



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:02 AM UTC

PDB ID : 4GPB / pdb_00004gpb
Title : COMPARISON OF THE BINDING OF GLUCOSE AND GLUCOSE-1-PHOSPHATE DERIVATIVES TO T-STATE GLYCOGEN PHOSPHORYLASE B
Authors : Martin, J.L.; Johnson, L.N.
Deposited on : 1990-06-04
Resolution : 2.30 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

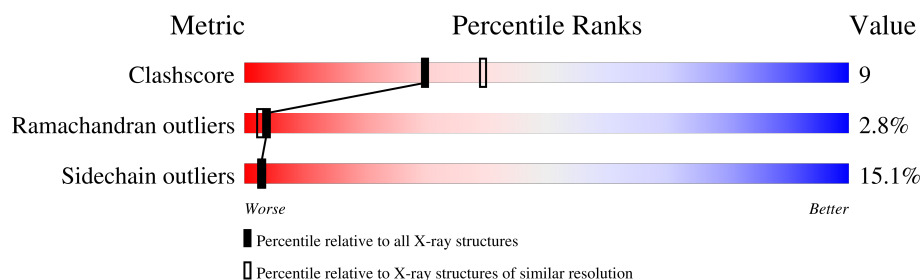
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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	 54% 33% 9% . .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7430 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.

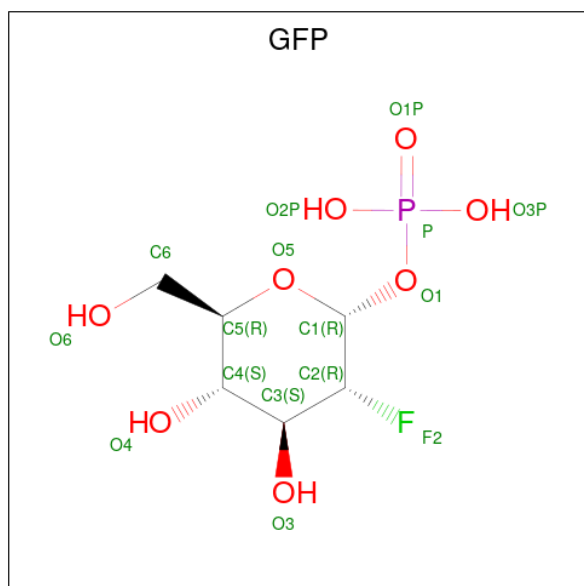
- Molecule 1 is a protein called GLYCOGEN PHOSPHORYLASE B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	833	6779	4320	1197	1232	30	0	0	0

There is a discrepancy between the modelled and reference sequences:

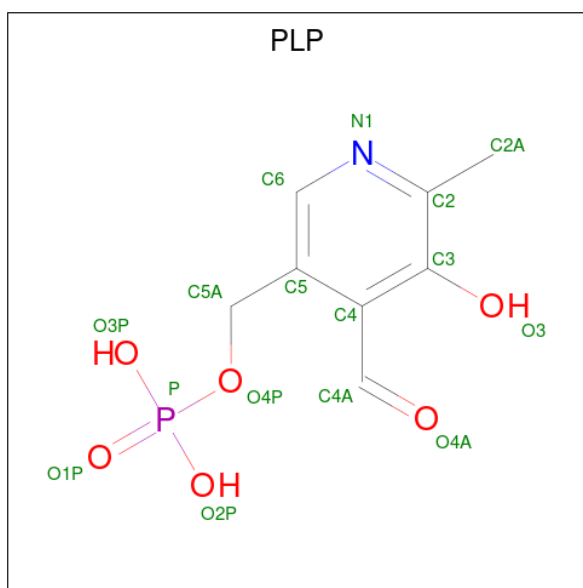
Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	conflict	UNP P00489

- Molecule 2 is 2-deoxy-2-fluoro-1-O-phosphono-alpha-D-glucopyranose (CCD ID: GFP) (formula: $C_6H_{12}FO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	O	P		
2	A	1	16	6	1	8	1	0	0
2	A	1	16	6	1	8	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.

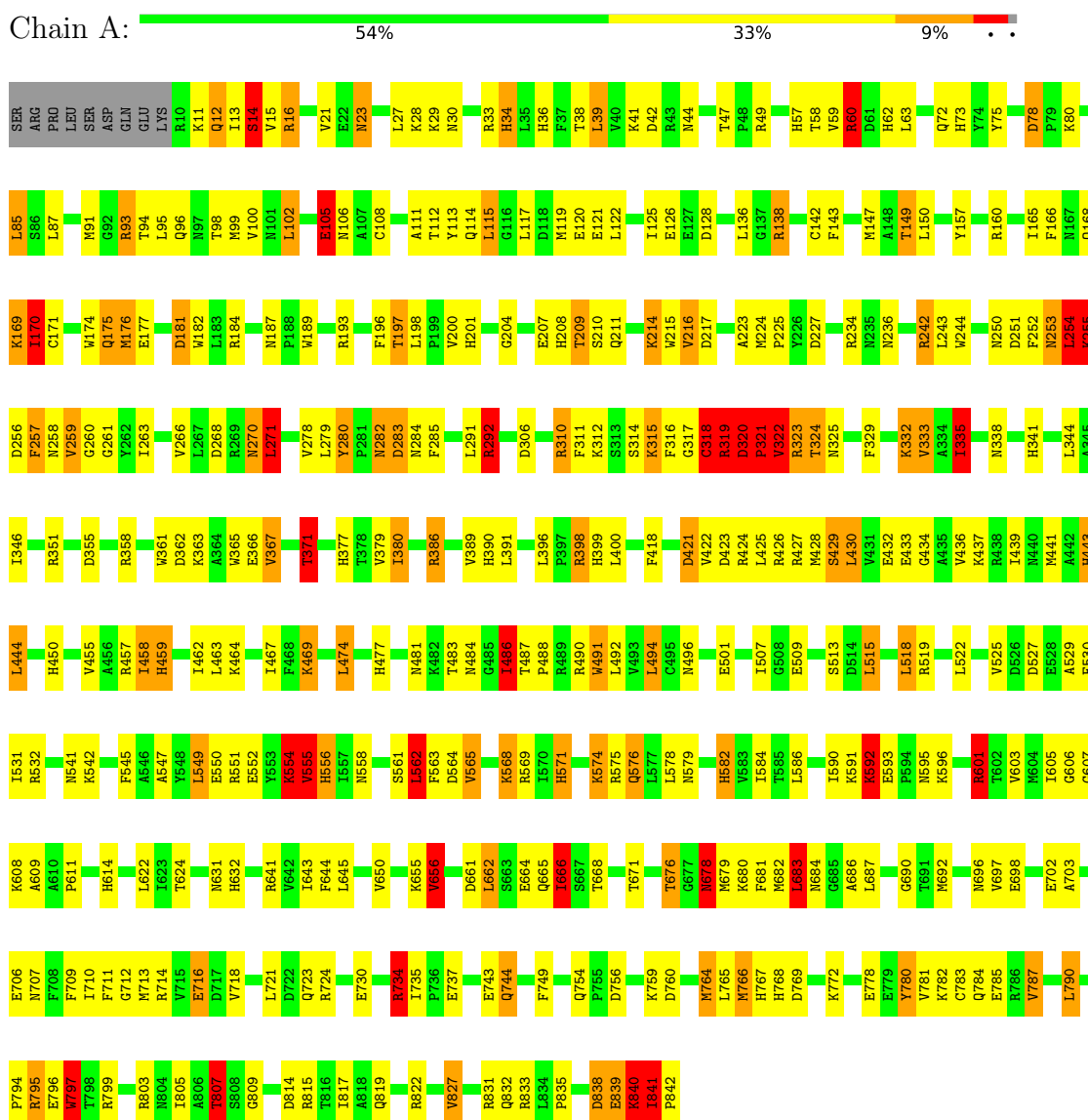
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	604	Total	O	0	0
			604	604		

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)	8.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7430	wwPDB-VP
Average B, all atoms (Å ²)	37.0	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: GFP, 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	1.21	37/6933 (0.5%)	2.11	287/9381 (3.1%)

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 (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	371	THR	CA-CB	9.29	1.68	1.53
1	A	335	ILE	CA-CB	8.04	1.64	1.54
1	A	459	HIS	CD2-NE2	-7.77	1.29	1.37
1	A	787	VAL	CA-CB	7.47	1.64	1.54
1	A	62	HIS	CD2-NE2	-7.45	1.29	1.37
1	A	57	HIS	CD2-NE2	-7.37	1.29	1.37
1	A	208	HIS	CD2-NE2	-7.25	1.29	1.37
1	A	201	HIS	CD2-NE2	-7.22	1.29	1.37
1	A	34	HIS	CD2-NE2	-7.08	1.30	1.37
1	A	632	HIS	CD2-NE2	-7.08	1.30	1.37
1	A	36	HIS	CD2-NE2	-6.65	1.30	1.37
1	A	73	HIS	CD2-NE2	-6.41	1.30	1.37
1	A	768	HIS	CD2-NE2	-6.36	1.30	1.37
1	A	571	HIS	CD2-NE2	-6.35	1.30	1.37
1	A	614	HIS	CD2-NE2	-6.31	1.30	1.37
1	A	165	ILE	CA-CB	6.23	1.62	1.54
1	A	399	HIS	CD2-NE2	-6.20	1.31	1.37
1	A	556	HIS	CD2-NE2	-6.10	1.31	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	34	HIS	CG-ND1	-6.07	1.31	1.38
1	A	582	HIS	CD2-NE2	-5.99	1.31	1.37
1	A	643	ILE	CA-CB	5.98	1.62	1.54
1	A	201	HIS	CG-ND1	-5.95	1.31	1.38
1	A	632	HIS	CG-ND1	-5.95	1.31	1.38
1	A	341	HIS	CD2-NE2	-5.94	1.31	1.37
1	A	443	HIS	CD2-NE2	-5.93	1.31	1.37
1	A	377	HIS	CD2-NE2	-5.83	1.31	1.37
1	A	767	HIS	CD2-NE2	-5.81	1.31	1.37
1	A	377	HIS	CG-ND1	-5.68	1.32	1.38
1	A	565	VAL	CA-CB	5.68	1.61	1.54
1	A	477	HIS	CD2-NE2	-5.49	1.31	1.37
1	A	208	HIS	CG-ND1	-5.49	1.32	1.38
1	A	450	HIS	CD2-NE2	-5.45	1.31	1.37
1	A	582	HIS	CG-ND1	-5.45	1.32	1.38
1	A	571	HIS	CG-ND1	-5.36	1.32	1.38
1	A	390	HIS	CD2-NE2	-5.30	1.32	1.37
1	A	57	HIS	CG-ND1	-5.22	1.32	1.38
1	A	443	HIS	CG-ND1	-5.04	1.32	1.38

All (287) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	838	ASP	N-CA-C	13.44	130.04	110.42
1	A	255	LYS	N-CA-C	11.92	127.70	108.63
1	A	666	ILE	N-CA-CB	-11.52	92.23	111.23
1	A	555	VAL	N-CA-C	10.42	131.01	109.34
1	A	656	VAL	CB-CA-C	-9.83	99.14	112.02
1	A	257	PHE	N-CA-C	9.77	116.79	108.78
1	A	484	ASN	OD1-CG-ND2	-9.58	113.02	122.60
1	A	258	ASN	CA-CB-CG	9.37	121.97	112.60
1	A	362	ASP	CA-CB-CG	-9.33	103.27	112.60
1	A	666	ILE	CA-CB-CG1	-9.26	94.65	110.40
1	A	807	THR	N-CA-CB	-9.08	96.22	111.20
1	A	72	GLN	OE1-CD-NE2	-9.01	113.59	122.60
1	A	838	ASP	CA-CB-CG	-8.92	103.68	112.60
1	A	666	ILE	CA-CB-CG2	8.79	125.44	110.50
1	A	490	ARG	CB-CA-C	-8.53	97.49	110.88
1	A	256	ASP	N-CA-C	-8.52	93.87	107.93
1	A	216	VAL	N-CA-CB	-8.49	100.64	112.52
1	A	838	ASP	O-C-N	8.45	132.57	123.11
1	A	696	ASN	CA-CB-CG	8.35	120.94	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	HIS	CB-CG-CD2	-8.32	120.39	131.20
1	A	767	HIS	CB-CG-CD2	-8.31	120.39	131.20
1	A	840	LYS	CA-C-N	-8.30	116.62	122.59
1	A	840	LYS	C-N-CA	-8.30	116.62	122.59
1	A	458	ILE	N-CA-CB	8.28	121.17	110.57
1	A	208	HIS	CB-CG-CD2	-8.22	120.51	131.20
1	A	15	VAL	CA-C-O	8.19	131.02	120.78
1	A	16	ARG	N-CA-C	-8.06	104.43	112.97
1	A	282	ASN	N-CA-C	8.03	122.12	107.99
1	A	59	VAL	CA-C-O	-8.01	112.36	120.85
1	A	283	ASP	CA-CB-CG	7.98	120.58	112.60
1	A	614	HIS	CB-CG-CD2	-7.92	120.91	131.20
1	A	575	ARG	N-CA-C	7.82	121.83	111.28
1	A	23	ASN	CA-CB-CG	-7.75	104.85	112.60
1	A	592	LYS	CG-CD-CE	7.73	129.07	111.30
1	A	458	ILE	CB-CA-C	-7.62	102.04	112.02
1	A	529	ALA	N-CA-C	-7.60	102.13	111.40
1	A	60	ARG	CA-CB-CG	7.59	129.27	114.10
1	A	312	LYS	CA-CB-CG	-7.57	98.96	114.10
1	A	841	ILE	N-CA-C	-7.55	100.13	107.76
1	A	253	ASN	O-C-N	7.53	132.69	122.83
1	A	558	ASN	O-C-N	-7.50	115.15	121.23
1	A	285	PHE	CA-CB-CG	7.44	121.24	113.80
1	A	744	GLN	OE1-CD-NE2	-7.41	115.19	122.60
1	A	80	LYS	N-CA-C	-7.37	99.37	110.28
1	A	527	ASP	CA-CB-CG	7.36	119.96	112.60
1	A	62	HIS	CB-CG-ND1	7.28	133.63	122.70
1	A	592	LYS	CB-CG-CD	7.20	127.86	111.30
1	A	464	LYS	CB-CG-CD	-7.14	94.89	111.30
1	A	822	ARG	N-CA-C	7.13	119.13	111.36
1	A	563	PHE	CA-CB-CG	7.13	120.93	113.80
1	A	797	TRP	CG-CD2-CE3	7.12	141.02	133.90
1	A	666	ILE	CB-CA-C	7.10	122.93	111.29
1	A	807	THR	CB-CA-C	7.04	122.42	111.02
1	A	501	GLU	CA-C-O	-7.03	113.46	120.70
1	A	656	VAL	N-CA-CB	7.00	119.52	110.57
1	A	365	TRP	CG-CD2-CE3	6.97	140.87	133.90
1	A	30	ASN	OD1-CG-ND2	-6.94	115.66	122.60
1	A	797	TRP	CB-CG-CD1	-6.92	116.52	126.90
1	A	584	ILE	N-CA-C	-6.92	104.03	110.53
1	A	564	ASP	CA-CB-CG	6.91	119.51	112.60
1	A	207	GLU	N-CA-C	-6.91	98.47	109.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	LEU	N-CA-C	6.89	118.68	111.03
1	A	115	LEU	N-CA-C	-6.89	103.41	114.09
1	A	333	VAL	CG1-CB-CG2	-6.81	95.81	110.80
1	A	575	ARG	CB-CG-CD	-6.81	95.64	111.30
1	A	682	MET	CA-C-O	-6.80	113.21	120.42
1	A	595	ASN	OD1-CG-ND2	-6.78	115.82	122.60
1	A	678	ASN	OD1-CG-ND2	-6.75	115.85	122.60
1	A	323	ARG	N-CA-C	-6.75	96.43	110.80
1	A	196	PHE	CA-CB-CG	6.73	120.53	113.80
1	A	767	HIS	CB-CG-ND1	6.65	132.68	122.70
1	A	282	ASN	N-CA-CB	-6.63	100.47	110.35
1	A	200	VAL	N-CA-C	-6.62	98.58	108.12
1	A	665	GLN	OE1-CD-NE2	-6.61	115.99	122.60
1	A	321	PRO	CA-C-N	6.58	133.81	121.97
1	A	321	PRO	C-N-CA	6.58	133.81	121.97
1	A	469	LYS	CA-CB-CG	6.58	127.26	114.10
1	A	574	LYS	CA-C-N	6.56	132.08	122.63
1	A	574	LYS	C-N-CA	6.56	132.08	122.63
1	A	565	VAL	N-CA-C	6.56	117.57	108.12
1	A	494	LEU	N-CA-CB	-6.52	100.95	110.47
1	A	310	ARG	NE-CZ-NH2	-6.52	113.33	119.20
1	A	250	ASN	N-CA-C	6.49	121.33	113.41
1	A	490	ARG	N-CA-CB	6.49	119.42	110.01
1	A	683	LEU	CB-CA-C	-6.49	96.94	110.17
1	A	255	LYS	CA-C-O	6.45	128.44	121.02
1	A	93	ARG	CB-CG-CD	-6.45	96.48	111.30
1	A	282	ASN	CB-CG-ND2	6.43	126.05	116.40
1	A	606	GLY	O-C-N	-6.43	117.64	123.36
1	A	578	LEU	N-CA-C	-6.42	104.36	111.36
1	A	325	ASN	OD1-CG-ND2	-6.42	116.18	122.60
1	A	712	GLY	O-C-N	6.38	129.51	122.68
1	A	78	ASP	CA-CB-CG	6.38	118.98	112.60
1	A	209	THR	O-C-N	6.36	131.26	123.44
1	A	338	ASN	OD1-CG-ND2	-6.33	116.27	122.60
1	A	256	ASP	CA-C-O	6.30	127.67	119.98
1	A	491	TRP	CG-CD2-CE3	6.26	140.16	133.90
1	A	575	ARG	NE-CZ-NH2	-6.24	113.58	119.20
1	A	315	LYS	N-CA-C	-6.23	104.94	114.16
1	A	556	HIS	N-CA-C	6.22	124.06	110.80
1	A	236	ASN	N-CA-C	6.22	120.45	112.86
1	A	579	ASN	CA-CB-CG	6.22	118.82	112.60
1	A	486	ILE	CA-CB-CG1	-6.17	99.91	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	784	GLN	CG-CD-NE2	6.16	125.64	116.40
1	A	723	GLN	CA-C-N	6.16	128.44	120.44
1	A	723	GLN	C-N-CA	6.16	128.44	120.44
1	A	632	HIS	CA-CB-CG	-6.15	107.65	113.80
1	A	609	ALA	O-C-N	-6.11	116.36	123.27
1	A	259	VAL	N-CA-C	6.09	122.01	109.34
1	A	253	ASN	CA-C-N	6.07	133.13	121.54
1	A	253	ASN	C-N-CA	6.07	133.13	121.54
1	A	714	ARG	O-C-N	-6.07	115.58	122.68
1	A	198	LEU	O-C-N	-6.06	117.58	121.88
1	A	562	LEU	N-CA-C	-6.06	100.87	109.96
1	A	72	GLN	CG-CD-NE2	6.06	125.48	116.40
1	A	681	PHE	CA-CB-CG	6.05	119.85	113.80
1	A	422	VAL	CA-C-O	-6.04	112.36	119.85
1	A	271	LEU	N-CA-C	-6.03	97.95	110.80
1	A	614	HIS	CB-CG-ND1	6.03	131.75	122.70
1	A	554	LYS	N-CA-C	6.03	123.64	110.80
1	A	121	GLU	CA-CB-CG	6.02	126.15	114.10
1	A	365	TRP	CB-CG-CD1	-6.00	117.89	126.90
1	A	258	ASN	OD1-CG-ND2	-6.00	116.60	122.60
1	A	207	GLU	N-CA-CB	5.99	120.33	110.69
1	A	72	GLN	CB-CG-CD	5.98	122.77	112.60
1	A	324	THR	CA-C-O	5.98	129.06	120.51
1	A	428	MET	CA-CB-CG	-5.98	102.14	114.10
1	A	766	MET	CG-SD-CE	5.98	114.05	100.90
1	A	684	ASN	OD1-CG-ND2	-5.96	116.64	122.60
1	A	507	ILE	N-CA-C	5.94	117.87	112.29
1	A	558	ASN	CA-CB-CG	5.94	118.54	112.60
1	A	614	HIS	CA-C-O	-5.93	114.59	120.82
1	A	696	ASN	OD1-CG-ND2	-5.92	116.68	122.60
1	A	106	ASN	N-CA-C	5.91	117.80	111.36
1	A	711	PHE	N-CA-C	-5.90	100.60	108.74
1	A	683	LEU	N-CA-CB	5.88	120.68	110.39
1	A	366	GLU	N-CA-C	-5.87	104.96	111.36
1	A	496	ASN	CA-C-N	5.87	125.41	119.19
1	A	496	ASN	C-N-CA	5.87	125.41	119.19
1	A	682	MET	CG-SD-CE	5.86	113.80	100.90
1	A	214	LYS	CB-CG-CD	-5.86	97.83	111.30
1	A	734	ARG	CB-CG-CD	5.85	124.75	111.30
1	A	270	ASN	OD1-CG-ND2	-5.84	116.76	122.60
1	A	530	PHE	CA-CB-CG	-5.84	107.96	113.80
1	A	96	GLN	CA-CB-CG	-5.83	102.44	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	519	ARG	CA-CB-CG	-5.82	102.47	114.10
1	A	182	TRP	N-CA-C	5.81	119.63	112.54
1	A	735	ILE	CA-C-N	5.81	125.50	119.05
1	A	735	ILE	C-N-CA	5.81	125.50	119.05
1	A	367	VAL	O-C-N	-5.80	116.22	121.91
1	A	457	ARG	CA-C-O	-5.80	114.41	120.55
1	A	481	ASN	OD1-CG-ND2	-5.79	116.81	122.60
1	A	509	GLU	O-C-N	-5.79	114.83	122.42
1	A	386	ARG	CB-CG-CD	-5.75	98.07	111.30
1	A	100	VAL	N-CA-C	-5.74	104.73	110.30
1	A	459	HIS	CB-CG-CD2	-5.74	123.74	131.20
1	A	362	ASP	CA-C-O	-5.73	114.34	120.42
1	A	12	GLN	CA-CB-CG	-5.70	102.71	114.10
1	A	399	HIS	CB-CG-CD2	-5.69	123.80	131.20
1	A	784	GLN	OE1-CD-NE2	-5.69	116.91	122.60
1	A	166	PHE	N-CA-C	5.68	117.62	110.24
1	A	474	LEU	O-C-N	-5.67	115.97	122.09
1	A	833	ARG	CA-CB-CG	5.67	125.44	114.10
1	A	282	ASN	OD1-CG-ND2	-5.66	116.94	122.60
1	A	63	LEU	N-CA-CB	-5.66	102.21	110.47
1	A	713	MET	CA-CB-CG	5.63	125.37	114.10
1	A	558	ASN	CA-C-O	-5.63	115.63	119.29
1	A	317	GLY	CA-C-N	5.62	132.28	121.54
1	A	317	GLY	C-N-CA	5.62	132.28	121.54
1	A	605	ILE	CA-C-N	5.60	126.78	121.46
1	A	605	ILE	C-N-CA	5.60	126.78	121.46
1	A	270	ASN	CB-CG-ND2	5.60	124.80	116.40
1	A	57	HIS	CB-CG-CD2	-5.59	123.93	131.20
1	A	678	ASN	CA-CB-CG	5.57	118.17	112.60
1	A	434	GLY	N-CA-C	-5.56	102.68	110.63
1	A	142	CYS	N-CA-C	-5.56	105.30	111.36
1	A	201	HIS	CB-CG-CD2	-5.56	123.98	131.20
1	A	250	ASN	CA-CB-CG	-5.54	107.06	112.60
1	A	436	VAL	N-CA-C	-5.54	99.25	107.51
1	A	840	LYS	CA-CB-CG	5.54	125.18	114.10
1	A	532	ARG	CA-CB-CG	5.53	125.16	114.10
1	A	282	ASN	CA-CB-CG	5.51	118.11	112.60
1	A	832	GLN	OE1-CD-NE2	-5.50	117.10	122.60
1	A	631	ASN	OD1-CG-ND2	-5.49	117.11	122.60
1	A	91	MET	N-CA-C	5.49	118.19	111.82
1	A	780	TYR	CA-C-O	-5.48	115.05	120.70
1	A	113	TYR	N-CA-C	-5.47	105.01	110.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	486	ILE	CA-CB-CG2	5.47	119.79	110.50
1	A	686	ALA	N-CA-C	-5.46	101.23	109.85
1	A	160	ARG	CB-CG-CD	-5.46	98.75	111.30
1	A	541	ASN	OD1-CG-ND2	-5.45	117.15	122.60
1	A	346	ILE	CA-C-O	-5.45	112.65	119.95
1	A	396	LEU	CA-C-O	-5.44	115.74	121.29
1	A	797	TRP	CE2-CD2-CG	-5.44	100.67	107.20
1	A	486	ILE	N-CA-CB	-5.43	102.31	112.36
1	A	322	VAL	CA-C-N	5.43	131.91	121.54
1	A	322	VAL	C-N-CA	5.43	131.91	121.54
1	A	365	TRP	CE2-CD2-CG	-5.43	100.69	107.20
1	A	650	VAL	O-C-N	-5.43	116.51	121.94
1	A	494	LEU	CB-CA-C	5.42	118.72	109.24
1	A	595	ASN	CB-CG-ND2	5.42	124.53	116.40
1	A	390	HIS	CB-CG-CD2	-5.42	124.16	131.20
1	A	318	CYS	N-CA-C	-5.41	99.27	110.80
1	A	319	ARG	CB-CG-CD	5.40	123.72	111.30
1	A	713	MET	N-CA-CB	-5.40	102.03	109.97
1	A	215	TRP	N-CA-C	-5.40	99.93	108.73
1	A	611	PRO	N-CA-C	5.40	120.94	113.65
1	A	671	THR	O-C-N	-5.39	114.70	122.36
1	A	707	ASN	CA-C-O	5.39	125.86	119.56
1	A	835	PRO	O-C-N	5.39	129.73	122.89
1	A	579	ASN	CB-CG-ND2	5.38	124.47	116.40
1	A	85	LEU	O-C-N	-5.38	117.09	123.22
1	A	197	THR	CA-CB-OG1	-5.37	101.55	109.60
1	A	358	ARG	N-CA-C	5.36	119.12	112.58
1	A	814	ASP	N-CA-C	-5.36	105.09	111.69
1	A	120	GLU	CA-C-O	-5.35	114.85	120.63
1	A	175	GLN	OE1-CD-NE2	-5.35	117.25	122.60
1	A	655	LYS	CA-CB-CG	-5.33	103.43	114.10
1	A	676	THR	CA-C-O	5.33	124.82	118.69
1	A	128	ASP	CA-CB-CG	5.33	117.93	112.60
1	A	216	VAL	CB-CA-C	5.33	118.71	110.82
1	A	380	ILE	CA-C-N	5.33	125.14	119.28
1	A	380	ILE	C-N-CA	5.33	125.14	119.28
1	A	207	GLU	CB-CA-C	-5.32	99.80	109.38
1	A	361	TRP	CG-CD2-CE3	5.32	139.22	133.90
1	A	278	VAL	N-CA-C	5.32	116.32	108.45
1	A	576	GLN	OE1-CD-NE2	-5.31	117.29	122.60
1	A	838	ASP	CA-C-O	5.31	126.26	120.95
1	A	280	TYR	CA-C-N	5.29	126.45	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	TYR	C-N-CA	5.29	126.45	119.84
1	A	666	ILE	N-CA-C	5.28	120.31	109.34
1	A	94	THR	O-C-N	-5.27	115.87	122.35
1	A	270	ASN	CA-C-O	5.26	127.48	121.58
1	A	785	GLU	N-CA-C	-5.26	105.61	112.23
1	A	584	ILE	CA-C-O	-5.25	115.23	121.05
1	A	678	ASN	CB-CG-ND2	5.24	124.26	116.40
1	A	263	ILE	N-CA-C	-5.23	105.28	110.62
1	A	644	PHE	CA-CB-CG	-5.23	108.57	113.80
1	A	78	ASP	CA-C-N	5.22	125.96	120.11
1	A	78	ASP	C-N-CA	5.22	125.96	120.11
1	A	181	ASP	CA-CB-CG	5.21	117.81	112.60
1	A	121	GLU	CB-CA-C	-5.20	102.72	110.88
1	A	656	VAL	N-CA-C	5.20	115.42	110.53
1	A	601	ARG	CA-CB-CG	5.20	124.50	114.10
1	A	244	TRP	CB-CG-CD1	-5.18	119.13	126.90
1	A	484	ASN	CB-CG-ND2	5.18	124.17	116.40
1	A	119	MET	CB-CA-C	-5.17	102.77	110.88
1	A	797	TRP	NE1-CE2-CZ2	-5.16	122.35	130.10
1	A	421	ASP	CA-CB-CG	5.16	117.76	112.60
1	A	624	THR	N-CA-C	-5.15	105.85	111.82
1	A	754	GLN	CA-C-N	5.14	124.45	118.85
1	A	754	GLN	C-N-CA	5.14	124.45	118.85
1	A	60	ARG	CB-CG-CD	5.13	123.11	111.30
1	A	338	ASN	CB-CG-ND2	5.13	124.10	116.40
1	A	390	HIS	CA-CB-CG	5.13	118.93	113.80
1	A	105	GLU	N-CA-C	5.12	117.26	111.11
1	A	819	GLN	CB-CG-CD	-5.12	103.89	112.60
1	A	44	ASN	CA-CB-CG	5.12	117.72	112.60
1	A	292	ARG	CA-C-O	-5.12	115.43	120.70
1	A	389	VAL	CA-C-O	-5.12	115.95	121.27
1	A	737	GLU	N-CA-C	-5.12	105.83	111.71
1	A	170	ILE	O-C-N	-5.11	116.71	122.94
1	A	283	ASP	N-CA-C	-5.11	102.13	110.20
1	A	668	THR	N-CA-C	-5.10	102.31	109.96
1	A	768	HIS	CB-CG-CD2	-5.10	124.57	131.20
1	A	60	ARG	CG-CD-NE	5.10	123.21	112.00
1	A	367	VAL	N-CA-CB	-5.10	104.59	110.55
1	A	661	ASP	N-CA-C	-5.10	106.75	113.12
1	A	558	ASN	CA-C-N	5.09	124.81	119.82
1	A	558	ASN	C-N-CA	5.09	124.81	119.82
1	A	149	THR	CA-CB-OG1	-5.07	102.00	109.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	THR	CA-CB-OG1	-5.06	102.01	109.60
1	A	532	ARG	N-CA-CB	-5.06	102.44	110.28
1	A	429	SER	CA-C-O	5.05	126.00	120.95
1	A	662	LEU	CA-C-N	5.04	129.48	122.77
1	A	662	LEU	C-N-CA	5.04	129.48	122.77
1	A	483	THR	O-C-N	5.04	129.04	122.89
1	A	551	ARG	CA-C-N	5.04	127.74	120.38
1	A	551	ARG	C-N-CA	5.04	127.74	120.38
1	A	73	HIS	CB-CG-CD2	-5.04	124.65	131.20
1	A	718	VAL	N-CA-C	-5.04	105.63	110.72
1	A	361	TRP	CE2-CD2-CG	-5.03	101.16	107.20
1	A	547	ALA	N-CA-C	-5.02	105.72	111.14
1	A	797	TRP	CB-CA-C	-5.02	103.00	110.88
1	A	766	MET	N-CA-C	5.01	117.64	111.82
1	A	189	TRP	CA-C-O	-5.01	113.91	119.67
1	A	827	VAL	CG1-CB-CG2	-5.01	99.78	110.80

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	6779	0	6729	116	0
2	A	32	0	20	0	0
3	A	15	0	7	0	0
4	A	604	0	0	18	0
All	All	7430	0	6756	116	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 9.

All (116) 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:225:PRO:HB2	1:A:242:ARG:HD2	1.60	0.82
1:A:515:LEU:HD22	1:A:518:LEU:HD22	1.65	0.77
1:A:367:VAL:O	1:A:371:THR:HG22	1.85	0.76
1:A:593:GLU:HB2	1:A:596:LYS:HD2	1.73	0.70
1:A:730:GLU:O	1:A:734:ARG:HG2	1.91	0.70
1:A:692:MET:HG3	1:A:697:VAL:HG22	1.74	0.69
1:A:99:MET:HE2	1:A:108:CYS:SG	2.33	0.68
1:A:716:GLU:HB2	4:A:1115:HOH:O	1.93	0.66
1:A:463:LEU:HA	1:A:467:ILE:HG23	1.79	0.64
1:A:78:ASP:HB3	1:A:315:LYS:HZ1	1.65	0.62
1:A:756:ASP:HB2	1:A:759:LYS:HD3	1.82	0.62
1:A:78:ASP:HB3	1:A:315:LYS:NZ	2.15	0.61
1:A:329:PHE:O	1:A:333:VAL:HG12	2.01	0.61
1:A:441:MET:HE3	1:A:444:LEU:HD12	1.84	0.59
1:A:703:ALA:HA	1:A:807:THR:HG21	1.85	0.57
1:A:430:LEU:HD22	1:A:443:HIS:HB3	1.85	0.57
1:A:315:LYS:O	1:A:318:CYS:HB2	2.04	0.57
1:A:841:ILE:HD13	1:A:842:PRO:HD2	1.84	0.57
1:A:28:LYS:HG2	1:A:115:LEU:HD22	1.87	0.57
1:A:143:PHE:O	1:A:147:MET:HG3	2.05	0.56
1:A:455:VAL:H	1:A:459:HIS:HD2	1.53	0.56
1:A:794:PRO:HA	4:A:1072:HOH:O	2.06	0.56
1:A:169:LYS:HG3	1:A:176:MET:HB3	1.88	0.55
1:A:698:GLU:O	1:A:702:GLU:HB2	2.08	0.54
1:A:157:TYR:OH	1:A:310:ARG:NH2	2.41	0.54
1:A:122:LEU:HA	1:A:125:ILE:HD12	1.90	0.53
1:A:545:PHE:CZ	1:A:656:VAL:HG13	2.44	0.53
1:A:678:ASN:HD22	1:A:679:MET:H	1.57	0.53
1:A:292:ARG:NH2	4:A:1421:HOH:O	2.41	0.53
1:A:379:VAL:HG22	4:A:1443:HOH:O	2.08	0.53
1:A:486:ILE:CD1	1:A:676:THR:HB	2.38	0.53
1:A:515:LEU:HB3	1:A:809:GLY:HA2	1.91	0.53
1:A:28:LYS:HG3	1:A:111:ALA:HB1	1.92	0.52
1:A:525:VAL:O	1:A:531:ILE:HD11	2.09	0.52
1:A:664:GLU:OE1	1:A:666:ILE:HD13	2.10	0.52
1:A:463:LEU:HA	1:A:467:ILE:CG2	2.40	0.52
1:A:561:SER:HB2	1:A:601:ARG:HA	1.92	0.52
1:A:795:ARG:O	1:A:799:ARG:HG3	2.10	0.51
1:A:75:TYR:HB2	4:A:1009:HOH:O	2.10	0.50
1:A:815:ARG:HB2	4:A:1485:HOH:O	2.11	0.50
1:A:251:ASP:O	1:A:255:LYS:N	2.45	0.49
1:A:168:GLN:HG3	1:A:175:GLN:HG3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:ILE:HG12	1:A:680:LYS:CG	2.43	0.48
1:A:592:LYS:HE2	4:A:1140:HOH:O	2.13	0.48
1:A:486:ILE:HG12	1:A:680:LYS:HG2	1.95	0.48
1:A:790:LEU:HD13	1:A:797:TRP:CD1	2.49	0.48
1:A:759:LYS:HE2	4:A:1539:HOH:O	2.14	0.47
1:A:85:LEU:HD13	1:A:335:ILE:HD12	1.97	0.47
1:A:197:THR:HA	1:A:223:ALA:O	2.15	0.47
1:A:187:ASN:ND2	4:A:1036:HOH:O	2.48	0.47
1:A:105:GLU:HB2	4:A:1019:HOH:O	2.14	0.46
1:A:98:THR:O	1:A:102:LEU:HB2	2.15	0.46
1:A:764:MET:HE1	4:A:1339:HOH:O	2.15	0.46
1:A:311:PHE:HE1	1:A:332:LYS:HG3	1.81	0.46
1:A:321:PRO:O	1:A:322:VAL:HB	2.15	0.46
1:A:171:CYS:HB2	1:A:176:MET:SD	2.56	0.45
1:A:562:LEU:HB3	1:A:601:ARG:HB3	1.98	0.45
1:A:423:ASP:O	1:A:427:ARG:HG3	2.15	0.45
1:A:138:ARG:HB3	4:A:1520:HOH:O	2.16	0.45
1:A:204:GLY:HA2	1:A:217:ASP:O	2.16	0.45
1:A:550:GLU:O	1:A:554:LYS:HA	2.16	0.45
1:A:703:ALA:CA	1:A:807:THR:HG21	2.46	0.45
1:A:487:THR:HA	1:A:488:PRO:HD2	1.78	0.45
1:A:268:ASP:O	1:A:271:LEU:HB2	2.17	0.44
1:A:181:ASP:O	1:A:184:ARG:HG3	2.17	0.44
1:A:251:ASP:CG	1:A:252:PHE:N	2.76	0.44
1:A:709:PHE:HB3	1:A:783:CYS:SG	2.57	0.44
1:A:316:PHE:HA	1:A:319:ARG:O	2.17	0.44
1:A:112:THR:HG23	1:A:117:LEU:HB2	2.00	0.43
1:A:488:PRO:O	1:A:492:LEU:HB3	2.18	0.43
1:A:764:MET:HE2	1:A:769:ASP:HA	2.00	0.43
1:A:721:LEU:HD23	1:A:772:LYS:HD3	1.99	0.43
1:A:170:ILE:HA	1:A:174:TRP:O	2.19	0.43
1:A:796:GLU:OE1	1:A:799:ARG:NH1	2.52	0.43
1:A:386:ARG:HA	1:A:439:ILE:O	2.19	0.43
1:A:181:ASP:O	1:A:184:ARG:NH1	2.52	0.43
1:A:433:GLU:OE2	1:A:437:LYS:NZ	2.51	0.43
1:A:335:ILE:O	1:A:335:ILE:HG13	2.15	0.43
1:A:441:MET:CE	1:A:444:LEU:HD12	2.48	0.43
1:A:554:LYS:HE2	4:A:1332:HOH:O	2.19	0.43
1:A:569:ARG:HD2	1:A:608:LYS:O	2.19	0.42
1:A:839:GLU:O	1:A:840:LYS:NZ	2.52	0.42
1:A:254:LEU:HD21	1:A:266:VAL:HG22	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:LEU:HB2	1:A:683:LEU:HD22	2.00	0.42
1:A:790:LEU:HB3	1:A:797:TRP:CD1	2.54	0.42
1:A:355:ASP:OD1	1:A:398:ARG:NH1	2.53	0.42
1:A:690:GLY:O	1:A:710:ILE:HA	2.19	0.42
1:A:351:ARG:O	1:A:355:ASP:HB2	2.19	0.42
1:A:582:HIS:HB2	1:A:780:TYR:CE2	2.54	0.42
1:A:280:TYR:OH	1:A:291:LEU:HB3	2.20	0.42
1:A:34:HIS:O	1:A:38:THR:HB	2.20	0.42
1:A:749:PHE:HB2	4:A:1537:HOH:O	2.20	0.42
1:A:744:GLN:HA	4:A:1537:HOH:O	2.20	0.42
1:A:93:ARG:NH1	1:A:126:GLU:O	2.53	0.42
1:A:568:LYS:O	1:A:607:GLY:HA3	2.20	0.41
1:A:724:ARG:NH2	4:A:1533:HOH:O	2.53	0.41
1:A:227:ASP:OD1	1:A:242:ARG:HD3	2.20	0.41
1:A:571:HIS:HB3	1:A:574:LYS:HG3	2.01	0.41
1:A:803:ARG:NH2	4:A:1315:HOH:O	2.46	0.41
1:A:257:PHE:CD1	1:A:257:PHE:N	2.88	0.41
1:A:678:ASN:ND2	1:A:679:MET:H	2.17	0.41
1:A:14:SER:HB3	1:A:16:ARG:CG	2.50	0.41
1:A:542:LYS:NZ	4:A:1517:HOH:O	2.52	0.41
1:A:549:LEU:HG	1:A:555:VAL:HG21	2.03	0.41
1:A:60:ARG:HG2	1:A:60:ARG:HH11	1.85	0.41
1:A:29:LYS:HE2	1:A:29:LYS:HB2	1.86	0.41
1:A:418:PHE:CD2	1:A:424:ARG:HD3	2.56	0.41
1:A:149:THR:O	1:A:831:ARG:HD2	2.21	0.40
1:A:319:ARG:NH1	1:A:320:ASP:OD1	2.54	0.40
1:A:549:LEU:HA	1:A:549:LEU:HD12	1.83	0.40
1:A:421:ASP:O	1:A:425:LEU:HD23	2.21	0.40
1:A:39:LEU:HD12	1:A:39:LEU:HA	1.92	0.40
1:A:49:ARG:HA	1:A:125:ILE:HG21	2.04	0.40
1:A:193:ARG:HH11	1:A:193:ARG:HD2	1.69	0.40
1:A:487:THR:O	1:A:491:TRP:HB2	2.21	0.40
1:A:805:ILE:HG21	1:A:805:ILE:HD13	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	831/842 (99%)	753 (91%)	55 (7%)	23 (3%)	4 2

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	VAL
1	A	114	GLN
1	A	254	LEU
1	A	259	VAL
1	A	318	CYS
1	A	320	ASP
1	A	321	PRO
1	A	322	VAL
1	A	323	ARG
1	A	324	THR
1	A	555	VAL
1	A	556	HIS
1	A	839	GLU
1	A	210	SER
1	A	261	GLY
1	A	314	SER
1	A	840	LYS
1	A	14	SER
1	A	271	LEU
1	A	319	ARG
1	A	554	LYS
1	A	284	ASN
1	A	260	GLY

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	722/731 (99%)	613 (85%)	109 (15%)	3 3

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	12	GLN
1	A	13	ILE
1	A	14	SER
1	A	23	ASN
1	A	27	LEU
1	A	33	ARG
1	A	39	LEU
1	A	41	LYS
1	A	42	ASP
1	A	47	THR
1	A	60	ARG
1	A	87	LEU
1	A	102	LEU
1	A	105	GLU
1	A	136	LEU
1	A	138	ARG
1	A	150	LEU
1	A	169	LYS
1	A	170	ILE
1	A	176	MET
1	A	177	GLU
1	A	209	THR
1	A	211	GLN
1	A	214	LYS
1	A	216	VAL
1	A	224	MET
1	A	234	ARG
1	A	242	ARG
1	A	243	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	253	ASN
1	A	254	LEU
1	A	255	LYS
1	A	270	ASN
1	A	271	LEU
1	A	279	LEU
1	A	282	ASN
1	A	283	ASP
1	A	292	ARG
1	A	306	ASP
1	A	319	ARG
1	A	322	VAL
1	A	332	LYS
1	A	335	ILE
1	A	344	LEU
1	A	363	LYS
1	A	371	THR
1	A	380	ILE
1	A	391	LEU
1	A	398	ARG
1	A	400	LEU
1	A	426	ARG
1	A	429	SER
1	A	430	LEU
1	A	432	GLU
1	A	444	LEU
1	A	458	ILE
1	A	462	ILE
1	A	469	LYS
1	A	474	LEU
1	A	486	ILE
1	A	494	LEU
1	A	513	SER
1	A	515	LEU
1	A	518	LEU
1	A	522	LEU
1	A	549	LEU
1	A	552	GLU
1	A	554	LYS
1	A	562	LEU
1	A	565	VAL
1	A	568	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	576	GLN
1	A	586	LEU
1	A	590	ILE
1	A	591	LYS
1	A	592	LYS
1	A	601	ARG
1	A	603	VAL
1	A	622	LEU
1	A	641	ARG
1	A	645	LEU
1	A	656	VAL
1	A	662	LEU
1	A	666	ILE
1	A	678	ASN
1	A	683	LEU
1	A	687	LEU
1	A	706	GLU
1	A	716	GLU
1	A	734	ARG
1	A	743	GLU
1	A	760	ASP
1	A	764	MET
1	A	765	LEU
1	A	766	MET
1	A	778	GLU
1	A	781	VAL
1	A	782	LYS
1	A	787	VAL
1	A	790	LEU
1	A	795	ARG
1	A	797	TRP
1	A	807	THR
1	A	817	ILE
1	A	827	VAL
1	A	838	ASP
1	A	840	LYS
1	A	841	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	34	HIS
1	A	57	HIS
1	A	62	HIS
1	A	187	ASN
1	A	390	HIS
1	A	453	ASN
1	A	484	ASN
1	A	496	ASN
1	A	541	ASN
1	A	595	ASN
1	A	678	ASN
1	A	767	HIS
1	A	768	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	GFP	A	900	-	15,16,16	1.11	2 (13%)	22,24,24	2.23	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GFP	A	901	-	15,16,16	1.79	4 (26%)	22,24,24	2.47	4 (18%)
3	PLP	A	999	1	15,15,16	1.77	1 (6%)	21,22,23	1.26	3 (14%)

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	GFP	A	900	-	-	1/6/27/27	0/1/1/1
2	GFP	A	901	-	-	3/6/27/27	0/1/1/1
3	PLP	A	999	1	-	1/6/6/8	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	PLP	C3-C2	-5.17	1.35	1.41
2	A	901	GFP	C2-C1	4.05	1.56	1.52
2	A	900	GFP	C2-C1	2.86	1.55	1.52
2	A	901	GFP	O5-C1	2.71	1.48	1.41
2	A	901	GFP	C4-C5	2.54	1.58	1.53
2	A	900	GFP	O5-C1	2.12	1.47	1.41
2	A	901	GFP	C6-C5	2.03	1.58	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	GFP	F2-C2-C1	9.93	119.04	107.62
2	A	900	GFP	F2-C2-C1	6.53	115.13	107.62
2	A	900	GFP	F2-C2-C3	4.73	112.91	108.81
2	A	900	GFP	C1-C2-C3	-3.96	104.76	110.54
2	A	901	GFP	F2-C2-C3	3.40	111.76	108.81
2	A	900	GFP	O3-C3-C4	-3.13	102.99	110.38
2	A	901	GFP	C1-C2-C3	-2.50	106.90	110.54
3	A	999	PLP	C5-C6-N1	-2.40	119.93	123.83
3	A	999	PLP	O2P-P-O1P	2.37	120.06	110.83
2	A	901	GFP	O1-C1-C2	2.15	112.32	108.38
3	A	999	PLP	C6-C5-C4	2.15	119.86	118.10

There are no chirality outliers.

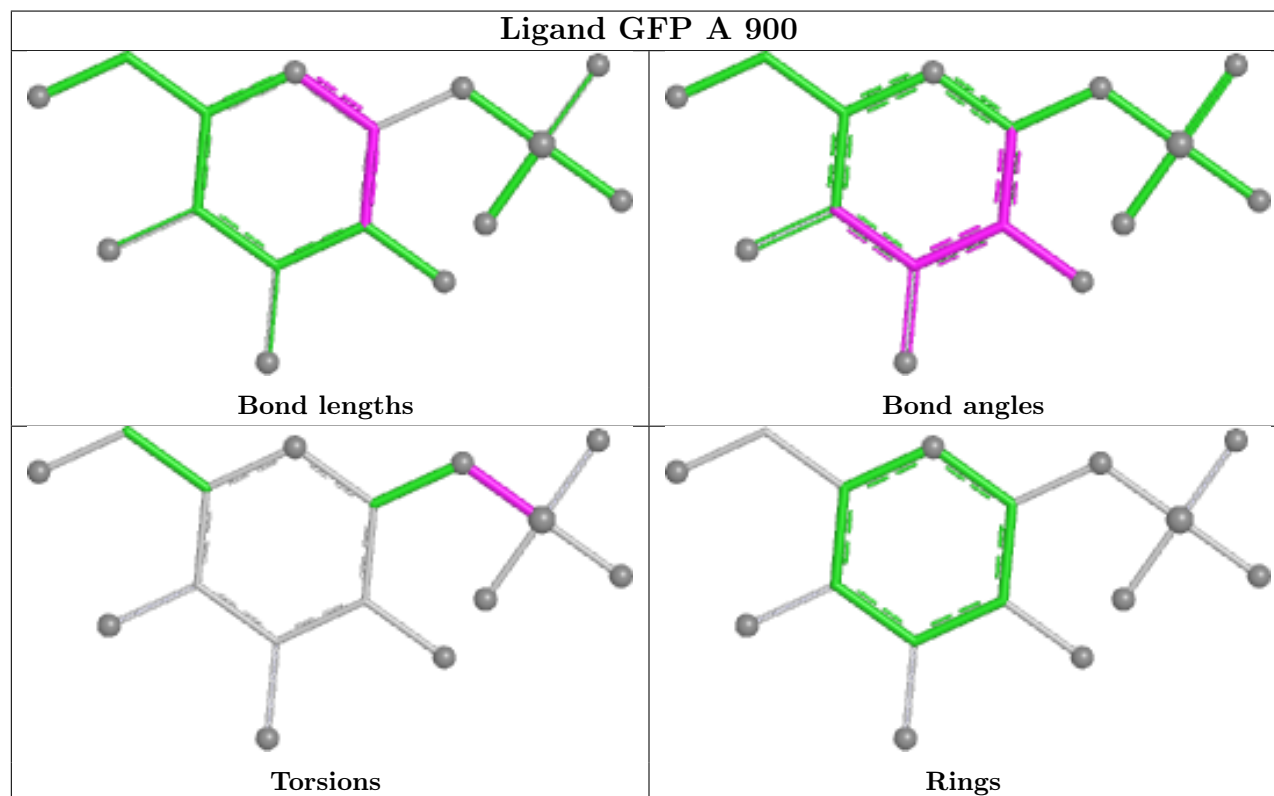
All (5) torsion outliers are listed below:

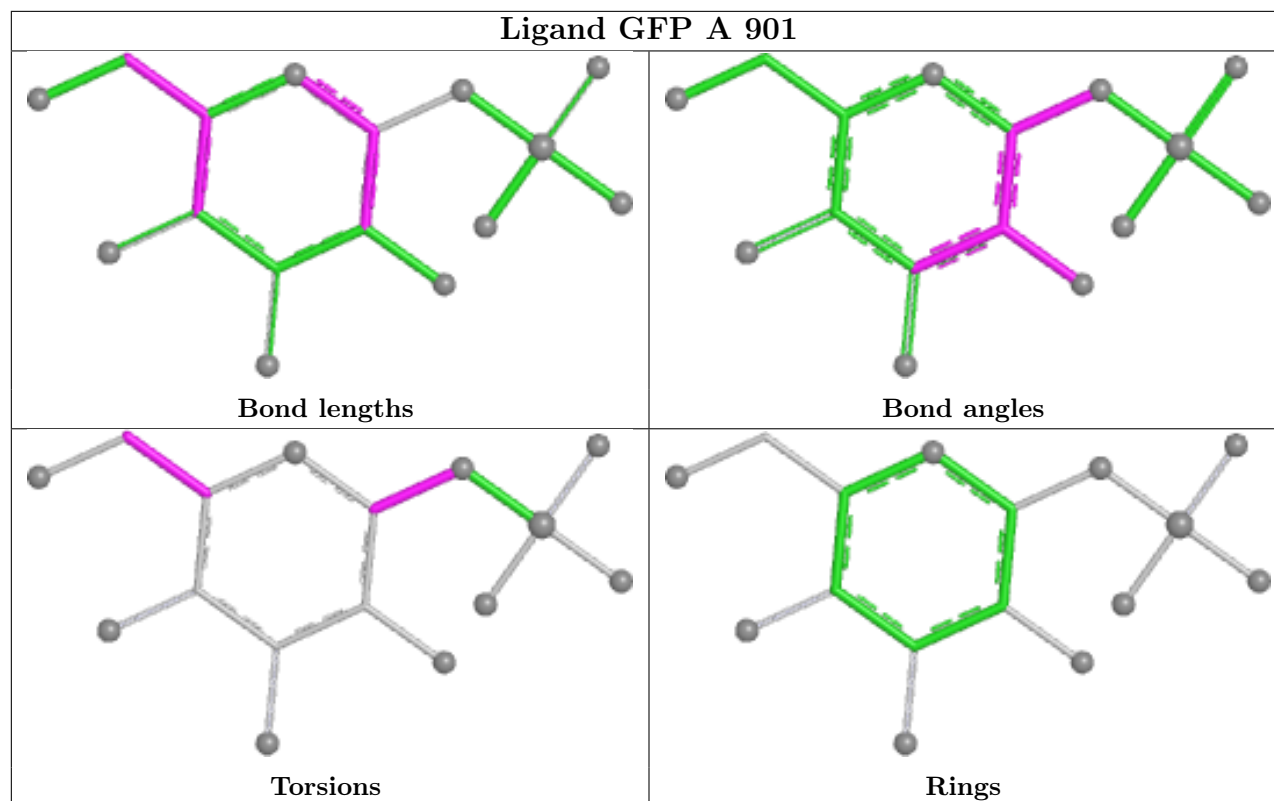
Mol	Chain	Res	Type	Atoms
2	A	901	GFP	O5-C1-O1-P
2	A	901	GFP	C4-C5-C6-O6
2	A	901	GFP	O5-C5-C6-O6
2	A	900	GFP	C1-O1-P-O3P
3	A	999	PLP	C4-C5-C5A-O4P

There are no ring outliers.

No monomer is involved in short contacts.

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.