Full wwPDB X-ray Structure Validation Report (i)

Sep 14, 2023 – 06:29 AM EDT

PDB ID	:	9GAC
Title	:	PRECURSOR OF THE T152C 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 (i) 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 (i)) were used in the production of this report:

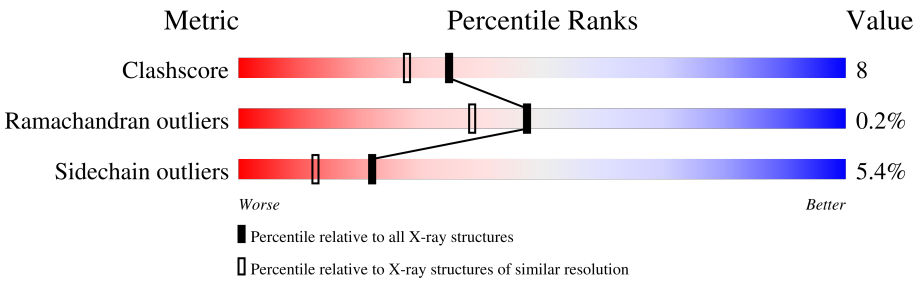
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	295	67% 21% 5% • 5%
1	C	295	72% 19% • • 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4423 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.

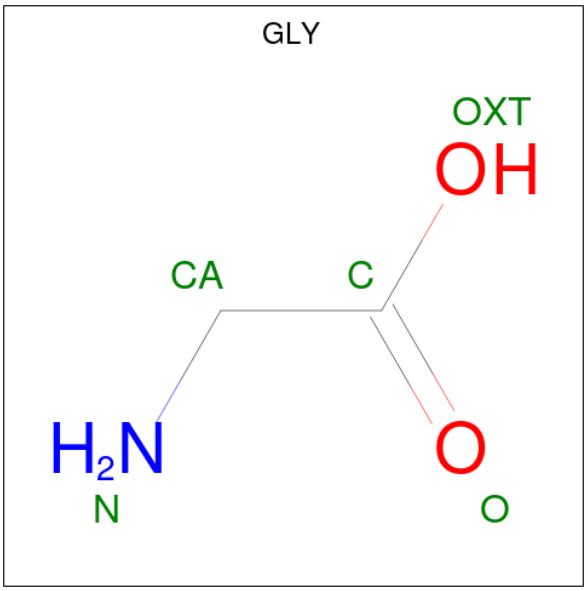
- Molecule 1 is a protein called PROTEIN (GLYCOSYLASPARAGINASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	280	2130	1331	381	404	14	0	0	0
1	C	280	2132	1333	382	403	14	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	CYS	THR	engineered mutation	UNP Q47898
C	452	CYS	THR	engineered mutation	UNP Q47898

- Molecule 2 is GLYCINE (three-letter code: GLY) (formula: $C_2H_5NO_2$).



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

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	76	76	76	0	0
			Total	O		
3	C	75	75	75	0	0

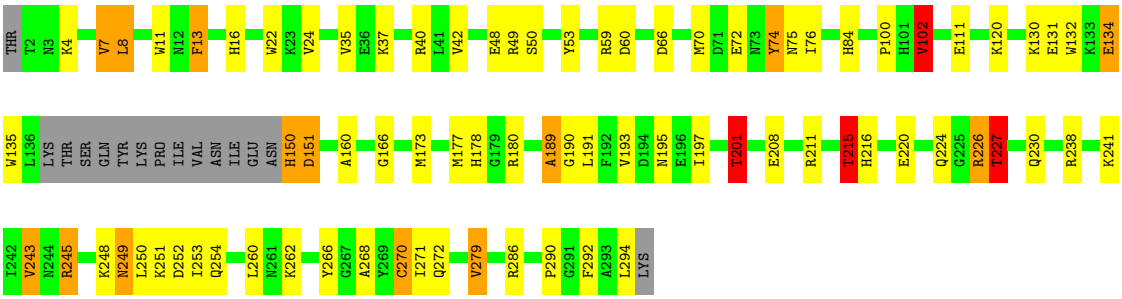
3 Residue-property plots (i)

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.

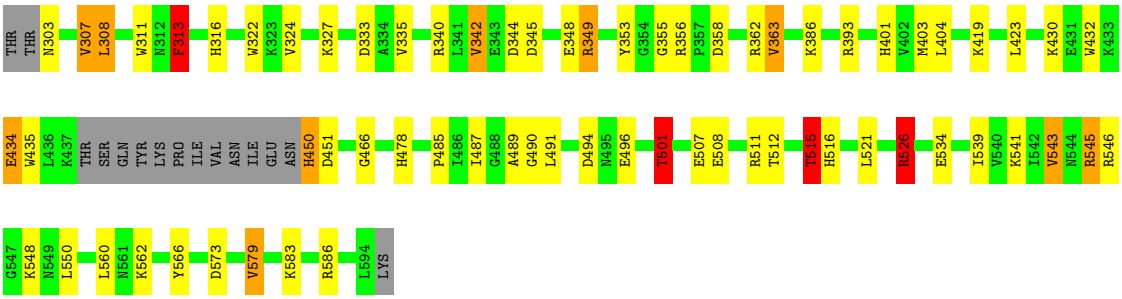
• Molecule 1: PROTEIN (GLYCOSYLASPARAGINASE)

Chain A: 67% 21% 5% • 5%



• Molecule 1: PROTEIN (GLYCOSYLASPARAGINASE)

Chain C: 72% 19% • • 5%



4 Data and refinement statistics (i)

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	46.30Å 52.80Å 62.40Å 80.80° 90.50° 105.10°	Depositor
Resolution (Å)	6.00 – 1.90	Depositor
% Data completeness (in resolution range)	92.8 (6.00-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	5.60	Depositor
Refinement program	XTALVIEW, X-PLOR 3.1	Depositor
R, R_{free}	0.232 , 0.278	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4423	wwPDB-VP
Average B, all atoms (Å^2)	10.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.95	1/2165 (0.0%)	2.00	66/2919 (2.3%)
1	C	0.96	0/2167	2.02	62/2920 (2.1%)
All	All	0.95	1/4332 (0.0%)	2.01	128/5839 (2.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	270	CYS	CA-CB	-5.21	1.42	1.53

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	211	ARG	NE-CZ-NH2	-26.46	107.07	120.30
1	C	511	ARG	NE-CZ-NH2	-25.85	107.38	120.30
1	A	40	ARG	NE-CZ-NH2	-25.66	107.47	120.30
1	C	340	ARG	NE-CZ-NH2	-23.14	108.73	120.30
1	C	526	ARG	NE-CZ-NH1	22.86	131.73	120.30
1	C	526	ARG	NE-CZ-NH2	-19.79	110.41	120.30
1	C	340	ARG	NE-CZ-NH1	18.87	129.73	120.30
1	A	40	ARG	NE-CZ-NH1	17.16	128.88	120.30
1	C	543	VAL	CG1-CB-CG2	-14.47	87.75	110.90
1	A	211	ARG	NE-CZ-NH1	13.55	127.07	120.30
1	C	362	ARG	NE-CZ-NH2	-13.12	113.74	120.30
1	A	59	ARG	NE-CZ-NH2	-12.72	113.94	120.30
1	C	511	ARG	NE-CZ-NH1	12.21	126.40	120.30
1	A	243	VAL	CG1-CB-CG2	-11.58	92.37	110.90
1	A	226	ARG	NE-CZ-NH2	-11.46	114.57	120.30
1	A	215	THR	N-CA-CB	-11.29	88.85	110.30
1	C	515	THR	N-CA-CB	-10.32	90.68	110.30
1	A	53	TYR	CA-C-N	9.83	135.86	116.20
1	A	245	ARG	NE-CZ-NH1	9.65	125.12	120.30
1	A	7	VAL	CB-CA-C	-9.10	94.12	111.40
1	C	545	ARG	NE-CZ-NH1	8.86	124.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	VAL	CG1-CB-CG2	8.81	125.00	110.90
1	C	511	ARG	CA-CB-CG	8.69	132.52	113.40
1	C	307	VAL	CB-CA-C	-8.55	95.15	111.40
1	A	74	TYR	CB-CG-CD1	-8.49	115.91	121.00
1	A	211	ARG	CD-NE-CZ	8.32	135.25	123.60
1	A	135	TRP	CD1-CG-CD2	8.28	112.92	106.30
1	C	573	ASP	CB-CG-OD2	-8.05	111.06	118.30
1	A	226	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	A	132	TRP	CE2-CD2-CG	-7.99	100.91	107.30
1	C	494	ASP	CB-CG-OD1	7.90	125.41	118.30
1	C	432	TRP	CD1-CG-CD2	7.85	112.58	106.30
1	A	132	TRP	CD1-CG-CD2	7.81	112.55	106.30
1	A	49	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	A	270	CYS	CB-CA-C	-7.57	95.26	110.40
1	A	22	TRP	CD1-CG-CD2	7.54	112.33	106.30
1	A	135	TRP	CE2-CD2-CG	-7.44	101.34	107.30
1	C	526	ARG	CD-NE-CZ	7.43	134.00	123.60
1	C	435	TRP	CD1-CG-CD2	7.41	112.23	106.30
1	C	573	ASP	CB-CG-OD1	7.36	124.93	118.30
1	C	511	ARG	CD-NE-CZ	7.29	133.81	123.60
1	A	102	VAL	N-CA-CB	-7.19	95.68	111.50
1	C	340	ARG	CD-NE-CZ	7.10	133.53	123.60
1	C	432	TRP	CE2-CD2-CG	-7.08	101.64	107.30
1	C	487	ILE	CA-C-N	7.07	130.34	116.20
1	A	40	ARG	CB-CG-CD	-6.86	93.77	111.60
1	A	24	VAL	CG1-CB-CG2	-6.86	99.93	110.90
1	A	35	VAL	CA-CB-CG1	-6.85	100.62	110.90
1	A	59	ARG	CB-CG-CD	-6.84	93.82	111.60
1	C	435	TRP	CE2-CD2-CG	-6.82	101.84	107.30
1	C	541	LYS	CA-CB-CG	-6.75	98.55	113.40
1	A	49	ARG	NE-CZ-NH2	-6.75	116.93	120.30
1	C	308	LEU	CA-CB-CG	6.74	130.80	115.30
1	A	22	TRP	CE2-CD2-CG	-6.72	101.92	107.30
1	C	322	TRP	CD1-CG-CD2	6.72	111.67	106.30
1	A	227	THR	N-CA-CB	-6.71	97.56	110.30
1	C	322	TRP	CE2-CD2-CG	-6.66	101.97	107.30
1	C	393	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	A	35	VAL	CA-CB-CG2	6.52	120.68	110.90
1	C	579	VAL	CB-CA-C	-6.47	99.11	111.40
1	C	340	ARG	CB-CG-CD	-6.43	94.89	111.60
1	A	211	ARG	CA-CB-CG	6.41	127.49	113.40
1	C	335	VAL	CA-CB-CG1	-6.38	101.34	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	241	LYS	CA-CB-CG	-6.37	99.39	113.40
1	A	53	TYR	O-C-N	-6.31	112.47	123.20
1	C	363	VAL	CG1-CB-CG2	-6.29	100.84	110.90
1	A	8	LEU	CA-CB-CG	6.28	129.74	115.30
1	A	40	ARG	CD-NE-CZ	6.25	132.34	123.60
1	A	211	ARG	CG-CD-NE	-6.21	98.75	111.80
1	C	560	LEU	CA-CB-CG	6.21	129.58	115.30
1	A	201	THR	N-CA-CB	6.20	122.08	110.30
1	C	511	ARG	NH1-CZ-NH2	6.20	126.22	119.40
1	C	487	ILE	O-C-N	-6.19	112.67	123.20
1	A	40	ARG	CG-CD-NE	-6.16	98.87	111.80
1	A	189	ALA	CA-C-N	6.14	128.47	116.20
1	C	451	ASP	CB-CG-OD2	6.10	123.79	118.30
1	C	313	PHE	CB-CG-CD2	-6.10	116.53	120.80
1	C	403	MET	CG-SD-CE	6.07	109.91	100.20
1	A	279	VAL	CB-CA-C	-6.04	99.92	111.40
1	C	333	ASP	CB-CG-OD1	6.03	123.72	118.30
1	C	353	TYR	CB-CG-CD2	-6.03	117.39	121.00
1	A	260	LEU	CA-CB-CG	5.95	128.97	115.30
1	A	226	ARG	CA-CB-CG	5.93	126.45	113.40
1	A	227	THR	OG1-CB-CG2	5.85	123.46	110.00
1	C	511	ARG	CG-CD-NE	-5.83	99.57	111.80
1	C	356	ARG	NE-CZ-NH2	5.82	123.21	120.30
1	A	211	ARG	NH1-CZ-NH2	5.82	125.81	119.40
1	A	7	VAL	N-CA-CB	5.81	124.27	111.50
1	C	434	GLU	CB-CG-CD	5.79	129.83	114.20
1	A	215	THR	CB-CA-C	5.75	127.13	111.60
1	C	345	ASP	CB-CG-OD1	5.70	123.43	118.30
1	C	303	ASN	CA-CB-CG	-5.65	100.97	113.40
1	A	252	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	11	TRP	CE2-CD2-CG	-5.62	102.81	107.30
1	C	342	VAL	CG1-CB-CG2	-5.60	101.94	110.90
1	C	508	GLU	OE1-CD-OE2	-5.60	116.58	123.30
1	C	307	VAL	N-CA-CB	5.59	123.80	111.50
1	C	450	HIS	CA-CB-CG	5.55	123.04	113.60
1	A	134	GLU	CB-CG-CD	5.52	129.11	114.20
1	A	102	VAL	CB-CA-C	5.52	121.89	111.40
1	A	238	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	C	349	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	74	TYR	CD1-CG-CD2	5.47	123.92	117.90
1	A	7	VAL	CA-CB-CG1	-5.46	102.72	110.90
1	A	173	MET	CG-SD-CE	5.36	108.77	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	ASP	N-CA-C	5.32	125.37	111.00
1	A	150	HIS	CA-CB-CG	5.31	122.63	113.60
1	C	307	VAL	CA-CB-CG1	-5.27	103.00	110.90
1	A	270	CYS	N-CA-CB	5.26	120.08	110.60
1	C	583	LYS	CA-C-N	5.25	126.70	116.20
1	C	340	ARG	CA-CB-CG	5.25	124.95	113.40
1	C	450	HIS	O-C-N	-5.24	114.32	122.70
1	A	131	GLU	OE1-CD-OE2	-5.22	117.03	123.30
1	C	324	VAL	CG1-CB-CG2	-5.21	102.56	110.90
1	A	37	LYS	CB-CA-C	-5.21	99.99	110.40
1	C	358	ASP	CB-CG-OD1	5.19	122.97	118.30
1	C	335	VAL	CA-CB-CG2	5.18	118.67	110.90
1	A	66	ASP	CB-CG-OD1	5.16	122.95	118.30
1	A	151	ASP	CB-CG-OD2	5.16	122.95	118.30
1	C	583	LYS	CB-CG-CD	5.16	125.02	111.60
1	A	13	PHE	CB-CG-CD1	5.16	124.41	120.80
1	A	243	VAL	CA-CB-CG2	5.16	118.64	110.90
1	C	327	LYS	CA-CB-CG	-5.15	102.08	113.40
1	C	515	THR	CB-CA-C	5.12	125.43	111.60
1	C	501	THR	N-CA-CB	5.12	120.03	110.30
1	A	40	ARG	CA-CB-CG	5.11	124.65	113.40
1	C	450	HIS	CA-C-N	5.11	128.44	117.20
1	A	208	GLU	OE1-CD-OE2	-5.07	117.22	123.30

There are no chirality outliers.

There are no planarity outliers.

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	2130	0	2117	49	0
1	C	2132	0	2123	38	0
2	A	5	0	2	0	0
2	C	5	0	2	0	0
3	A	76	0	0	0	0
3	C	75	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4423	0	4244	71	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 8.

All (71) 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	0.89
1:A:249:ASN:HD22	1:A:251:LYS:H	1.34	0.75
1:A:250:LEU:HD23	1:A:294:LEU:HD13	1.74	0.70
1:A:216:HIS:CD2	1:C:516:HIS:HD2	2.08	0.68
1:C:308:LEU:HD22	1:C:579:VAL:HG13	1.76	0.67
1:A:8:LEU:HD22	1:A:279:VAL:HG13	1.76	0.67
1:A:227:THR:HG22	1:A:230:GLN:H	1.60	0.66
1:C:430:LYS:O	1:C:434:GLU:HG3	1.97	0.65
1:A:220:GLU:HG3	1:A:224:GLN:HE21	1.61	0.65
1:A:245:ARG:NH2	1:C:496:GLU:HG2	2.12	0.64
1:A:130:LYS:O	1:A:134:GLU:HG3	1.98	0.63
1:A:74:TYR:OH	1:C:545:ARG:NH2	2.32	0.63
1:C:489:ALA:O	1:C:515:THR:HB	1.98	0.62
1:A:189:ALA:O	1:A:215:THR:HB	2.01	0.61
1:A:42:VAL:HG13	1:A:48:GLU:HG2	1.83	0.60
1:A:75:ASN:ND2	1:C:546:ARG:HE	2.00	0.59
1:C:526:ARG:HD3	1:C:534:GLU:OE1	2.03	0.58
1:A:216:HIS:HD2	1:C:516:HIS:CD2	2.10	0.57
1:A:76:ILE:HG13	1:A:102:VAL:HG22	1.88	0.56
1:A:177:MET:HE2	1:C:404:LEU:HD21	1.87	0.56
1:A:177:MET:CE	1:C:404:LEU:HD21	2.36	0.56
1:A:249:ASN:ND2	1:A:251:LYS:H	2.01	0.56
1:A:4:LYS:NZ	1:A:160:ALA:O	2.39	0.54
1:A:216:HIS:HE1	3:C:683:HOH:O	1.93	0.51
1:C:466:GLY:HA3	1:C:491:LEU:HD11	1.92	0.50
1:A:8:LEU:CD2	1:A:279:VAL:HG13	2.41	0.50
1:A:245:ARG:HH22	1:C:496:GLU:HG2	1.76	0.50
1:C:308:LEU:CD2	1:C:579:VAL:HG13	2.42	0.49
1:A:180:ARG:HG3	1:C:401:HIS:CD2	2.46	0.49
1:C:430:LYS:NZ	1:C:434:GLU:OE2	2.45	0.49
1:C:543:VAL:HG11	1:C:550:LEU:HD13	1.95	0.49
1:A:190:GLY:O	1:A:201:THR:HG22	2.12	0.49
1:A:70:MET:HG2	1:A:193:VAL:HB	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ALA:HB3	1:A:290:PRO:HB3	1.94	0.48
1:A:243:VAL:HG23	1:A:248:LYS:HB2	1.96	0.47
1:C:490:GLY:O	1:C:501:THR:HG22	2.15	0.47
1:A:130:LYS:NZ	1:A:134:GLU:OE2	2.48	0.47
1:A:177:MET:HE3	1:C:404:LEU:HD11	1.96	0.47
1:A:177:MET:H	1:C:401:HIS:HE1	1.63	0.46
1:A:102:VAL:HB	1:C:507:GLU:HG3	1.96	0.46
1:A:270:CYS:O	1:A:292:PHE:HA	2.15	0.46
1:C:363:VAL:HG11	1:C:423:LEU:HB2	1.98	0.46
1:C:308:LEU:HD11	1:C:566:TYR:HB2	1.97	0.46
1:C:512:THR:HG21	1:C:539:ILE:HG12	1.97	0.46
1:A:177:MET:HE2	1:A:177:MET:HB2	1.79	0.45
1:A:249:ASN:HD22	1:A:251:LYS:N	2.09	0.45
1:A:111:GLU:OE2	1:C:478:HIS:HD2	2.00	0.45
1:C:311:TRP:HB2	1:C:313:PHE:CE1	2.51	0.45
1:C:311:TRP:HB3	1:C:450:HIS:ND1	2.32	0.45
1:C:543:VAL:HG23	1:C:548:LYS:HB2	1.98	0.45
1:A:8:LEU:HD11	1:A:266:TYR:HB2	1.99	0.44
1:A:243:VAL:HG11	1:A:250:LEU:CD1	2.48	0.43
1:C:342:VAL:HG13	1:C:348:GLU:HG2	2.01	0.43
1:C:562:LYS:HA	1:C:562:LYS:HD2	1.70	0.43
1:A:177:MET:H	1:C:401:HIS:CE1	2.37	0.43
1:A:72:GLU:O	1:A:195:ASN:HB2	2.18	0.43
1:A:271:ILE:HG22	1:A:272:GLN:HG3	2.00	0.42
1:C:342:VAL:CG1	1:C:348:GLU:HG2	2.49	0.42
1:A:243:VAL:HG11	1:A:250:LEU:HD13	1.99	0.42
1:C:311:TRP:CE2	1:C:450:HIS:HA	2.55	0.42
1:C:344:ASP:OD1	1:C:386:LYS:HE3	2.19	0.42
1:C:521:LEU:HB3	1:C:526:ARG:HD2	2.01	0.42
1:A:197:ILE:HD13	1:A:197:ILE:HG21	1.85	0.42
1:A:60:ASP:OD2	1:A:178:HIS:HB2	2.20	0.41
1:A:84:HIS:HB3	1:A:120:LYS:HG3	2.02	0.41
1:A:195:ASN:O	1:A:262:LYS:HD3	2.21	0.41
1:A:166:GLY:HA3	1:A:191:LEU:HD11	2.01	0.41
1:A:272:GLN:HG2	1:A:294:LEU:HD23	2.02	0.41
1:C:349:ARG:O	1:C:355:GLY:HA2	2.20	0.41
1:A:111:GLU:OE2	1:C:478:HIS:CD2	2.73	0.41
1:A:191:LEU:N	1:A:215:THR:HG21	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	276/295 (94%)	264 (96%)	11 (4%)	1 (0%)	34 24
1	C	276/295 (94%)	270 (98%)	6 (2%)	0	100 100
All	All	552/590 (94%)	534 (97%)	17 (3%)	1 (0%)	47 38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	ASP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	223/238 (94%)	208 (93%)	15 (7%)	16 7
1	C	223/238 (94%)	214 (96%)	9 (4%)	31 22
All	All	446/476 (94%)	422 (95%)	24 (5%)	22 13

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	13	PHE
1	A	16	HIS
1	A	50	SER
1	A	100	PRO

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Mol	Chain	Res	Type
1	A	102	VAL
1	A	150	HIS
1	A	201	THR
1	A	215	THR
1	A	226	ARG
1	A	227	THR
1	A	249	ASN
1	A	253	ILE
1	A	254	GLN
1	A	286	ARG
1	C	307	VAL
1	C	313	PHE
1	C	316	HIS
1	C	419	LYS
1	C	485	PRO
1	C	501	THR
1	C	515	THR
1	C	526	ARG
1	C	586	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	150	HIS
1	A	216	HIS
1	A	224	GLN
1	A	249	ASN
1	C	312	ASN
1	C	375	ASN
1	C	478	HIS
1	C	516	HIS
1	C	576	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 monosaccharides 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	$\#\|Z\| > 2$
2	GLY	C	596	-	4,4,4	1.31	1 (25%)	3,4,4	1.54	1 (33%)
2	GLY	A	296	-	4,4,4	1.38	1 (25%)	3,4,4	1.20	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	-	-	0/2/2/2	-
2	GLY	A	296	-	-	0/2/2/2	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	296	GLY	OXT-C	-2.62	1.21	1.30
2	C	596	GLY	OXT-C	-2.46	1.22	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	596	GLY	OXT-C-CA	2.01	121.44	113.45

There are no chirality outliers.

There are no torsion outliers.

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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.