



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:14 AM UTC

PDB ID : 1GPY / pdb_00001gpy
Title : CRYSTALLOGRAPHIC BINDING STUDIES ON THE ALLOSTERIC INHIBITOR GLUCOSE-6-PHOSPHATE TO T STATE GLYCOGEN PHOSPHORYLASE B
Authors : Johnson, L.N.
Deposited on : 1993-03-31
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 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

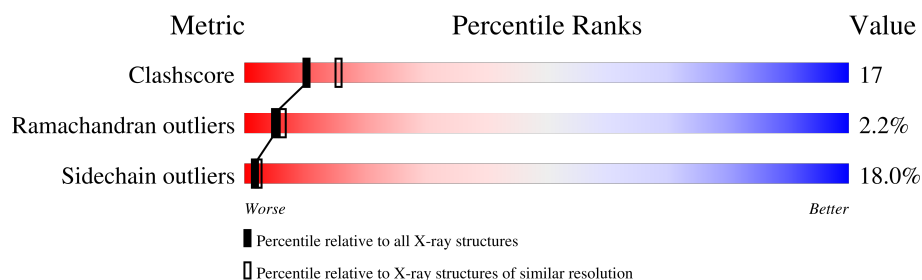
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	842	

2 Entry composition [i](#)

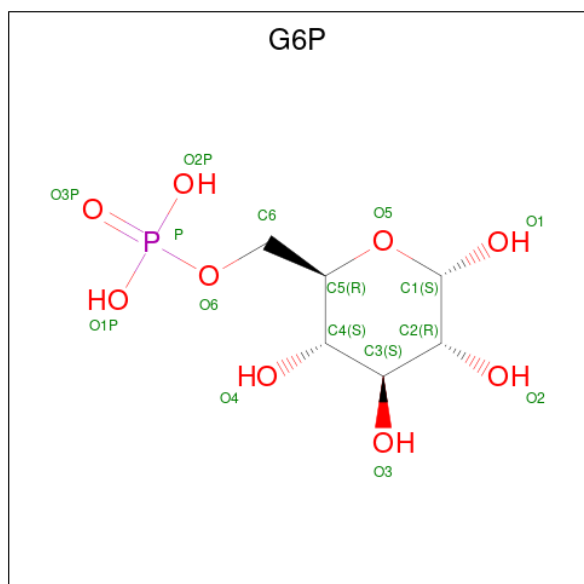
There are 4 unique types of molecules in this entry. The entry contains 7431 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

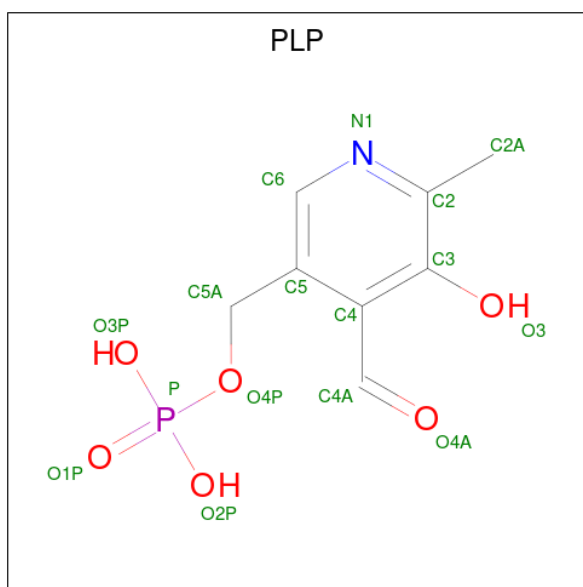
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	828	6727	4286	1186	1225	30	39	0	0

- Molecule 2 is 6-O-phosphono-alpha-D-glucopyranose (CCD ID: G6P) (formula: $C_6H_{13}O_9P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
2	A	1	16	6	9	1	0	0

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	673	Total	O	0	0
			673	673		



P794	R795	E796	W797	T798	R799	M800	V801	I802	R803	A806	T807	S808	G809	K810	T816	I817	I824	W825	G826	V827	E828	R831	Q832	R833	L834	P835	A836	P837	D838	E839	K840	I841	PRD
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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) – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.203 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7431	wwPDB-VP
Average B, all atoms (Å ²)	31.0	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: G6P, 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	1.58	62/6880 (0.9%)	2.40	447/9313 (4.8%)

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	10

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	308	ILE	C-N	33.65	1.78	1.33
1	A	309	ARG	C-N	27.68	1.73	1.33
1	A	20	GLY	C-N	16.77	1.54	1.33
1	A	17	GLY	C-N	9.64	1.46	1.33
1	A	16	ARG	NE-CZ	9.47	1.43	1.33
1	A	406	ILE	CA-CB	8.24	1.63	1.54
1	A	433	GLU	CA-CB	8.00	1.64	1.53
1	A	459	HIS	CD2-NE2	-7.93	1.29	1.37
1	A	614	HIS	CD2-NE2	-7.63	1.29	1.37
1	A	34	HIS	CD2-NE2	-7.61	1.29	1.37
1	A	341	HIS	CD2-NE2	-7.53	1.29	1.37
1	A	377	HIS	CD2-NE2	-7.43	1.29	1.37
1	A	450	HIS	CD2-NE2	-7.37	1.29	1.37
1	A	208	HIS	CD2-NE2	-7.32	1.29	1.37
1	A	656	VAL	CA-CB	7.26	1.64	1.54
1	A	371	THR	CA-CB	7.24	1.65	1.53
1	A	14	SER	CA-C	7.09	1.67	1.52
1	A	477	HIS	CD2-NE2	-7.06	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	582	HIS	CD2-NE2	-6.80	1.30	1.37
1	A	459	HIS	CG-ND1	-6.77	1.30	1.38
1	A	278	VAL	CA-CB	6.76	1.63	1.54
1	A	443	HIS	CD2-NE2	-6.75	1.30	1.37
1	A	571	HIS	CD2-NE2	-6.72	1.30	1.37
1	A	555	VAL	CA-CB	6.70	1.63	1.54
1	A	323	ARG	CZ-NH1	6.68	1.42	1.32
1	A	62	HIS	CD2-NE2	-6.66	1.30	1.37
1	A	201	HIS	CD2-NE2	-6.62	1.30	1.37
1	A	125	ILE	CA-CB	6.49	1.62	1.54
1	A	284	ASN	CA-CB	6.35	1.63	1.53
1	A	795	ARG	CA-CB	6.33	1.63	1.53
1	A	237	VAL	CA-CB	6.27	1.61	1.54
1	A	838	ASP	CA-C	6.21	1.60	1.53
1	A	836	ALA	CA-C	6.21	1.60	1.52
1	A	73	HIS	CD2-NE2	-6.17	1.31	1.37
1	A	399	HIS	CD2-NE2	-6.14	1.31	1.37
1	A	450	HIS	CG-ND1	-6.11	1.31	1.38
1	A	320	ASP	CA-CB	6.09	1.63	1.53
1	A	323	ARG	NE-CZ	6.05	1.39	1.33
1	A	817	ILE	CA-CB	5.92	1.61	1.54
1	A	36	HIS	CD2-NE2	-5.87	1.31	1.37
1	A	34	HIS	CG-ND1	-5.80	1.31	1.38
1	A	378	THR	C-N	-5.69	1.27	1.33
1	A	57	HIS	CD2-NE2	-5.65	1.31	1.37
1	A	325	ASN	CA-C	-5.64	1.45	1.52
1	A	240	THR	CA-CB	5.60	1.63	1.53
1	A	346	ILE	CA-CB	5.56	1.61	1.54
1	A	341	HIS	CG-ND1	-5.55	1.32	1.38
1	A	838	ASP	C-O	5.52	1.29	1.23
1	A	299	VAL	CA-CB	5.51	1.61	1.54
1	A	536	LYS	CA-CB	-5.40	1.44	1.53
1	A	643	ILE	CA-CB	5.36	1.60	1.54
1	A	257	PHE	CA-CB	5.33	1.59	1.52
1	A	335	ILE	CA-CB	5.33	1.63	1.55
1	A	259	VAL	CA-CB	5.28	1.61	1.54
1	A	593	GLU	CA-CB	-5.23	1.47	1.53
1	A	260	GLY	C-N	5.20	1.41	1.33
1	A	381	PRO	C-N	-5.17	1.27	1.33
1	A	367	VAL	CA-CB	5.17	1.60	1.54
1	A	767	HIS	CD2-NE2	-5.12	1.32	1.37
1	A	556	HIS	CD2-NE2	-5.11	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	22	GLU	CA-C	5.03	1.59	1.52
1	A	123	GLU	CA-CB	-5.03	1.45	1.53

All (447) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	381	PRO	O-C-N	-14.50	105.79	122.17
1	A	255	LYS	N-CA-C	14.23	131.68	108.34
1	A	763	ASN	CA-CB-CG	-11.69	100.91	112.60
1	A	696	ASN	CA-CB-CG	11.46	124.06	112.60
1	A	217	ASP	CA-CB-CG	10.87	123.47	112.60
1	A	325	ASN	N-CA-C	10.83	126.55	108.90
1	A	832	GLN	N-CA-C	10.51	123.33	110.41
1	A	43	ARG	NE-CZ-NH2	-10.48	109.77	119.20
1	A	28	LYS	CA-CB-CG	10.42	134.95	114.10
1	A	117	LEU	N-CA-C	10.24	126.33	113.43
1	A	753	LYS	CA-CB-CG	9.98	134.07	114.10
1	A	264	GLN	OE1-CD-NE2	-9.82	112.78	122.60
1	A	213	ALA	N-CA-C	-9.72	94.85	110.20
1	A	321	PRO	O-C-N	9.59	135.59	122.64
1	A	760	ASP	CA-CB-CG	9.46	122.06	112.60
1	A	253	ASN	CA-CB-CG	-9.40	103.20	112.60
1	A	423	ASP	CA-CB-CG	-9.16	103.44	112.60
1	A	457	ARG	NE-CZ-NH2	-9.09	111.02	119.20
1	A	255	LYS	N-CA-CB	-9.06	96.54	110.77
1	A	678	ASN	CA-CB-CG	9.04	121.64	112.60
1	A	338	ASN	OD1-CG-ND2	-8.92	113.68	122.60
1	A	47	THR	N-CA-CB	-8.91	99.25	110.03
1	A	252	PHE	CA-CB-CG	-8.89	104.91	113.80
1	A	552	GLU	N-CA-C	8.81	122.04	111.82
1	A	321	PRO	CA-N-CD	-8.77	99.72	112.00
1	A	754	GLN	CA-CB-CG	8.76	131.63	114.10
1	A	724	ARG	CA-CB-CG	8.76	131.61	114.10
1	A	767	HIS	CB-CG-CD2	-8.51	120.14	131.20
1	A	601	ARG	NE-CZ-NH2	-8.51	111.54	119.20
1	A	20	GLY	O-C-N	-8.50	111.64	122.70
1	A	277	ARG	CA-CB-CG	-8.47	97.17	114.10
1	A	319	ARG	N-CA-C	-8.46	92.78	110.80
1	A	527	ASP	CA-CB-CG	8.44	121.04	112.60
1	A	484	ASN	OD1-CG-ND2	-8.44	114.16	122.60
1	A	422	VAL	N-CA-CB	-8.42	101.16	110.51
1	A	51	TYR	N-CA-C	8.39	121.26	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	ARG	CA-C-O	-8.34	110.67	120.10
1	A	455	VAL	N-CA-C	8.34	120.13	112.29
1	A	43	ARG	NE-CZ-NH1	8.33	129.83	121.50
1	A	838	ASP	CA-CB-CG	8.32	120.92	112.60
1	A	235	ASN	OD1-CG-ND2	-8.29	114.31	122.60
1	A	734	ARG	O-C-N	-8.25	112.18	122.17
1	A	236	ASN	N-CA-C	8.25	123.30	113.23
1	A	579	ASN	OD1-CG-ND2	-8.22	114.38	122.60
1	A	486	ILE	CA-CB-CG1	-8.21	96.44	110.40
1	A	703	ALA	N-CA-C	8.18	122.52	112.54
1	A	284	ASN	OD1-CG-ND2	-8.13	114.47	122.60
1	A	595	ASN	OD1-CG-ND2	-8.12	114.48	122.60
1	A	318	CYS	O-C-N	8.10	130.95	123.50
1	A	211	GLN	N-CA-C	-8.04	100.53	111.87
1	A	507	ILE	N-CA-C	7.98	119.75	112.17
1	A	338	ASN	CB-CG-ND2	7.98	128.37	116.40
1	A	275	ILE	CB-CA-C	-7.94	101.42	112.14
1	A	789	ALA	N-CA-C	-7.94	102.70	111.36
1	A	558	ASN	CA-CB-CG	7.91	120.51	112.60
1	A	727	ASN	CA-CB-CG	-7.88	104.72	112.60
1	A	95	LEU	N-CA-C	7.86	119.63	111.14
1	A	754	GLN	N-CA-CB	-7.85	96.40	110.37
1	A	235	ASN	CB-CG-ND2	7.83	128.14	116.40
1	A	549	LEU	CA-C-O	-7.83	112.60	120.82
1	A	332	LYS	CG-CD-CE	7.82	129.29	111.30
1	A	187	ASN	OD1-CG-ND2	-7.76	114.83	122.60
1	A	253	ASN	CB-CG-ND2	7.70	127.95	116.40
1	A	367	VAL	N-CA-C	-7.70	103.19	110.42
1	A	314	SER	O-C-N	7.64	132.75	122.59
1	A	325	ASN	CA-CB-CG	-7.60	105.00	112.60
1	A	37	PHE	N-CA-C	7.56	119.60	111.36
1	A	315	LYS	CG-CD-CE	7.56	128.69	111.30
1	A	413	ARG	NE-CZ-NH2	-7.55	112.40	119.20
1	A	486	ILE	CA-CB-CG2	7.55	123.34	110.50
1	A	760	ASP	N-CA-CB	-7.54	98.38	110.14
1	A	464	LYS	CA-CB-CG	7.53	129.17	114.10
1	A	576	GLN	CG-CD-NE2	7.51	127.67	116.40
1	A	579	ASN	CB-CG-ND2	7.49	127.64	116.40
1	A	516	ASP	CA-CB-CG	7.47	120.07	112.60
1	A	729	GLN	CG-CD-NE2	7.46	127.58	116.40
1	A	564	ASP	CA-CB-CG	7.45	120.05	112.60
1	A	641	ARG	N-CA-C	-7.44	96.19	108.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	254	LEU	CA-C-N	-7.43	112.30	122.77
1	A	254	LEU	C-N-CA	-7.43	112.30	122.77
1	A	407	ASN	O-C-N	7.42	129.80	122.09
1	A	326	PHE	CA-CB-CG	-7.40	106.40	113.80
1	A	638	ASP	N-CA-C	7.36	121.17	112.93
1	A	253	ASN	OD1-CG-ND2	-7.36	115.25	122.60
1	A	771	PHE	CA-CB-CG	-7.35	106.45	113.80
1	A	210	SER	N-CA-C	7.35	126.46	110.80
1	A	541	ASN	OD1-CG-ND2	-7.34	115.26	122.60
1	A	321	PRO	N-CA-C	7.33	127.57	112.47
1	A	47	THR	CB-CA-C	7.33	119.41	108.86
1	A	197	THR	CA-CB-OG1	-7.32	98.62	109.60
1	A	650	VAL	CA-C-O	-7.32	113.46	121.29
1	A	270	ASN	CA-CB-CG	-7.28	105.32	112.60
1	A	367	VAL	CA-C-O	-7.28	112.74	121.18
1	A	251	ASP	CA-CB-CG	-7.27	105.33	112.60
1	A	486	ILE	N-CA-CB	-7.27	103.23	112.60
1	A	323	ARG	N-CA-C	-7.26	96.20	109.56
1	A	691	THR	O-C-N	-7.25	114.44	122.84
1	A	576	GLN	OE1-CD-NE2	-7.24	115.36	122.60
1	A	91	MET	N-CA-C	7.21	120.18	111.82
1	A	242	ARG	NE-CZ-NH2	-7.19	112.73	119.20
1	A	817	ILE	CA-C-O	-7.19	113.07	121.05
1	A	242	ARG	NE-CZ-NH1	7.12	128.62	121.50
1	A	317	GLY	N-CA-C	-7.12	103.46	115.34
1	A	371	THR	N-CA-C	-7.09	104.26	113.12
1	A	239	ASN	CA-CB-CG	7.08	119.68	112.60
1	A	322	VAL	N-CA-C	-7.08	94.62	109.34
1	A	563	PHE	CA-CB-CG	7.06	120.86	113.80
1	A	689	ILE	O-C-N	-7.05	115.46	122.93
1	A	807	THR	N-CA-CB	-7.03	99.83	110.73
1	A	324	THR	CA-CB-OG1	-7.03	99.06	109.60
1	A	754	GLN	O-C-N	-7.02	113.25	121.32
1	A	270	ASN	CB-CG-ND2	7.01	126.92	116.40
1	A	274	ASN	OD1-CG-ND2	-7.00	115.60	122.60
1	A	795	ARG	CB-CG-CD	7.00	127.39	111.30
1	A	121	GLU	CA-CB-CG	6.97	128.05	114.10
1	A	536	LYS	O-C-N	6.95	129.59	122.09
1	A	325	ASN	O-C-N	6.92	131.53	123.30
1	A	641	ARG	CA-CB-CG	6.86	127.81	114.10
1	A	216	VAL	N-CA-CB	-6.85	100.93	112.44
1	A	643	ILE	O-C-N	-6.83	115.96	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	834	LEU	N-CA-C	-6.82	100.16	110.39
1	A	713	MET	CG-SD-CE	-6.79	85.96	100.90
1	A	457	ARG	NE-CZ-NH1	6.78	128.28	121.50
1	A	759	LYS	CA-CB-CG	-6.76	100.57	114.10
1	A	29	LYS	N-CA-CB	-6.74	100.18	110.16
1	A	318	CYS	CB-CA-C	6.71	120.77	111.51
1	A	49	ARG	CA-C-O	-6.69	113.33	120.42
1	A	540	GLU	CB-CG-CD	6.69	123.97	112.60
1	A	801	VAL	CA-C-O	-6.69	114.31	121.27
1	A	308	ILE	CA-C-N	6.68	129.24	120.28
1	A	308	ILE	C-N-CA	6.68	129.24	120.28
1	A	306	ASP	CA-CB-CG	6.66	119.25	112.60
1	A	387	TRP	CG-CD2-CE3	6.65	140.55	133.90
1	A	32	ASN	N-CA-C	6.64	118.52	111.28
1	A	324	THR	CA-C-N	-6.64	113.63	122.99
1	A	324	THR	C-N-CA	-6.64	113.63	122.99
1	A	724	ARG	CD-NE-CZ	6.59	133.63	124.40
1	A	335	ILE	CB-CG1-CD1	-6.58	99.98	113.80
1	A	729	GLN	OE1-CD-NE2	-6.56	116.04	122.60
1	A	340	THR	N-CA-CB	-6.56	98.91	110.39
1	A	763	ASN	N-CA-CB	-6.55	100.47	110.16
1	A	436	VAL	N-CA-C	-6.54	95.73	109.34
1	A	282	ASN	CB-CG-ND2	-6.54	106.59	116.40
1	A	536	LYS	CB-CG-CD	-6.52	96.30	111.30
1	A	483	THR	CA-CB-OG1	-6.51	99.84	109.60
1	A	271	LEU	N-CA-C	-6.50	104.11	111.07
1	A	614	HIS	CB-CG-CD2	-6.50	122.75	131.20
1	A	399	HIS	CA-C-O	-6.49	113.67	120.55
1	A	316	PHE	N-CA-C	-6.48	106.58	114.75
1	A	480	GLN	OE1-CD-NE2	-6.47	116.12	122.60
1	A	294	LYS	CG-CD-CE	-6.45	96.46	111.30
1	A	282	ASN	OD1-CG-ND2	6.45	129.05	122.60
1	A	33	ARG	CB-CA-C	-6.44	100.77	110.88
1	A	284	ASN	CB-CG-ND2	6.43	126.04	116.40
1	A	399	HIS	CA-CB-CG	-6.43	107.37	113.80
1	A	178	GLU	CA-CB-CG	-6.40	101.29	114.10
1	A	251	ASP	CA-C-N	-6.40	110.16	122.06
1	A	251	ASP	C-N-CA	-6.40	110.16	122.06
1	A	25	THR	N-CA-CB	-6.39	100.72	110.12
1	A	120	GLU	CB-CG-CD	6.39	123.46	112.60
1	A	494	LEU	O-C-N	-6.39	115.13	122.03
1	A	114	GLN	OE1-CD-NE2	-6.38	116.22	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	390	HIS	CB-CG-CD2	-6.38	122.91	131.20
1	A	239	ASN	OD1-CG-ND2	-6.34	116.26	122.60
1	A	321	PRO	CA-C-N	6.33	133.36	121.97
1	A	321	PRO	C-N-CA	6.33	133.36	121.97
1	A	477	HIS	CB-CG-CD2	-6.33	122.97	131.20
1	A	582	HIS	CB-CG-CD2	-6.29	123.03	131.20
1	A	408	GLN	N-CA-CB	-6.28	100.27	109.82
1	A	836	ALA	O-C-N	-6.26	114.12	121.32
1	A	235	ASN	N-CA-C	6.25	122.34	113.02
1	A	118	ASP	CA-C-O	6.24	129.43	120.51
1	A	435	ALA	O-C-N	6.23	130.88	122.59
1	A	529	ALA	N-CA-C	-6.23	104.38	112.23
1	A	37	PHE	O-C-N	-6.23	115.05	122.15
1	A	368	THR	N-CA-C	6.23	118.58	111.11
1	A	253	ASN	CA-C-O	6.22	127.12	119.97
1	A	320	ASP	CA-C-N	6.21	127.60	119.84
1	A	320	ASP	C-N-CA	6.21	127.60	119.84
1	A	225	PRO	N-CA-C	6.20	121.24	111.38
1	A	399	HIS	CB-CG-CD2	-6.18	123.16	131.20
1	A	491	TRP	CG-CD2-CE3	6.18	140.08	133.90
1	A	318	CYS	N-CA-C	-6.17	96.48	107.28
1	A	549	LEU	N-CA-C	-6.17	104.47	111.07
1	A	778	GLU	CB-CA-C	-6.17	101.19	110.88
1	A	182	TRP	N-CA-C	6.13	120.49	112.89
1	A	467	ILE	N-CA-C	6.13	117.68	111.00
1	A	638	ASP	CA-C-O	6.13	127.13	119.59
1	A	452	VAL	N-CA-C	-6.12	99.54	108.11
1	A	181	ASP	N-CA-CB	-6.12	101.36	110.60
1	A	825	TRP	CG-CD2-CE3	6.12	140.02	133.90
1	A	106	ASN	CA-CB-CG	6.12	118.72	112.60
1	A	404	TYR	CA-C-O	-6.12	113.94	120.42
1	A	530	PHE	CA-CB-CG	-6.11	107.69	113.80
1	A	263	ILE	CA-C-O	-6.10	114.70	121.17
1	A	551	ARG	NE-CZ-NH2	6.08	124.67	119.20
1	A	734	ARG	CA-CB-CG	6.08	126.25	114.10
1	A	107	ALA	CA-C-O	-6.07	114.45	120.70
1	A	29	LYS	CA-CB-CG	6.07	126.24	114.10
1	A	519	ARG	CA-CB-CG	-6.06	101.98	114.10
1	A	30	ASN	CA-C-O	-6.06	113.52	120.24
1	A	31	PHE	N-CA-C	-6.04	103.86	111.11
1	A	123	GLU	CA-CB-CG	-6.03	102.03	114.10
1	A	125	ILE	CB-CG1-CD1	6.02	126.44	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	396	LEU	CA-C-N	6.02	125.50	119.24
1	A	396	LEU	C-N-CA	6.02	125.50	119.24
1	A	110	GLU	CB-CG-CD	6.02	122.83	112.60
1	A	769	ASP	N-CA-C	6.02	117.81	109.15
1	A	565	VAL	N-CA-C	6.01	116.78	108.12
1	A	576	GLN	N-CA-C	-6.00	104.86	111.82
1	A	259	VAL	O-C-N	5.99	129.79	122.72
1	A	27	LEU	CA-C-N	5.97	128.28	120.28
1	A	27	LEU	C-N-CA	5.97	128.28	120.28
1	A	764	MET	N-CA-C	-5.97	104.90	111.82
1	A	33	ARG	CA-CB-CG	5.95	126.00	114.10
1	A	551	ARG	NE-CZ-NH1	-5.95	115.55	121.50
1	A	49	ARG	N-CA-C	-5.95	104.88	111.36
1	A	681	PHE	CA-CB-CG	5.93	119.73	113.80
1	A	430	LEU	N-CA-C	-5.92	105.55	112.89
1	A	720	ARG	CB-CG-CD	-5.91	97.70	111.30
1	A	768	HIS	CB-CG-CD2	-5.91	123.52	131.20
1	A	467	ILE	CB-CA-C	-5.90	104.34	112.24
1	A	535	ALA	N-CA-C	5.88	119.71	112.54
1	A	131	LEU	N-CA-CB	-5.87	102.32	110.65
1	A	408	GLN	OE1-CD-NE2	-5.86	116.74	122.60
1	A	313	SER	CA-C-O	5.85	126.94	120.80
1	A	73	HIS	CB-CG-CD2	-5.84	123.60	131.20
1	A	270	ASN	OD1-CG-ND2	-5.84	116.76	122.60
1	A	665	GLN	CG-CD-NE2	5.84	125.16	116.40
1	A	839	GLU	CB-CG-CD	5.84	122.52	112.60
1	A	36	HIS	CB-CG-CD2	-5.83	123.62	131.20
1	A	838	ASP	N-CA-C	5.83	117.59	109.31
1	A	25	THR	CA-C-N	5.83	128.02	120.44
1	A	25	THR	C-N-CA	5.83	128.02	120.44
1	A	33	ARG	N-CA-CB	5.83	118.46	110.01
1	A	224	MET	CA-CB-CG	-5.82	102.46	114.10
1	A	16	ARG	CA-C-N	5.82	130.50	122.06
1	A	16	ARG	C-N-CA	5.82	130.50	122.06
1	A	94	THR	O-C-N	-5.81	114.71	122.49
1	A	570	ILE	CA-C-O	5.80	127.59	120.74
1	A	255	LYS	O-C-N	5.79	130.05	123.27
1	A	641	ARG	N-CA-CB	-5.79	100.78	110.80
1	A	23	ASN	N-CA-C	5.79	118.37	111.71
1	A	754	GLN	N-CA-C	-5.79	97.02	109.81
1	A	156	GLY	CA-C-O	-5.78	115.88	120.91
1	A	459	HIS	CB-CG-CD2	-5.78	123.68	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	592	LYS	CB-CG-CD	5.78	124.59	111.30
1	A	613	TYR	N-CA-C	-5.78	97.82	107.99
1	A	393	GLU	CB-CG-CD	-5.78	102.78	112.60
1	A	323	ARG	NE-CZ-NH2	-5.76	114.02	119.20
1	A	49	ARG	CA-CB-CG	5.76	125.62	114.10
1	A	26	GLU	CA-C-O	-5.75	114.79	120.82
1	A	601	ARG	CA-CB-CG	5.73	125.56	114.10
1	A	109	ASP	N-CA-C	5.73	117.60	111.36
1	A	478	LYS	CG-CD-CE	-5.72	98.15	111.30
1	A	216	VAL	CA-C-O	-5.71	115.67	121.67
1	A	250	ASN	CA-C-O	5.71	126.61	120.55
1	A	275	ILE	N-CA-CB	5.71	118.31	110.54
1	A	665	GLN	CB-CG-CD	5.71	122.31	112.60
1	A	238	VAL	CG1-CB-CG2	-5.71	98.25	110.80
1	A	789	ALA	CA-C-O	-5.71	114.37	120.42
1	A	439	ILE	CB-CG1-CD1	-5.68	101.86	113.80
1	A	654	GLU	O-C-N	-5.68	114.87	122.43
1	A	408	GLN	CG-CD-NE2	5.68	124.92	116.40
1	A	481	ASN	OD1-CG-ND2	-5.68	116.92	122.60
1	A	551	ARG	CA-CB-CG	5.68	125.46	114.10
1	A	309	ARG	O-C-N	5.67	128.13	122.12
1	A	514	ASP	CA-CB-CG	5.67	118.27	112.60
1	A	560	ASN	OD1-CG-ND2	-5.67	116.93	122.60
1	A	601	ARG	NE-CZ-NH1	5.67	127.17	121.50
1	A	554	LYS	CB-CG-CD	-5.66	98.28	111.30
1	A	18	LEU	O-C-N	5.66	129.79	122.89
1	A	264	GLN	CG-CD-NE2	5.66	124.88	116.40
1	A	256	ASP	O-C-N	-5.65	115.08	122.59
1	A	367	VAL	CG1-CB-CG2	-5.64	98.38	110.80
1	A	303	THR	N-CA-C	5.64	117.43	111.28
1	A	759	LYS	CA-C-N	5.64	132.13	121.81
1	A	759	LYS	C-N-CA	5.64	132.13	121.81
1	A	196	PHE	CA-C-O	-5.63	112.94	119.59
1	A	227	ASP	CA-CB-CG	5.63	118.23	112.60
1	A	224	MET	CG-SD-CE	5.63	113.29	100.90
1	A	641	ARG	CB-CA-C	5.63	119.89	109.70
1	A	636	VAL	CA-C-O	-5.62	114.69	120.71
1	A	370	LYS	CA-CB-CG	5.62	125.35	114.10
1	A	16	ARG	O-C-N	-5.62	114.50	122.15
1	A	377	HIS	O-C-N	-5.62	115.44	122.35
1	A	32	ASN	OD1-CG-ND2	-5.62	116.98	122.60
1	A	78	ASP	O-C-N	-5.61	114.87	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	PHE	N-CA-C	5.60	117.56	110.33
1	A	62	HIS	O-C-N	-5.59	114.75	122.46
1	A	47	THR	OG1-CB-CG2	5.58	120.46	109.30
1	A	258	ASN	CA-C-N	-5.58	113.34	121.71
1	A	258	ASN	C-N-CA	-5.58	113.34	121.71
1	A	474	LEU	N-CA-C	-5.58	104.60	111.40
1	A	250	ASN	CA-CB-CG	-5.57	107.03	112.60
1	A	807	THR	CA-CB-OG1	-5.57	101.25	109.60
1	A	778	GLU	N-CA-CB	5.56	118.07	110.01
1	A	470	ASP	CA-C-N	5.56	128.18	120.29
1	A	470	ASP	C-N-CA	5.56	128.18	120.29
1	A	257	PHE	CA-C-O	5.56	130.66	122.38
1	A	542	LYS	CA-C-N	5.55	128.18	120.29
1	A	542	LYS	C-N-CA	5.55	128.18	120.29
1	A	399	HIS	CB-CG-ND1	5.55	131.03	122.70
1	A	541	ASN	CB-CG-ND2	5.55	124.73	116.40
1	A	238	VAL	CA-C-O	5.54	125.16	120.22
1	A	716	GLU	N-CA-C	5.54	118.03	111.33
1	A	141	ALA	CA-C-N	5.52	127.67	120.28
1	A	141	ALA	C-N-CA	5.52	127.67	120.28
1	A	534	VAL	CA-C-O	-5.51	115.32	121.05
1	A	767	HIS	O-C-N	-5.50	116.52	122.19
1	A	322	VAL	CA-CB-CG2	-5.50	101.05	110.40
1	A	284	ASN	CA-CB-CG	5.50	118.10	112.60
1	A	627	GLY	O-C-N	-5.50	116.91	122.19
1	A	455	VAL	N-CA-CB	-5.50	104.06	112.15
1	A	610	ALA	CA-C-N	5.50	126.71	119.84
1	A	610	ALA	C-N-CA	5.50	126.71	119.84
1	A	280	TYR	CA-C-N	5.49	126.70	119.84
1	A	280	TYR	C-N-CA	5.49	126.70	119.84
1	A	793	ASN	CA-C-N	5.49	125.32	119.28
1	A	793	ASN	C-N-CA	5.49	125.32	119.28
1	A	565	VAL	CA-C-O	5.48	126.17	120.36
1	A	597	PHE	CA-C-N	5.47	130.68	122.75
1	A	597	PHE	C-N-CA	5.47	130.68	122.75
1	A	318	CYS	N-CA-CB	-5.47	102.50	111.74
1	A	558	ASN	CA-C-N	5.45	126.65	119.84
1	A	558	ASN	C-N-CA	5.45	126.65	119.84
1	A	446	ILE	CA-C-N	5.44	127.51	120.44
1	A	446	ILE	C-N-CA	5.44	127.51	120.44
1	A	839	GLU	CA-C-N	-5.44	114.69	123.23
1	A	839	GLU	C-N-CA	-5.44	114.69	123.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	676	THR	N-CA-C	-5.43	107.91	114.75
1	A	836	ALA	N-CA-CB	-5.43	100.70	110.37
1	A	452	VAL	O-C-N	-5.43	117.40	123.26
1	A	365	TRP	CA-C-N	5.42	127.49	120.44
1	A	365	TRP	C-N-CA	5.42	127.49	120.44
1	A	650	VAL	CG1-CB-CG2	-5.42	98.88	110.80
1	A	684	ASN	OD1-CG-ND2	-5.42	117.18	122.60
1	A	532	ARG	CA-CB-CG	5.42	124.93	114.10
1	A	477	HIS	CB-CG-ND1	5.41	130.82	122.70
1	A	445	CYS	O-C-N	-5.41	116.50	122.07
1	A	642	VAL	CB-CA-C	-5.40	103.10	110.77
1	A	418	PHE	CA-C-N	5.40	126.59	119.84
1	A	418	PHE	C-N-CA	5.40	126.59	119.84
1	A	407	ASN	OD1-CG-ND2	-5.40	117.20	122.60
1	A	32	ASN	CA-C-O	-5.39	114.83	120.55
1	A	292	ARG	CB-CG-CD	5.39	123.70	111.30
1	A	828	GLU	CB-CG-CD	5.39	121.76	112.60
1	A	208	HIS	CB-CG-CD2	-5.38	124.20	131.20
1	A	793	ASN	CA-C-O	5.37	126.20	120.08
1	A	763	ASN	N-CA-C	5.37	117.21	111.36
1	A	300	VAL	N-CA-C	5.37	115.46	110.42
1	A	645	LEU	CA-C-N	5.36	128.38	120.82
1	A	645	LEU	C-N-CA	5.36	128.38	120.82
1	A	477	HIS	CA-CB-CG	5.36	119.16	113.80
1	A	710	ILE	CA-CB-CG2	-5.36	101.39	110.50
1	A	257	PHE	CA-CB-CG	5.35	119.15	113.80
1	A	824	ILE	O-C-N	-5.35	117.86	121.98
1	A	719	ASP	CB-CA-C	-5.34	102.50	110.88
1	A	787	VAL	N-CA-CB	-5.33	104.31	110.55
1	A	778	GLU	O-C-N	5.33	127.56	122.07
1	A	649	ARG	NE-CZ-NH2	-5.33	114.41	119.20
1	A	16	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	A	389	VAL	CB-CA-C	-5.32	105.07	112.04
1	A	63	LEU	CA-C-O	5.31	125.75	119.48
1	A	490	ARG	N-CA-C	5.31	117.75	111.33
1	A	571	HIS	ND1-CG-CD2	5.31	111.41	106.10
1	A	544	LYS	N-CA-C	-5.30	105.19	110.97
1	A	15	VAL	O-C-N	5.30	129.20	122.57
1	A	365	TRP	CE2-CD2-CG	-5.30	100.84	107.20
1	A	309	ARG	NE-CZ-NH2	5.30	123.97	119.20
1	A	311	PHE	CA-C-O	-5.28	112.95	120.51
1	A	710	ILE	CA-CB-CG1	5.28	119.38	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	743	GLU	CA-CB-CG	-5.28	103.55	114.10
1	A	70	THR	CA-C-O	-5.26	114.92	120.55
1	A	387	TRP	CE2-CD2-CG	-5.26	100.88	107.20
1	A	215	TRP	CE2-CD2-CG	-5.26	100.89	107.20
1	A	593	GLU	N-CA-CB	-5.26	102.68	110.99
1	A	310	ARG	N-CA-C	-5.25	105.23	111.69
1	A	734	ARG	CG-CD-NE	5.25	123.56	112.00
1	A	174	TRP	CE2-CD2-CG	-5.25	100.90	107.20
1	A	469	LYS	CA-C-O	-5.24	115.31	120.82
1	A	412	ASN	CA-CB-CG	5.24	117.84	112.60
1	A	767	HIS	CB-CG-ND1	5.24	130.55	122.70
1	A	597	PHE	O-C-N	5.23	129.27	122.89
1	A	779	GLU	CB-CG-CD	-5.23	103.71	112.60
1	A	224	MET	CA-C-N	5.23	125.13	119.85
1	A	224	MET	C-N-CA	5.23	125.13	119.85
1	A	400	LEU	CA-C-O	-5.23	112.95	119.38
1	A	20	GLY	CA-C-N	5.23	127.25	120.56
1	A	20	GLY	C-N-CA	5.23	127.25	120.56
1	A	258	ASN	N-CA-C	5.22	117.45	109.62
1	A	421	ASP	CA-CB-CG	5.21	117.81	112.60
1	A	566	GLN	OE1-CD-NE2	-5.21	117.39	122.60
1	A	90	TYR	CA-CB-CG	5.20	123.27	113.90
1	A	169	LYS	CA-C-N	-5.19	116.75	123.19
1	A	169	LYS	C-N-CA	-5.19	116.75	123.19
1	A	684	ASN	CA-CB-CG	-5.19	107.41	112.60
1	A	740	GLN	OE1-CD-NE2	-5.19	117.41	122.60
1	A	244	TRP	CE2-CD2-CG	-5.18	100.98	107.20
1	A	370	LYS	CG-CD-CE	5.18	123.23	111.30
1	A	244	TRP	CG-CD2-CE3	5.18	139.08	133.90
1	A	472	TYR	N-CA-CB	-5.18	102.50	110.12
1	A	22	GLU	CA-C-O	5.17	126.25	120.82
1	A	136	LEU	CD1-CG-CD2	-5.16	99.44	110.80
1	A	777	TYR	CA-C-O	-5.16	115.38	120.70
1	A	208	HIS	CA-C-N	5.16	129.71	122.79
1	A	208	HIS	C-N-CA	5.16	129.71	122.79
1	A	216	VAL	O-C-N	5.15	128.76	123.04
1	A	422	VAL	O-C-N	-5.15	116.79	121.94
1	A	208	HIS	CB-CG-ND1	5.14	130.42	122.70
1	A	259	VAL	N-CA-C	-5.13	102.23	109.21
1	A	377	HIS	CB-CG-CD2	-5.13	124.53	131.20
1	A	533	ASP	N-CA-C	-5.13	105.14	111.40
1	A	376	ASN	OD1-CG-ND2	-5.13	117.47	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	712	GLY	O-C-N	5.13	127.78	122.91
1	A	753	LYS	N-CA-CB	5.12	119.15	110.49
1	A	629	VAL	N-CA-CB	-5.12	104.49	110.64
1	A	386	ARG	CA-CB-CG	5.12	124.34	114.10
1	A	266	VAL	N-CA-C	-5.12	105.42	111.00
1	A	365	TRP	CG-CD2-CE3	5.12	139.02	133.90
1	A	168	GLN	CA-C-O	5.11	125.95	120.38
1	A	782	LYS	CA-C-O	-5.11	115.44	120.70
1	A	197	THR	CA-CB-CG2	5.11	119.18	110.50
1	A	634	PRO	N-CA-C	-5.11	107.48	113.86
1	A	334	ALA	CA-C-O	-5.10	114.01	120.28
1	A	149	THR	CA-CB-OG1	-5.09	101.96	109.60
1	A	100	VAL	N-CA-CB	-5.09	105.07	110.62
1	A	424	ARG	NE-CZ-NH2	-5.08	114.63	119.20
1	A	431	VAL	CA-C-N	5.08	129.34	122.19
1	A	431	VAL	C-N-CA	5.08	129.34	122.19
1	A	313	SER	O-C-N	5.07	127.99	122.11
1	A	79	PRO	CA-N-CD	-5.07	104.90	112.00
1	A	642	VAL	N-CA-CB	5.06	118.22	111.64
1	A	522	LEU	O-C-N	-5.06	116.05	122.27
1	A	640	LEU	CA-C-O	5.05	125.93	120.32
1	A	67	TRP	CE2-CD2-CG	-5.05	101.14	107.20
1	A	277	ARG	CB-CG-CD	5.04	122.89	111.30
1	A	381	PRO	CA-C-N	5.03	130.35	120.99
1	A	381	PRO	C-N-CA	5.03	130.35	120.99
1	A	491	TRP	CB-CG-CD1	-5.03	119.36	126.90
1	A	21	VAL	CA-C-O	-5.02	115.47	121.05
1	A	387	TRP	CB-CG-CD1	-5.02	119.37	126.90
1	A	710	ILE	CG1-CB-CG2	-5.01	95.67	110.70
1	A	487	THR	CA-CB-CG2	5.01	119.01	110.50
1	A	106	ASN	CB-CA-C	-5.00	102.34	110.85
1	A	431	VAL	CA-C-O	-5.00	114.81	120.66
1	A	438	ARG	CB-CG-CD	-5.00	99.80	111.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	16	ARG	Mainchain
1	A	185	TYR	Sidechain
1	A	20	GLY	Mainchain
1	A	318	CYS	Mainchain

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Mol	Chain	Res	Type	Group
1	A	381	PRO	Mainchain
1	A	472	TYR	Sidechain
1	A	51	TYR	Sidechain
1	A	777	TYR	Sidechain
1	A	831	ARG	Sidechain
1	A	840	LYS	Mainchain

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	6727	0	6655	228	2
2	A	16	0	11	2	0
3	A	15	0	6	0	0
4	A	673	0	0	34	2
All	All	7431	0	6672	228	2

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 17.

All (228) 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:309:ARG:C	1:A:310:ARG:N	1.73	1.46
1:A:308:ILE:C	1:A:309:ARG:N	1.78	1.42
1:A:841:ILE:CB	4:A:1672:HOH:O	1.77	1.29
1:A:67:TRP:HE1	1:A:240:THR:HG22	1.35	0.91
1:A:730:GLU:O	1:A:734:ARG:HB2	1.78	0.83
1:A:225:PRO:HB2	1:A:242:ARG:HD2	1.65	0.79
1:A:756:ASP:HA	1:A:759:LYS:HD3	1.65	0.79
1:A:528:GLU:HG3	1:A:532:ARG:HH12	1.48	0.78
1:A:833:ARG:HD2	1:A:833:ARG:N	1.99	0.78
1:A:309:ARG:NH2	1:A:310:ARG:HG3	2.00	0.77
1:A:437:LYS:HE2	4:A:1540:HOH:O	1.86	0.76
1:A:528:GLU:HG3	1:A:532:ARG:NH1	2.01	0.75
1:A:309:ARG:HH21	1:A:310:ARG:HG3	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:794:PRO:HG3	4:A:1640:HOH:O	1.86	0.75
1:A:593:GLU:HG2	1:A:596:LYS:HE3	1.68	0.75
1:A:703:ALA:HA	1:A:807:THR:HG21	1.70	0.72
1:A:316:PHE:HA	1:A:319:ARG:HE	1.54	0.71
1:A:304:LEU:HD23	1:A:307:ILE:HD12	1.73	0.70
1:A:322:VAL:HG13	1:A:323:ARG:H	1.57	0.69
1:A:30:ASN:HB2	1:A:58:THR:HG23	1.76	0.68
1:A:47:THR:HG21	4:A:1564:HOH:O	1.95	0.66
1:A:340:THR:HG22	1:A:385:GLU:OE1	1.96	0.65
1:A:833:ARG:HD2	1:A:833:ARG:H	1.60	0.65
1:A:82:ILE:HD11	1:A:827:VAL:HG21	1.79	0.65
1:A:314:SER:O	1:A:316:PHE:HB2	1.99	0.63
1:A:405:GLU:HA	1:A:408:GLN:HE21	1.64	0.63
1:A:548:TYR:CE2	1:A:552:GLU:HG3	2.33	0.62
1:A:138:ARG:HB3	4:A:1507:HOH:O	1.99	0.62
1:A:651:SER:O	1:A:655:LYS:HD2	2.00	0.62
1:A:252:PHE:CE1	1:A:256:ASP:HB2	2.34	0.62
1:A:196:PHE:CE1	1:A:309:ARG:NH1	2.67	0.62
1:A:256:ASP:HB3	1:A:258:ASN:CG	2.25	0.62
1:A:392:LEU:HB3	1:A:400:LEU:HG	1.81	0.61
1:A:309:ARG:C	1:A:310:ARG:CA	2.70	0.61
1:A:506:ARG:HG3	1:A:506:ARG:HH11	1.65	0.60
1:A:75:TYR:CZ	1:A:315:LYS:HE3	2.37	0.60
1:A:304:LEU:HD12	1:A:348:GLU:HG3	1.82	0.60
1:A:322:VAL:HG13	1:A:323:ARG:N	2.17	0.60
1:A:251:ASP:HB2	1:A:255:LYS:NZ	2.17	0.59
1:A:255:LYS:NZ	1:A:255:LYS:HB3	2.18	0.59
1:A:424:ARG:HH22	1:A:473:GLU:CD	2.10	0.59
1:A:404:TYR:O	1:A:408:GLN:HB2	2.03	0.59
1:A:335:ILE:HD11	1:A:337:LEU:HD13	1.84	0.59
1:A:252:PHE:CZ	1:A:256:ASP:HB2	2.38	0.59
1:A:404:TYR:HB3	4:A:1261:HOH:O	2.03	0.59
1:A:405:GLU:O	1:A:408:GLN:HB3	2.03	0.59
1:A:466:THR:O	1:A:469:LYS:HD2	2.00	0.59
1:A:204:GLY:HA3	1:A:218:THR:HG22	1.85	0.59
1:A:256:ASP:HB3	1:A:258:ASN:ND2	2.18	0.58
1:A:256:ASP:HB3	1:A:258:ASN:OD1	2.04	0.58
1:A:703:ALA:CA	1:A:807:THR:HG21	2.33	0.57
1:A:641:ARG:HG3	1:A:643:ILE:HD11	1.86	0.57
1:A:77:LYS:HD3	4:A:1567:HOH:O	2.04	0.57
1:A:582:HIS:HB2	1:A:780:TYR:HE2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:VAL:HG11	1:A:325:ASN:HB2	1.86	0.57
1:A:710:ILE:HD12	1:A:710:ILE:H	1.69	0.57
1:A:250:ASN:HA	1:A:269:ARG:HH12	1.69	0.56
1:A:319:ARG:NH2	1:A:320:ASP:HA	2.19	0.56
1:A:423:ASP:O	1:A:426:ARG:HG3	2.05	0.56
1:A:335:ILE:HD11	1:A:337:LEU:CD1	2.36	0.56
1:A:309:ARG:CA	1:A:310:ARG:N	2.65	0.56
1:A:514:ASP:HB2	1:A:831:ARG:NH2	2.20	0.56
1:A:227:ASP:OD1	1:A:242:ARG:HD3	2.05	0.56
1:A:207:GLU:HG2	1:A:214:LYS:HB3	1.87	0.55
1:A:321:PRO:O	1:A:322:VAL:HG12	2.06	0.55
1:A:65:GLY:O	1:A:69:ARG:HB2	2.06	0.55
1:A:692:MET:HE3	1:A:697:VAL:HG13	1.88	0.55
1:A:548:TYR:HA	1:A:551:ARG:HG3	1.88	0.55
1:A:548:TYR:HA	1:A:551:ARG:CG	2.37	0.55
1:A:303:THR:O	1:A:307:ILE:HG13	2.07	0.54
1:A:502:ILE:HA	1:A:505:GLU:HG3	1.88	0.54
1:A:582:HIS:HB2	1:A:780:TYR:CE2	2.42	0.54
1:A:831:ARG:O	1:A:833:ARG:NH1	2.40	0.54
1:A:225:PRO:CB	1:A:242:ARG:HD2	2.38	0.54
1:A:458:ILE:O	1:A:462:ILE:HG12	2.07	0.54
1:A:285:PHE:HE1	1:A:382:GLU:HB2	1.73	0.54
1:A:285:PHE:CE1	1:A:382:GLU:HB2	2.43	0.53
1:A:355:ASP:OD2	1:A:398:ARG:HD2	2.08	0.53
1:A:255:LYS:HB3	1:A:255:LYS:HZ2	1.74	0.53
1:A:706:GLU:H	1:A:706:GLU:CD	2.16	0.53
1:A:711:PHE:CE2	1:A:780:TYR:HB2	2.44	0.53
1:A:532:ARG:O	1:A:536:LYS:HG3	2.09	0.53
1:A:308:ILE:HG22	1:A:312:LYS:HD2	1.91	0.53
1:A:178:GLU:HG2	4:A:1584:HOH:O	2.10	0.52
1:A:516:ASP:HA	1:A:809:GLY:HA3	1.90	0.52
1:A:20:GLY:C	4:A:1204:HOH:O	2.53	0.52
1:A:183:LEU:CD2	1:A:187:ASN:HB2	2.40	0.52
1:A:312:LYS:HE2	4:A:1090:HOH:O	2.11	0.51
1:A:69:ARG:NH2	1:A:834:LEU:HD11	2.25	0.51
1:A:166:PHE:CE2	1:A:611:PRO:HD3	2.46	0.51
1:A:375:THR:HG23	1:A:453:ASN:HD21	1.75	0.51
1:A:753:LYS:HB3	4:A:1094:HOH:O	2.11	0.51
1:A:47:THR:O	1:A:50:ASP:HB2	2.11	0.51
1:A:166:PHE:HE2	1:A:611:PRO:HD3	1.76	0.51
1:A:319:ARG:NE	1:A:319:ARG:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:LYS:HE2	1:A:824:ILE:HD11	1.92	0.50
1:A:532:ARG:HH11	1:A:532:ARG:HG3	1.76	0.50
1:A:544:LYS:HD2	4:A:1222:HOH:O	2.09	0.50
1:A:569:ARG:HD2	1:A:608:LYS:O	2.11	0.50
1:A:497:PRO:HB3	4:A:1416:HOH:O	2.12	0.50
1:A:43:ARG:CZ	4:A:1002:HOH:O	2.59	0.50
1:A:322:VAL:C	1:A:323:ARG:HD2	2.37	0.50
1:A:490:ARG:HA	1:A:494:LEU:HB3	1.93	0.50
1:A:647:ASN:O	1:A:649:ARG:HG2	2.11	0.50
1:A:831:ARG:HG3	4:A:1268:HOH:O	2.10	0.50
1:A:529:ALA:HA	1:A:532:ARG:HD2	1.94	0.50
1:A:93:ARG:HD3	1:A:126:GLU:O	2.12	0.50
1:A:455:VAL:H	1:A:459:HIS:HD2	1.58	0.50
1:A:361:TRP:CZ3	1:A:409:ARG:HD2	2.47	0.50
1:A:82:ILE:CD1	1:A:827:VAL:HG21	2.41	0.49
1:A:157:TYR:OH	1:A:310:ARG:NH2	2.44	0.49
1:A:117:LEU:HD11	4:A:1002:HOH:O	2.11	0.49
1:A:417:ALA:C	1:A:419:PRO:HD3	2.38	0.49
1:A:569:ARG:O	1:A:574:LYS:HD3	2.13	0.49
1:A:93:ARG:HD2	1:A:126:GLU:HB3	1.95	0.49
1:A:386:ARG:NH2	4:A:1180:HOH:O	2.45	0.49
1:A:754:GLN:NE2	1:A:757:LEU:HD13	2.28	0.49
1:A:365:TRP:CH2	1:A:448:GLY:HA2	2.47	0.48
1:A:405:GLU:HA	1:A:408:GLN:NE2	2.29	0.48
1:A:732:TYR:CZ	1:A:739:ARG:HG3	2.48	0.48
1:A:91:MET:HB2	1:A:129:ALA:HB3	1.96	0.48
1:A:110:GLU:OE2	1:A:114:GLN:NE2	2.46	0.48
1:A:250:ASN:HA	1:A:269:ARG:NH1	2.27	0.48
1:A:486:ILE:CD1	1:A:676:THR:HB	2.44	0.48
1:A:515:LEU:HB3	1:A:809:GLY:HA2	1.95	0.48
1:A:490:ARG:HD2	4:A:1385:HOH:O	2.13	0.48
1:A:834:LEU:HD12	1:A:835:PRO:HD3	1.96	0.47
1:A:193:ARG:NH2	2:A:998:G6P:H2	2.29	0.47
1:A:316:PHE:O	1:A:320:ASP:HA	2.14	0.47
1:A:254:LEU:N	1:A:254:LEU:HD12	2.29	0.47
1:A:565:VAL:HG23	1:A:567:VAL:HG13	1.95	0.47
1:A:511:TYR:HA	1:A:514:ASP:O	2.14	0.47
1:A:698:GLU:O	1:A:702:GLU:HB2	2.15	0.46
1:A:66:ARG:HD2	1:A:837:PRO:HB3	1.97	0.46
1:A:558:ASN:HB2	1:A:638:ASP:OD2	2.16	0.46
1:A:184:ARG:HH11	1:A:184:ARG:HB3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:592:LYS:NZ	1:A:593:GLU:OE2	2.48	0.46
1:A:593:GLU:O	1:A:596:LYS:HG2	2.15	0.46
1:A:36:HIS:O	1:A:40:VAL:HA	2.16	0.46
1:A:723:GLN:HB2	4:A:1518:HOH:O	2.16	0.46
1:A:698:GLU:HB3	1:A:810:LYS:NZ	2.31	0.46
1:A:726:TYR:OH	1:A:774:PHE:HB2	2.16	0.46
1:A:338:ASN:OD1	1:A:377:HIS:NE2	2.49	0.46
1:A:146:SER:O	1:A:150:LEU:HG	2.17	0.45
1:A:20:GLY:O	1:A:24:VAL:HG23	2.17	0.45
1:A:236:ASN:HB3	1:A:836:ALA:HB3	1.98	0.45
1:A:358:ARG:HG2	1:A:358:ARG:HH11	1.82	0.45
1:A:33:ARG:HA	4:A:1560:HOH:O	2.16	0.45
1:A:455:VAL:H	1:A:459:HIS:CD2	2.34	0.45
1:A:521:LEU:HB2	1:A:806:ALA:HB2	1.99	0.45
1:A:408:GLN:HG2	4:A:1189:HOH:O	2.16	0.45
1:A:170:ILE:HA	1:A:174:TRP:O	2.17	0.45
1:A:795:ARG:O	1:A:799:ARG:HG3	2.17	0.45
1:A:181:ASP:HB3	1:A:184:ARG:NH2	2.32	0.44
1:A:793:ASN:HA	1:A:794:PRO:HD3	1.60	0.44
1:A:423:ASP:O	1:A:427:ARG:HG3	2.17	0.44
1:A:502:ILE:O	1:A:506:ARG:HD3	2.17	0.44
1:A:547:ALA:O	1:A:550:GLU:N	2.51	0.44
1:A:561:SER:HB2	1:A:601:ARG:HA	1.98	0.44
1:A:343:SER:HB3	1:A:445:CYS:SG	2.58	0.44
1:A:461:GLU:OE1	1:A:465:LYS:NZ	2.51	0.44
1:A:21:VAL:HG13	1:A:22:GLU:N	2.33	0.44
1:A:515:LEU:O	1:A:518:LEU:HB2	2.18	0.44
1:A:593:GLU:HB3	1:A:596:LYS:HG2	1.98	0.44
1:A:424:ARG:NH2	1:A:470:ASP:HA	2.32	0.44
1:A:57:HIS:HE1	4:A:1007:HOH:O	2.01	0.44
1:A:483:THR:O	1:A:816:THR:HG23	2.17	0.44
1:A:502:ILE:HD13	1:A:533:ASP:HB3	2.00	0.43
1:A:562:LEU:HD21	1:A:662:LEU:HB2	2.00	0.43
1:A:566:GLN:HA	4:A:1364:HOH:O	2.17	0.43
1:A:166:PHE:CD1	1:A:177:GLU:HB3	2.54	0.43
1:A:205:ARG:HG3	1:A:216:VAL:HG12	2.01	0.43
1:A:373:ALA:HB1	4:A:1255:HOH:O	2.18	0.43
1:A:118:ASP:HA	4:A:1419:HOH:O	2.18	0.43
1:A:678:ASN:HB2	1:A:699:MET:SD	2.58	0.43
1:A:589:ARG:NH1	1:A:737:GLU:OE1	2.52	0.43
1:A:544:LYS:NZ	4:A:1142:HOH:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:817:ILE:HD13	1:A:817:ILE:HA	1.91	0.43
1:A:160:ARG:HB2	1:A:243:LEU:HB3	1.99	0.43
1:A:605:ILE:O	1:A:644:PHE:HA	2.18	0.43
1:A:177:GLU:OE1	1:A:611:PRO:HG3	2.18	0.43
1:A:251:ASP:HB2	1:A:255:LYS:HZ2	1.83	0.43
1:A:328:ALA:HB2	4:A:1446:HOH:O	2.19	0.43
1:A:375:THR:HG23	1:A:453:ASN:ND2	2.33	0.43
1:A:767:HIS:HB2	1:A:768:HIS:CE1	2.54	0.43
1:A:501:GLU:O	1:A:505:GLU:HG3	2.19	0.42
1:A:234:ARG:NH1	4:A:1570:HOH:O	2.45	0.42
1:A:251:ASP:CG	1:A:252:PHE:N	2.76	0.42
1:A:459:HIS:O	1:A:463:LEU:HG	2.19	0.42
1:A:517:GLN:O	1:A:520:LYS:HG3	2.20	0.42
1:A:487:THR:HG23	1:A:490:ARG:HB3	2.02	0.42
1:A:759:LYS:O	1:A:763:ASN:HB2	2.18	0.42
1:A:421:ASP:O	1:A:425:LEU:HD13	2.19	0.42
1:A:533:ASP:HA	1:A:536:LYS:HE2	2.02	0.42
1:A:591:LYS:HD3	1:A:633:ASP:OD2	2.20	0.42
1:A:263:ILE:O	1:A:267:LEU:HG	2.20	0.42
1:A:359:LEU:HD23	1:A:359:LEU:HA	1.82	0.42
1:A:486:ILE:HG12	1:A:680:LYS:HG2	2.02	0.42
1:A:309:ARG:HE	1:A:309:ARG:HB3	1.24	0.41
1:A:340:THR:HG23	1:A:441:MET:HB3	2.01	0.41
1:A:484:ASN:ND2	4:A:1046:HOH:O	2.52	0.41
1:A:648:TYR:HA	1:A:652:LEU:HD23	2.01	0.41
1:A:549:LEU:HB3	1:A:550:GLU:OE1	2.20	0.41
1:A:330:PRO:HD3	1:A:367:VAL:HG13	2.01	0.41
1:A:457:ARG:HH22	1:A:701:GLU:CD	2.29	0.41
1:A:803:ARG:O	1:A:807:THR:HB	2.20	0.41
1:A:256:ASP:HB3	1:A:258:ASN:HD21	1.86	0.41
1:A:379:VAL:HG12	4:A:1649:HOH:O	2.20	0.41
1:A:275:ILE:HD12	1:A:294:LYS:HB3	2.01	0.41
1:A:103:ALA:HB2	1:A:234:ARG:HD2	2.02	0.41
1:A:63:LEU:C	1:A:63:LEU:HD23	2.46	0.41
1:A:754:GLN:OE1	1:A:757:LEU:HB2	2.20	0.41
1:A:344:LEU:HD22	4:A:1609:HOH:O	2.20	0.41
1:A:242:ARG:NH2	2:A:998:G6P:O3P	2.49	0.40
1:A:292:ARG:NH2	4:A:1408:HOH:O	2.53	0.40
1:A:548:TYR:CD1	1:A:548:TYR:C	2.99	0.40
1:A:593:GLU:HG2	1:A:596:LYS:CE	2.45	0.40
1:A:353:LEU:HB3	1:A:359:LEU:HD12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:ARG:NH1	1:A:552:GLU:CD	2.79	0.40
1:A:553:TYR:O	1:A:554:LYS:HG3	2.21	0.40
1:A:685:GLY:HA2	4:A:1650:HOH:O	2.21	0.40
1:A:117:LEU:HD21	4:A:1002:HOH:O	2.21	0.40
1:A:172:GLY:O	1:A:621:LYS:NZ	2.55	0.40
1:A:323:ARG:N	1:A:323:ARG:HD2	2.36	0.40
1:A:754:GLN:CD	1:A:757:LEU:HD13	2.47	0.40
1:A:83:TYR:CE2	1:A:333:VAL:HG13	2.57	0.40
1:A:251:ASP:HB2	1:A:255:LYS:HZ1	1.85	0.40
1:A:445:CYS:O	1:A:449:SER:HB2	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ALA:O	4:A:1064:HOH:O[7_556]	1.76	0.44
1:A:111:ALA:CB	4:A:1064:HOH:O[7_556]	2.13	0.07

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	826/842 (98%)	746 (90%)	62 (8%)	18 (2%)	5 6

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	GLY
1	A	321	PRO
1	A	322	VAL
1	A	324	THR
1	A	555	VAL

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Mol	Chain	Res	Type
1	A	837	PRO
1	A	312	LYS
1	A	320	ASP
1	A	436	VAL
1	A	705	GLU
1	A	203	TYR
1	A	435	ALA
1	A	611	PRO
1	A	260	GLY
1	A	319	ARG
1	A	489	ARG
1	A	15	VAL
1	A	835	PRO

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	715/731 (98%)	586 (82%)	129 (18%)	2 2

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	SER
1	A	18	LEU
1	A	23	ASN
1	A	26	GLU
1	A	29	LYS
1	A	38	THR
1	A	48	PRO
1	A	55	LEU
1	A	60	ARG
1	A	63	LEU
1	A	64	VAL
1	A	69	ARG
1	A	76	GLU

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Mol	Chain	Res	Type
1	A	77	LYS
1	A	82	ILE
1	A	85	LEU
1	A	102	LEU
1	A	110	GLU
1	A	114	GLN
1	A	127	GLU
1	A	131	LEU
1	A	138	ARG
1	A	144	LEU
1	A	152	LEU
1	A	159	ILE
1	A	165	ILE
1	A	170	ILE
1	A	176	MET
1	A	177	GLU
1	A	191	LYS
1	A	198	LEU
1	A	209	THR
1	A	211	GLN
1	A	214	LYS
1	A	216	VAL
1	A	217	ASP
1	A	224	MET
1	A	234	ARG
1	A	235	ASN
1	A	242	ARG
1	A	243	LEU
1	A	250	ASN
1	A	255	LYS
1	A	259	VAL
1	A	285	PHE
1	A	292	ARG
1	A	305	GLN
1	A	309	ARG
1	A	316	PHE
1	A	318	CYS
1	A	319	ARG
1	A	320	ASP
1	A	321	PRO
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	360	ASP
1	A	363	LYS
1	A	384	LEU
1	A	390	HIS
1	A	398	ARG
1	A	400	LEU
1	A	405	GLU
1	A	411	LEU
1	A	426	ARG
1	A	430	LEU
1	A	433	GLU
1	A	444	LEU
1	A	467	ILE
1	A	469	LYS
1	A	474	LEU
1	A	486	ILE
1	A	501	GLU
1	A	506	ARG
1	A	510	GLU
1	A	513	SER
1	A	515	LEU
1	A	519	ARG
1	A	522	LEU
1	A	523	SER
1	A	539	GLN
1	A	543	LEU
1	A	548	TYR
1	A	549	LEU
1	A	550	GLU
1	A	556	HIS
1	A	565	VAL
1	A	568	LYS
1	A	576	GLN
1	A	586	LEU
1	A	593	GLU
1	A	596	LYS
1	A	598	VAL
1	A	611	PRO
1	A	622	LEU
1	A	638	ASP

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Mol	Chain	Res	Type
1	A	641	ARG
1	A	645	LEU
1	A	649	ARG
1	A	655	LYS
1	A	662	LEU
1	A	665	GLN
1	A	666	ILE
1	A	687	LEU
1	A	692	MET
1	A	702	GLU
1	A	705	GLU
1	A	706	GLU
1	A	710	ILE
1	A	720	ARG
1	A	729	GLN
1	A	734	ARG
1	A	735	ILE
1	A	740	GLN
1	A	753	LYS
1	A	754	GLN
1	A	761	ILE
1	A	764	MET
1	A	765	LEU
1	A	779	GLU
1	A	790	LEU
1	A	797	TRP
1	A	800	MET
1	A	807	THR
1	A	827	VAL
1	A	831	ARG
1	A	838	ASP
1	A	839	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	72	GLN
1	A	101	ASN
1	A	187	ASN
1	A	219	GLN
1	A	235	ASN

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Mol	Chain	Res	Type
1	A	284	ASN
1	A	408	GLN
1	A	453	ASN
1	A	459	HIS
1	A	477	HIS
1	A	481	ASN
1	A	484	ASN
1	A	496	ASN
1	A	541	ASN
1	A	558	ASN
1	A	684	ASN
1	A	804	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](#)

2 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	PLP	A	999	1	15,15,16	2.12	5 (33%)	21,22,23	1.46	4 (19%)
2	G6P	A	998	-	16,16,16	1.71	5 (31%)	23,24,24	2.35	9 (39%)

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	PLP	A	999	1	-	0/6/6/8	0/1/1/1
2	G6P	A	998	-	-	2/6/26/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	PLP	C3-C2	-4.99	1.35	1.41
3	A	999	PLP	C5-C4	-3.19	1.36	1.40
2	A	998	G6P	C4-C3	-2.87	1.44	1.52
3	A	999	PLP	P-O2P	-2.81	1.44	1.54
3	A	999	PLP	P-O4P	-2.70	1.51	1.60
2	A	998	G6P	C3-C2	-2.68	1.45	1.52
3	A	999	PLP	C4A-C4	2.27	1.56	1.51
2	A	998	G6P	O5-C1	2.23	1.48	1.42
2	A	998	G6P	C1-C2	-2.17	1.47	1.52
2	A	998	G6P	O5-C5	2.14	1.49	1.44

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	998	G6P	O4-C4-C3	-4.65	99.41	110.38
2	A	998	G6P	O1-C1-O5	4.26	123.07	110.41
3	A	999	PLP	O4P-C5A-C5	-4.10	101.66	109.36
2	A	998	G6P	O2-C2-C3	-3.60	101.89	110.38
2	A	998	G6P	O1-C1-C2	-3.59	98.58	108.98
2	A	998	G6P	O6-C6-C5	3.41	120.60	108.99
2	A	998	G6P	O5-C5-C6	2.92	112.49	106.69
2	A	998	G6P	C1-C2-C3	2.75	115.96	110.36
2	A	998	G6P	C4-C3-C2	2.72	115.60	110.83
3	A	999	PLP	C4A-C4-C5	-2.34	118.53	120.94
3	A	999	PLP	C5-C6-N1	-2.33	120.04	123.83
2	A	998	G6P	O3-C3-C4	-2.18	105.23	110.38
3	A	999	PLP	O2P-P-O1P	2.16	119.24	110.83

There are no chirality outliers.

All (2) torsion outliers are listed below:

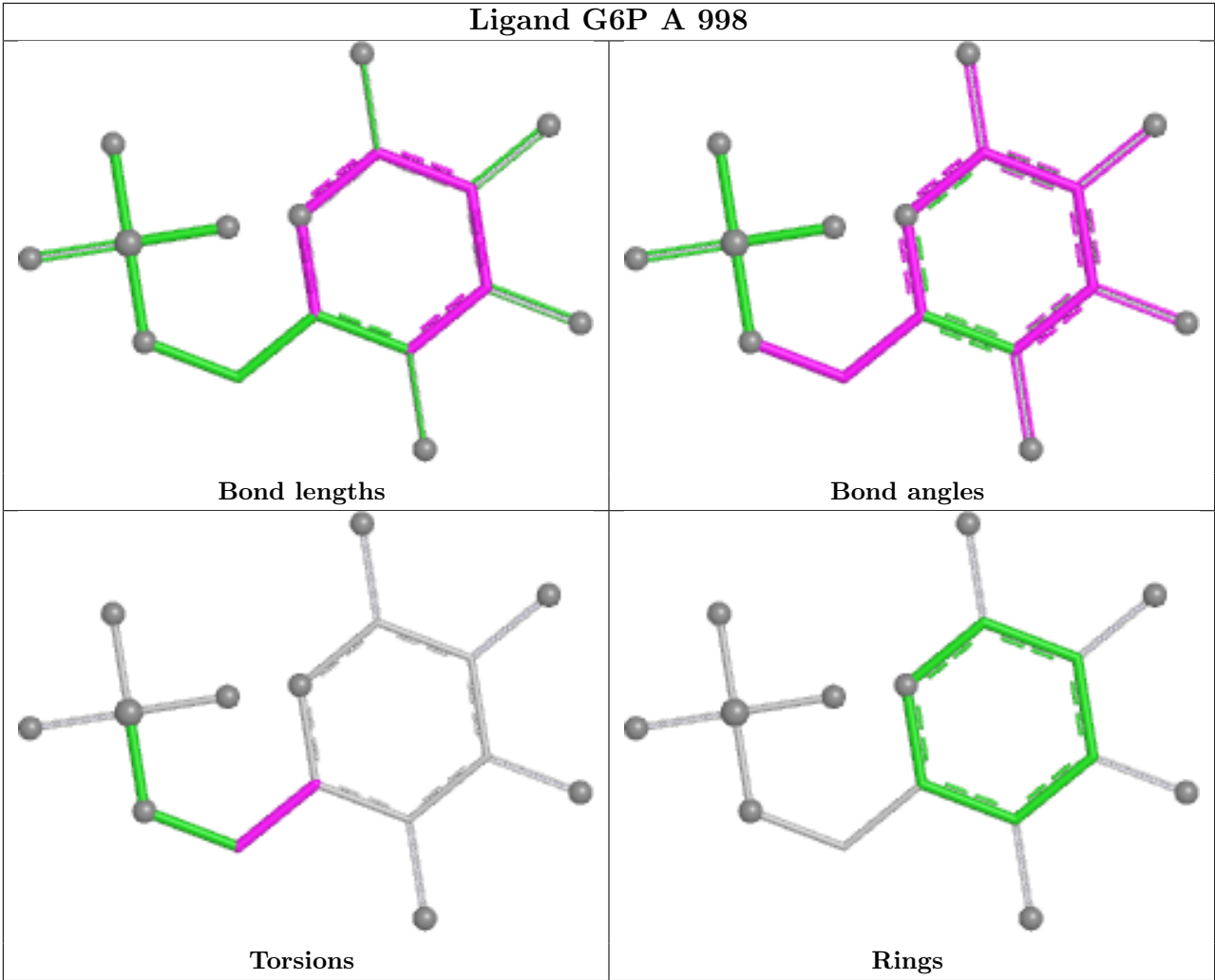
Mol	Chain	Res	Type	Atoms
2	A	998	G6P	C4-C5-C6-O6
2	A	998	G6P	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	998	G6P	2	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	308:ILE	C	309:ARG	N	1.78
1	A	309:ARG	C	310:ARG	N	1.73

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.