



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 07:46 PM UTC

PDB ID : 9GAF / pdb_00009gaf
Title : PRECURSOR OF THE W11F MUTANT GLYCOSYLASPARAGINASE
FROM FLAVOBACTERIUM MENINGOSEPTICUM
Authors : Guo, H.-C.; Xu, Q.
Deposited on : 1999-06-15
Resolution : 1.90 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
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

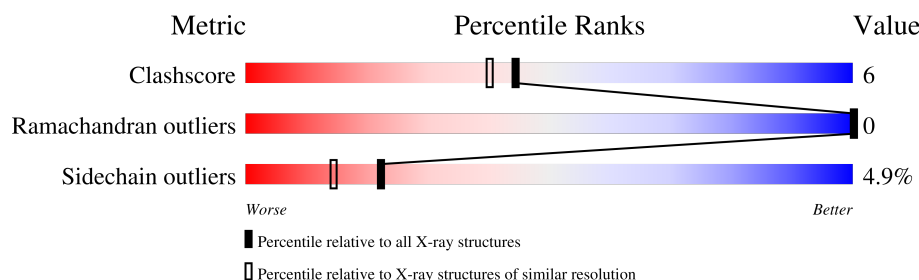
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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	295	77% 16% . . .
1	C	295	78% 17% . . .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4680 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.

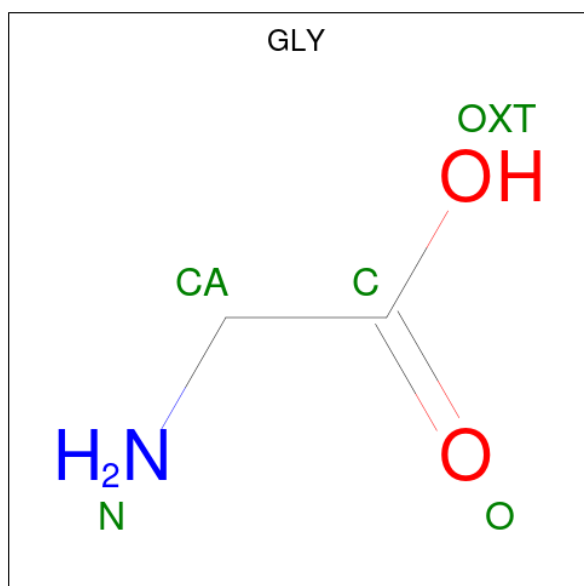
- Molecule 1 is a protein called PROTEIN (GLYCOSYLASPARAGINASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	4	0	0
			2214	1386	394	421	13			
1	C	292	Total	C	N	O	S	0	0	0
			2230	1396	397	424	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	PHE	TYR	engineered mutation	UNP Q47898
C	311	PHE	TYR	engineered mutation	UNP Q47898

- Molecule 2 is GLYCINE (CCD ID: GLY) (formula: C₂H₅NO₂).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	107	Total	O	0	0
			107	107		
3	C	119	Total	O	0	0
			119	119		

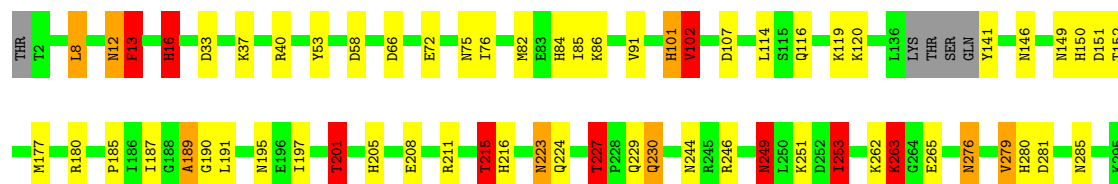
3 Residue-property plots

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.

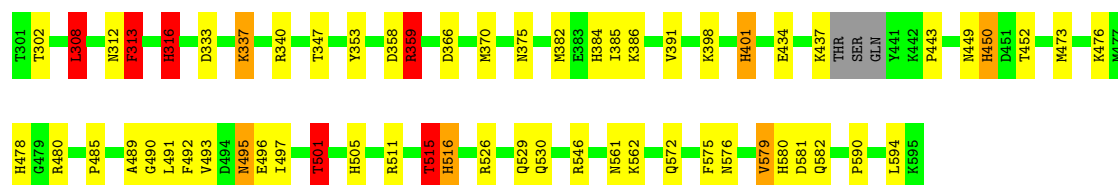
• Molecule 1: PROTEIN (GLYCOSYLASPARAGINASE)

Chain A: 



• Molecule 1: PROTEIN (GLYCOSYLASPARAGINASE)

Chain C: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	46.30 Å 52.80 Å 62.40 Å 80.80° 90.50° 105.10°	Depositor
Resolution (Å)	6.00 – 1.90	Depositor
% Data completeness (in resolution range)	97.5 (6.00-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	2.60	Depositor
Refinement program	XTALVIEW, X-PLOR 3.1	Depositor
R, R_{free}	0.196 , 0.239	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4680	wwPDB-VP
Average B, all atoms (Å ²)	8.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	1.04	8/2250 (0.4%)	1.76	48/3032 (1.6%)
1	C	1.06	10/2266 (0.4%)	1.69	37/3053 (1.2%)
All	All	1.05	18/4516 (0.4%)	1.73	85/6085 (1.4%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	478	HIS	CD2-NE2	-7.12	1.30	1.37
1	C	401	HIS	CD2-NE2	-7.04	1.30	1.37
1	A	150	HIS	CD2-NE2	-6.44	1.30	1.37
1	C	450	HIS	CD2-NE2	-6.17	1.31	1.37
1	A	253	ILE	CA-CB	5.90	1.65	1.55
1	C	316	HIS	CG-ND1	-5.85	1.31	1.38
1	C	316	HIS	CD2-NE2	-5.79	1.31	1.37
1	C	516	HIS	CD2-NE2	-5.70	1.31	1.37
1	A	84	HIS	CD2-NE2	-5.69	1.31	1.37
1	C	384	HIS	CD2-NE2	-5.58	1.31	1.37
1	A	16	HIS	CD2-NE2	-5.55	1.31	1.37
1	C	505	HIS	CD2-NE2	-5.47	1.31	1.37
1	C	580	HIS	CD2-NE2	-5.42	1.31	1.37
1	A	205	HIS	CD2-NE2	-5.34	1.31	1.37
1	A	101	HIS	CD2-NE2	-5.33	1.31	1.37
1	A	187	ILE	CA-CB	5.28	1.60	1.54
1	C	505	HIS	CG-ND1	-5.17	1.32	1.38
1	A	150	HIS	CG-ND1	-5.09	1.32	1.38

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	511	ARG	NE-CZ-NH2	-15.20	105.52	119.20
1	A	211	ARG	NE-CZ-NH2	-14.22	106.40	119.20
1	C	515	THR	N-CA-CB	-11.31	92.87	110.30
1	A	215	THR	N-CA-CB	-11.22	93.02	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	VAL	N-CA-CB	-10.99	97.28	112.12
1	C	359	ARG	CB-CG-CD	-10.91	86.20	111.30
1	C	511	ARG	NE-CZ-NH1	10.29	131.79	121.50
1	C	449	ASN	OD1-CG-ND2	-9.86	112.74	122.60
1	A	53	TYR	O-C-N	-9.43	112.36	122.07
1	A	102	VAL	CB-CA-C	9.33	119.80	110.65
1	A	211	ARG	NE-CZ-NH1	8.87	130.37	121.50
1	C	511	ARG	CD-NE-CZ	8.83	136.76	124.40
1	A	211	ARG	CD-NE-CZ	8.74	136.64	124.40
1	C	358	ASP	CA-CB-CG	8.64	121.24	112.60
1	A	12	ASN	CA-C-O	8.45	129.50	120.55
1	C	316	HIS	ND1-CG-CD2	8.43	114.53	106.10
1	A	224	GLN	OE1-CD-NE2	-8.04	114.56	122.60
1	A	276	ASN	CA-CB-CG	7.90	120.50	112.60
1	C	580	HIS	CB-CG-CD2	-7.78	121.08	131.20
1	C	313	PHE	CA-CB-CG	7.78	121.58	113.80
1	A	13	PHE	CA-CB-CG	7.77	121.57	113.80
1	A	149	ASN	OD1-CG-ND2	-7.70	114.90	122.60
1	A	40	ARG	NE-CZ-NH2	-7.61	112.35	119.20
1	A	151	ASP	N-CA-C	7.58	121.78	112.54
1	A	215	THR	OG1-CB-CG2	7.52	124.35	109.30
1	A	16	HIS	ND1-CG-CD2	7.32	113.42	106.10
1	A	280	HIS	CB-CG-CD2	-7.30	121.71	131.20
1	A	215	THR	CB-CA-C	7.28	125.24	110.38
1	C	515	THR	CB-CA-C	7.24	125.14	110.38
1	A	58	ASP	CA-CB-CG	7.16	119.76	112.60
1	A	40	ARG	CB-CG-CD	-7.12	94.93	111.30
1	A	66	ASP	CA-CB-CG	7.12	119.72	112.60
1	C	340	ARG	CB-CG-CD	-6.88	95.47	111.30
1	C	312	ASN	CA-C-O	-6.87	112.33	120.10
1	C	576	ASN	OD1-CG-ND2	-6.71	115.89	122.60
1	A	279	VAL	CB-CA-C	-6.70	100.71	110.63
1	C	579	VAL	CB-CA-C	-6.70	100.71	110.63
1	A	227	THR	N-CA-CB	-6.61	100.44	110.03
1	C	515	THR	OG1-CB-CG2	6.60	122.51	109.30
1	A	285	ASN	CA-CB-CG	6.58	119.18	112.60
1	A	230	GLN	OE1-CD-NE2	-6.55	116.05	122.60
1	C	495	ASN	OD1-CG-ND2	-6.49	116.11	122.60
1	C	511	ARG	CG-CD-NE	-6.47	97.77	112.00
1	A	280	HIS	CB-CG-ND1	6.40	132.31	122.70
1	A	53	TYR	N-CA-C	6.40	117.92	111.07
1	C	401	HIS	CB-CG-CD2	-6.39	122.89	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	TYR	CA-C-O	-6.35	114.16	120.82
1	C	384	HIS	CB-CG-CD2	-6.29	123.02	131.20
1	C	580	HIS	CB-CG-ND1	6.28	132.12	122.70
1	C	366	ASP	CA-CB-CG	6.22	118.82	112.60
1	A	211	ARG	CG-CD-NE	-6.17	98.43	112.00
1	A	281	ASP	CA-CB-CG	6.07	118.67	112.60
1	A	116	GLN	OE1-CD-NE2	-6.06	116.54	122.60
1	C	340	ARG	NE-CZ-NH2	-6.04	113.76	119.20
1	A	16	HIS	CB-CG-CD2	-5.98	123.43	131.20
1	C	511	ARG	CA-CB-CG	5.92	125.93	114.10
1	A	249	ASN	OD1-CG-ND2	-5.90	116.70	122.60
1	A	72	GLU	CB-CG-CD	5.86	122.57	112.60
1	C	449	ASN	CB-CG-ND2	5.85	125.17	116.40
1	A	211	ARG	CA-CB-CG	5.71	125.52	114.10
1	A	227	THR	CA-C-O	-5.67	114.30	120.87
1	A	189	ALA	CA-C-O	-5.64	113.16	119.98
1	C	581	ASP	CA-CB-CG	5.57	118.17	112.60
1	C	316	HIS	CG-CD2-NE2	-5.44	101.76	107.20
1	A	244	ASN	OD1-CG-ND2	-5.43	117.17	122.60
1	A	16	HIS	CG-CD2-NE2	-5.33	101.88	107.20
1	C	452	THR	CA-C-N	-5.28	116.26	123.12
1	C	452	THR	C-N-CA	-5.28	116.26	123.12
1	C	501	THR	N-CA-CB	5.24	120.67	111.55
1	C	582	GLN	OE1-CD-NE2	-5.22	117.38	122.60
1	C	302	THR	N-CA-C	-5.20	99.97	108.76
1	A	223	ASN	OD1-CG-ND2	-5.17	117.43	122.60
1	A	263	LYS	CG-CD-CE	5.16	123.16	111.30
1	C	561	ASN	CA-CB-CG	5.16	117.76	112.60
1	C	530	GLN	OE1-CD-NE2	-5.13	117.47	122.60
1	A	91	VAL	N-CA-C	-5.12	105.55	110.72
1	A	146	ASN	OD1-CG-ND2	-5.11	117.49	122.60
1	A	205	HIS	CB-CG-CD2	-5.11	124.56	131.20
1	C	308	LEU	CA-CB-CG	5.09	134.12	116.30
1	A	201	THR	N-CA-CB	5.08	120.38	111.55
1	C	391	VAL	N-CA-C	-5.04	105.63	110.72
1	A	107	ASP	CA-CB-CG	5.03	117.63	112.60
1	C	501	THR	CB-CA-C	-5.03	99.48	109.79
1	A	152	THR	CA-C-N	-5.00	116.61	123.12
1	A	152	THR	C-N-CA	-5.00	116.61	123.12

There are no chirality outliers.

There are no planarity outliers.

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	2214	0	2209	30	0
1	C	2230	0	2229	32	0
2	A	5	0	2	0	0
2	C	5	0	2	0	0
3	A	107	0	0	2	0
3	C	119	0	0	3	0
All	All	4680	0	4442	53	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 6.

All (53) 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:216:HIS:HD2	1:C:516:HIS:HD2	1.18	0.91
1:A:208:GLU:HG3	1:A:253:ILE:HD12	1.52	0.89
1:A:227:THR:HG22	1:A:230:GLN:H	1.43	0.84
1:A:33:ASP:O	1:A:37:LYS:HE2	1.92	0.69
1:A:8:LEU:HD22	1:A:279:VAL:HG13	1.77	0.67
1:A:12:ASN:ND2	1:A:276:ASN:HD21	1.93	0.66
1:A:189:ALA:O	1:A:215:THR:HB	1.97	0.65
1:C:308:LEU:HD22	1:C:579:VAL:HG13	1.78	0.64
1:C:489:ALA:O	1:C:515:THR:HB	1.97	0.64
1:C:495:ASN:O	1:C:562:LYS:HD3	2.00	0.62
1:C:347:THR:HG21	3:C:722:HOH:O	2.00	0.62
1:A:195:ASN:O	1:A:262:LYS:HD3	1.99	0.61
1:A:249:ASN:HD22	1:A:251:LYS:H	1.49	0.61
1:C:496:GLU:HB2	1:C:497:ILE:HD12	1.83	0.61
1:C:333:ASP:O	1:C:337:LYS:HE2	2.01	0.60
1:A:75:ASN:ND2	1:C:546:ARG:HE	2.02	0.57
1:A:76:ILE:HG13	1:A:102:VAL:HG22	1.87	0.57
1:A:114:LEU:HD21	1:A:120:LYS:HG3	1.90	0.54
1:A:216:HIS:CD2	1:C:516:HIS:HD2	2.10	0.52
1:A:227:THR:HB	1:A:230:GLN:CD	2.35	0.52
1:A:216:HIS:HD2	1:C:516:HIS:CD2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:359:ARG:HD3	1:C:476:LYS:O	2.12	0.49
1:C:575:PHE:O	1:C:590:PRO:HD2	2.13	0.49
1:A:197:ILE:HD13	1:A:223:ASN:HB2	1.95	0.48
1:C:313:PHE:HA	1:C:316:HIS:CE1	2.49	0.47
1:C:386:LYS:HE3	1:C:386:LYS:HB2	1.62	0.47
1:A:190:GLY:O	1:A:201:THR:HG22	2.15	0.46
1:A:263:LYS:HG3	3:A:814:HOH:O	2.16	0.46
1:C:398:LYS:NZ	3:C:615:HOH:O	2.46	0.46
1:C:490:GLY:O	1:C:501:THR:HG22	2.16	0.46
1:C:382:MET:HE3	1:C:385:ILE:HB	1.98	0.45
1:A:246:ARG:HE	1:C:375:ASN:ND2	2.14	0.45
1:C:353:TYR:HB2	1:C:386:LYS:HG3	1.99	0.45
1:A:177:MET:H	1:C:401:HIS:CE1	2.36	0.44
1:A:13:PHE:HA	1:A:16:HIS:NE2	2.32	0.44
1:A:86:LYS:HE3	1:A:86:LYS:HB2	1.67	0.44
1:A:101:HIS:CG	1:C:480:ARG:HG3	2.53	0.44
1:A:141:TYR:HA	3:A:748:HOH:O	2.17	0.44
1:C:434:GLU:OE1	1:C:437:LYS:NZ	2.51	0.43
1:C:443:PRO:CB	1:C:473:MET:HE2	2.48	0.43
1:C:450:HIS:HE1	3:C:801:HOH:O	2.00	0.43
1:A:13:PHE:HA	1:A:16:HIS:CE1	2.54	0.43
1:A:177:MET:H	1:C:401:HIS:HE1	1.66	0.43
1:C:316:HIS:ND1	1:C:316:HIS:N	2.66	0.42
1:A:82:MET:HE3	1:A:85:ILE:HB	2.01	0.42
1:C:313:PHE:HA	1:C:316:HIS:NE2	2.34	0.41
1:C:572:GLN:HG2	1:C:594:LEU:HD23	2.01	0.41
1:A:180:ARG:HG3	1:C:401:HIS:CD2	2.56	0.41
1:C:491:LEU:N	1:C:515:THR:HG21	2.35	0.41
1:A:263:LYS:NZ	1:A:265:GLU:CD	2.79	0.40
1:C:492:PHE:HB2	1:C:515:THR:HG23	2.03	0.40
1:A:191:LEU:N	1:A:215:THR:HG21	2.36	0.40
1:C:370:MET:HG2	1:C:493:VAL:HB	2.03	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	286/295 (97%)	279 (98%)	7 (2%)	0	100	100
1	C	288/295 (98%)	281 (98%)	7 (2%)	0	100	100
All	All	574/590 (97%)	560 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	233/238 (98%)	220 (94%)	13 (6%)	19	11
1	C	235/238 (99%)	225 (96%)	10 (4%)	26	18
All	All	468/476 (98%)	445 (95%)	23 (5%)	22	14

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	13	PHE
1	A	16	HIS
1	A	102	VAL
1	A	119	LYS
1	A	185	PRO
1	A	201	THR
1	A	215	THR
1	A	227	THR
1	A	229	GLN
1	A	249	ASN
1	A	253	ILE
1	A	263	LYS
1	C	308	LEU

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Mol	Chain	Res	Type
1	C	313	PHE
1	C	316	HIS
1	C	337	LYS
1	C	359	ARG
1	C	485	PRO
1	C	501	THR
1	C	515	THR
1	C	526	ARG
1	C	529	GLN

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	12	ASN
1	A	75	ASN
1	A	161	GLN
1	A	216	HIS
1	A	249	ASN
1	A	276	ASN
1	C	312	ASN
1	C	375	ASN
1	C	384	HIS
1	C	450	HIS
1	C	516	HIS
1	C	576	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	$\# Z > 2$
2	GLY	C	596	-	4,4,4	1.28	1 (25%)	3,4,4	0.98	0
2	GLY	A	296	-	4,4,4	1.40	1 (25%)	3,4,4	1.04	0

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	GLY	C	596	-	-	1/2/2/2	-
2	GLY	A	296	-	-	1/2/2/2	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	296	GLY	OXT-C	-2.64	1.22	1.30
2	C	596	GLY	OXT-C	-2.32	1.23	1.30

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	296	GLY	OXT-C-CA-N
2	C	596	GLY	OXT-C-CA-N

There are no ring outliers.

No monomer is involved in short contacts.

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.