47	108.99
3	A	930	AMP	C4-N9-C8	-2.11	103.52	105.74
3	A	930	AMP	O2'-C2'-C1'	-2.05	103.04	110.10
2	A	999	PLP	O3-C3-C4	2.01	123.36	118.10

There are no chirality outliers.

All (6) torsion outliers are listed below:

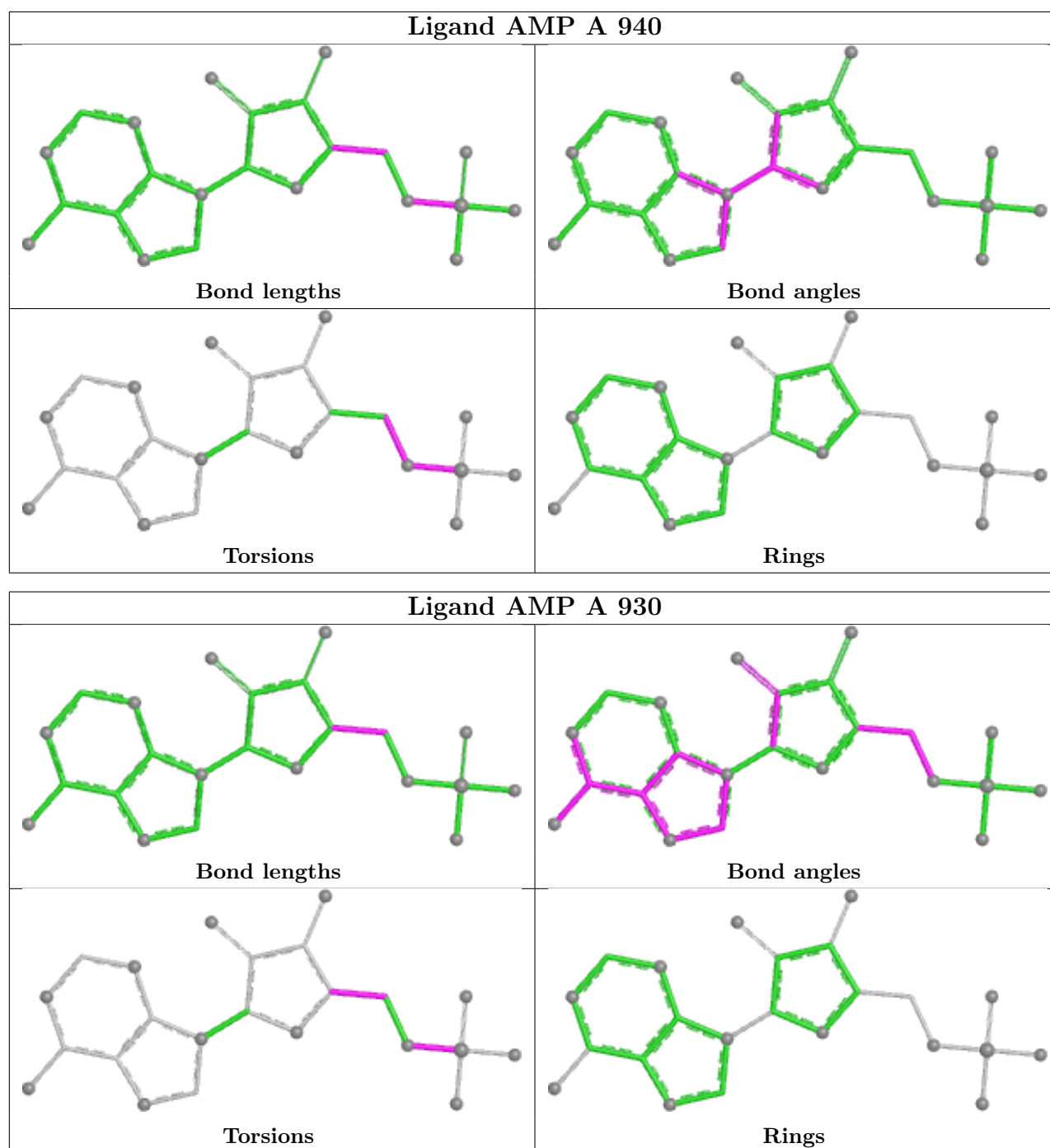
Mol	Chain	Res	Type	Atoms
2	A	999	PLP	C4-C5-C5A-O4P
3	A	940	AMP	C5'-O5'-P-O3P
3	A	930	AMP	O4'-C4'-C5'-O5'
3	A	930	AMP	C3'-C4'-C5'-O5'
3	A	940	AMP	C4'-C5'-O5'-P
3	A	930	AMP	C5'-O5'-P-O1P

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.