Full wwPDB X-ray Structure Validation Report ⓘ

Feb 2, 2016 – 12:02 AM GMT

PDB ID	:	9GAA
Title	:	PRECURSOR OF THE T152A MUTANT GLYCOSYLASPARAGINASE FROM FLAVOBACTERIUM MENINGOSEPTICUM
Authors	:	Guo, H.-C.; Xu, Q.
Deposited on	:	1999-06-15
Resolution	:	2.10 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

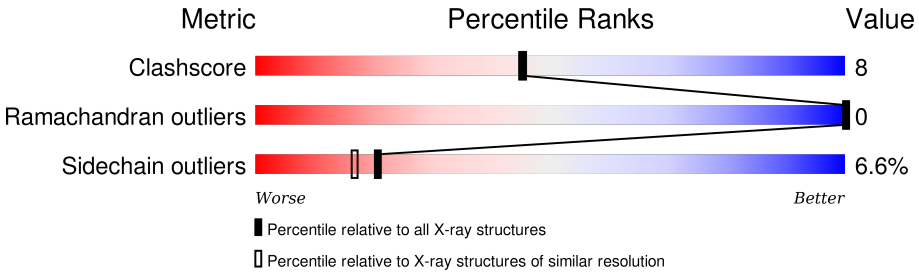
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.10 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	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	295	71% 18% • • 5%
1	C	295	68% 20% 5% • 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4362 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	279	Total	C	N	O	S	0	0	0
			2119	1325	378	403	13			
1	C	279	Total	C	N	O	S	0	0	0
			2119	1325	378	403	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	ALA	THR	MUTATION	UNP Q47898
C	452	ALA	THR	MUTATION	UNP Q47898

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	61	Total	O	0	0
			61	61		
2	C	63	Total	O	0	0
			63	63		

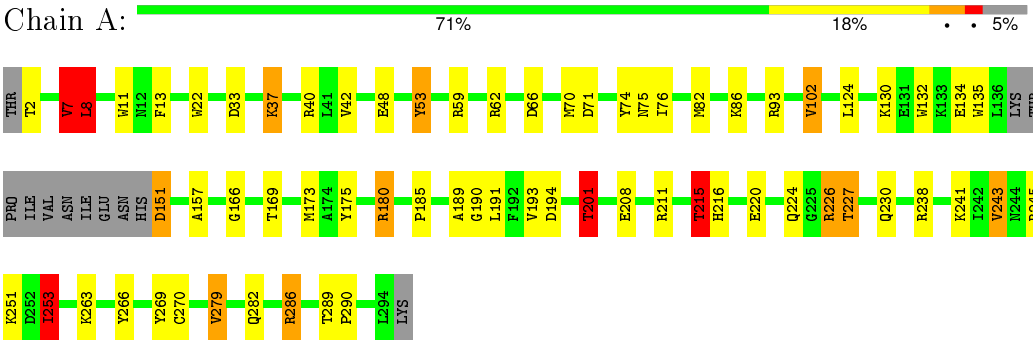
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

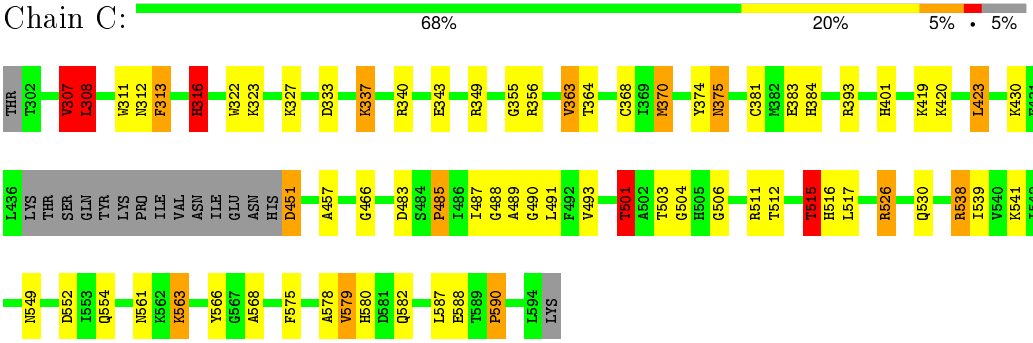
- Molecule 1: PROTEIN (GLYCOSYLASPARAGINASE)

Chain A:



- Molecule 1: PROTEIN (GLYCOSYLASPARAGINASE)

Chain C:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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 – 2.10	Depositor
% Data completeness (in resolution range)	89.8 (6.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	7.60	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.232 , 0.297	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4362	wwPDB-VP
Average B, all atoms (Å^2)	10.0	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	1.02	3/2153 (0.1%)	1.74	44/2903 (1.5%)
1	C	1.01	2/2153 (0.1%)	1.73	42/2903 (1.4%)
All	All	1.01	5/4306 (0.1%)	1.74	86/5806 (1.5%)

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	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	243	VAL	CA-CB	6.30	1.68	1.54
1	C	543	VAL	CA-CB	5.68	1.66	1.54
1	C	488	GLY	N-CA	5.55	1.54	1.46
1	A	169	THR	CA-CB	5.26	1.67	1.53
1	A	253	ILE	CA-CB	5.11	1.66	1.54

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	211	ARG	NE-CZ-NH2	-17.83	111.39	120.30
1	C	511	ARG	NE-CZ-NH2	-16.14	112.23	120.30
1	A	40	ARG	NE-CZ-NH2	-13.81	113.39	120.30
1	C	340	ARG	NE-CZ-NH2	-13.71	113.45	120.30
1	C	526	ARG	NE-CZ-NH1	12.96	126.78	120.30
1	C	526	ARG	NE-CZ-NH2	-11.34	114.63	120.30
1	A	215	THR	N-CA-CB	-9.37	92.50	110.30
1	A	22	TRP	CD1-CG-CD2	9.37	113.79	106.30
1	A	40	ARG	NE-CZ-NH1	8.95	124.77	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	226	ARG	NE-CZ-NH1	8.75	124.68	120.30
1	C	451	ASP	CB-CG-OD2	8.59	126.03	118.30
1	C	432	TRP	CD1-CG-CD2	8.49	113.09	106.30
1	A	22	TRP	CE2-CD2-CG	-8.27	100.69	107.30
1	A	132	TRP	CD1-CG-CD2	8.27	112.91	106.30
1	C	538	ARG	NE-CZ-NH2	-8.19	116.21	120.30
1	C	487	ILE	CA-C-N	8.07	132.34	116.20
1	C	393	ARG	NE-CZ-NH1	7.97	124.28	120.30
1	C	393	ARG	NE-CZ-NH2	-7.95	116.33	120.30
1	C	515	THR	N-CA-CB	-7.82	95.44	110.30
1	C	435	TRP	CD1-CG-CD2	7.79	112.53	106.30
1	A	7	VAL	CB-CA-C	-7.78	96.61	111.40
1	C	356	ARG	NE-CZ-NH2	-7.63	116.49	120.30
1	C	322	TRP	CD1-CG-CD2	7.43	112.24	106.30
1	A	135	TRP	CD1-CG-CD2	7.41	112.22	106.30
1	A	11	TRP	CE2-CD2-CG	-7.26	101.49	107.30
1	C	322	TRP	CE2-CD2-CG	-7.25	101.50	107.30
1	A	11	TRP	CD1-CG-CD2	7.23	112.08	106.30
1	C	432	TRP	CE2-CD2-CG	-7.15	101.58	107.30
1	C	307	VAL	CB-CA-C	-7.14	97.83	111.40
1	A	53	TYR	CA-C-N	7.10	130.41	116.20
1	C	435	TRP	CE2-CD2-CG	-7.08	101.63	107.30
1	A	8	LEU	CA-CB-CG	7.05	131.53	115.30
1	A	93	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	A	132	TRP	CE2-CD2-CG	-6.93	101.76	107.30
1	C	308	LEU	CA-CB-CG	6.76	130.84	115.30
1	A	211	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	A	180	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	A	173	MET	CG-SD-CE	6.65	110.84	100.20
1	A	135	TRP	CE2-CD2-CG	-6.65	101.98	107.30
1	C	311	TRP	CE2-CD2-CG	-6.64	101.99	107.30
1	A	201	THR	N-CA-CB	6.61	122.86	110.30
1	C	374	TYR	CB-CG-CD2	-6.60	117.04	121.00
1	A	238	ARG	NE-CZ-NH2	-6.45	117.07	120.30
1	C	487	ILE	O-C-N	-6.31	112.48	123.20
1	C	511	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	A	238	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	C	340	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	C	311	TRP	CD1-CG-CD2	6.11	111.18	106.30
1	A	82	MET	CG-SD-CE	6.10	109.95	100.20
1	A	40	ARG	CB-CG-CD	-5.96	96.10	111.60
1	C	313	PHE	CB-CG-CD2	-5.96	116.63	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	579	VAL	CB-CA-C	-5.92	100.16	111.40
1	A	227	THR	N-CA-CB	-5.89	99.11	110.30
1	C	316	HIS	ND1-CG-CD2	5.87	117.02	108.80
1	A	53	TYR	O-C-N	-5.77	113.39	123.20
1	A	71	ASP	CB-CG-OD1	5.76	123.49	118.30
1	A	93	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	C	432	TRP	CG-CD1-NE1	-5.63	104.47	110.10
1	A	59	ARG	CB-CG-CD	-5.62	96.98	111.60
1	A	66	ASP	CB-CG-OD1	5.62	123.35	118.30
1	A	279	VAL	CB-CA-C	-5.61	100.75	111.40
1	C	511	ARG	CA-CB-CG	5.58	125.67	113.40
1	A	270	CYS	CB-CA-C	-5.55	99.31	110.40
1	C	511	ARG	CG-CD-NE	-5.55	100.15	111.80
1	A	151	ASP	CB-CG-OD1	5.52	123.26	118.30
1	A	194	ASP	CB-CG-OD1	5.51	123.26	118.30
1	A	151	ASP	CA-CB-CG	5.50	125.50	113.40
1	C	451	ASP	CB-CG-OD1	-5.49	113.36	118.30
1	A	62	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	22	TRP	CG-CD1-NE1	-5.47	104.63	110.10
1	C	340	ARG	CB-CG-CD	-5.44	97.45	111.60
1	A	226	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	A	11	TRP	CG-CD1-NE1	-5.32	104.78	110.10
1	A	269	TYR	CB-CG-CD1	-5.31	117.82	121.00
1	A	37	LYS	CA-CB-CG	5.30	125.07	113.40
1	C	343	GLU	OE1-CD-OE2	-5.24	117.01	123.30
1	C	501	THR	N-CA-CB	5.24	120.25	110.30
1	A	132	TRP	CG-CD1-NE1	-5.24	104.86	110.10
1	C	451	ASP	C-N-CA	5.21	134.73	121.70
1	C	588	GLU	OE1-CD-OE2	-5.12	117.15	123.30
1	A	22	TRP	CG-CD2-CE3	5.11	138.50	133.90
1	C	375	ASN	N-CA-C	-5.08	97.28	111.00
1	C	370	MET	CA-CB-CG	5.06	121.90	113.30
1	C	363	VAL	CG1-CB-CG2	-5.04	102.84	110.90
1	C	313	PHE	CB-CG-CD1	5.01	124.31	120.80
1	C	322	TRP	CG-CD2-CE3	5.01	138.41	133.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	175	TYR	Sidechain
1	A	74	TYR	Sidechain

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	2119	0	2110	33	0
1	C	2119	0	2110	41	0
2	A	61	0	0	2	0
2	C	63	0	0	1	0
All	All	4362	0	4220	66	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 (66) 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	1.15	0.95
1:A:42:VAL:HG13	1:A:48:GLU:HG2	1.53	0.90
1:A:208:GLU:HG3	1:A:253:ILE:HD13	1.65	0.77
1:C:364:THR:HG22	1:C:383:GLU:HG3	1.74	0.68
1:A:249:ASN:HD22	1:A:251:LYS:H	1.42	0.66
1:C:489:ALA:O	1:C:515:THR:HB	1.97	0.65
1:A:216:HIS:HD2	1:C:516:HIS:CD2	2.07	0.64
1:A:216:HIS:CD2	1:C:516:HIS:HD2	2.06	0.64
1:A:76:ILE:HG13	1:A:102:VAL:HG22	1.82	0.62
1:C:563:LYS:HD2	1:C:563:LYS:H	1.64	0.62
1:A:70:MET:HG2	1:A:193:VAL:HB	1.83	0.61
1:C:312:ASN:ND2	1:C:587:LEU:HD21	2.16	0.59
1:C:483:ASP:OD1	1:C:506:GLY:HA2	2.04	0.58
1:C:308:LEU:HD11	1:C:566:TYR:HB2	1.87	0.57
1:C:512:THR:HG21	1:C:539:ILE:HG12	1.87	0.56
1:A:75:ASN:ND2	1:C:546:ARG:HE	2.04	0.55
1:C:308:LEU:HD22	1:C:579:VAL:HG13	1.88	0.55
1:A:220:GLU:HG3	1:A:224:GLN:HE21	1.71	0.55
1:A:7:VAL:HG13	1:A:157:ALA:HB2	1.90	0.54
1:A:246:ARG:HH21	1:C:375:ASN:HD22	1.55	0.53
1:C:384:HIS:HB3	1:C:420:LYS:HG3	1.90	0.53
1:C:323:LYS:O	1:C:327:LYS:HG2	2.09	0.52
1:A:8:LEU:HD22	1:A:279:VAL:HG13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:368:CYS:HB3	1:C:485:PRO:HA	1.90	0.52
1:A:249:ASN:ND2	1:A:251:LYS:H	2.07	0.51
1:C:307:VAL:HG23	1:C:580:HIS:HB3	1.92	0.51
1:C:307:VAL:HG13	1:C:457:ALA:HB2	1.92	0.51
1:A:8:LEU:HD11	1:A:266:TYR:HB2	1.93	0.50
1:A:130:LYS:O	1:A:134:GLU:HG3	2.10	0.50
1:A:246:ARG:HH21	1:C:375:ASN:ND2	2.09	0.50
1:C:466:GLY:HA3	1:C:491:LEU:HD11	1.93	0.50
1:A:241:LYS:O	1:A:245:ARG:HG3	2.12	0.49
1:C:503:THR:HG21	1:C:575:PHE:CD1	2.48	0.49
1:C:349:ARG:O	1:C:355:GLY:HA2	2.12	0.49
1:C:363:VAL:HG21	1:C:423:LEU:HB2	1.94	0.49
1:C:503:THR:HG21	1:C:575:PHE:CE1	2.49	0.48
1:A:180:ARG:HG3	1:C:401:HIS:CD2	2.48	0.48
1:A:190:GLY:O	1:A:201:THR:HG22	2.14	0.48
1:A:226:ARG:HD2	2:A:618:HOH:O	2.14	0.47
1:A:189:ALA:O	1:A:215:THR:HB	2.14	0.47
1:C:490:GLY:O	1:C:501:THR:HG22	2.14	0.47
1:C:333:ASP:O	1:C:337:LYS:HB2	2.16	0.46
1:A:166:GLY:HA3	1:A:191:LEU:HD11	1.96	0.46
1:C:504:GLY:HA3	1:C:554:GLN:O	2.16	0.46
1:C:316:HIS:N	1:C:316:HIS:ND1	2.63	0.46
1:C:541:LYS:O	1:C:545:ARG:HG3	2.17	0.45
1:A:227:THR:HB	1:A:230:GLN:CD	2.37	0.45
1:A:2:THR:HG23	1:A:263:LYS:HA	1.99	0.45
1:A:227:THR:HG22	1:A:230:GLN:H	1.82	0.45
1:C:526:ARG:HG2	1:C:530:GLN:HB3	1.99	0.45
1:C:364:THR:HB	1:C:381:CYS:HA	1.99	0.45
1:A:227:THR:HB	1:A:230:GLN:OE1	2.18	0.44
1:A:286:ARG:HA	2:A:690:HOH:O	2.17	0.44
1:C:561:ASN:OD1	1:C:563:LYS:HD2	2.17	0.44
1:A:75:ASN:HD22	1:C:546:ARG:HH21	1.64	0.44
1:C:568:ALA:HB3	1:C:590:PRO:HB3	2.00	0.43
1:C:430:LYS:O	1:C:434:GLU:HG3	2.19	0.42
1:A:33:ASP:O	1:A:37:LYS:HB2	2.19	0.42
1:C:517:LEU:HD21	1:C:538:ARG:HD2	2.01	0.42
1:A:246:ARG:HD3	1:A:246:ARG:HH11	1.69	0.42
1:A:289:THR:HA	1:A:290:PRO:HD2	1.74	0.41
1:C:312:ASN:HB2	2:C:679:HOH:O	2.20	0.41
1:C:549:ASN:HB3	1:C:552:ASP:OD2	2.20	0.41
1:C:308:LEU:HA	1:C:578:ALA:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:370:MET:HG2	1:C:493:VAL:HB	2.03	0.40
1:A:53:TYR:HB2	1:A:86:LYS:HG3	2.03	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	275/295 (93%)	265 (96%)	10 (4%)	0	100	100
1	C	275/295 (93%)	265 (96%)	10 (4%)	0	100	100
All	All	550/590 (93%)	530 (96%)	20 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	221/237 (93%)	207 (94%)	14 (6%)	22	18
1	C	221/237 (93%)	206 (93%)	15 (7%)	20	16
All	All	442/474 (93%)	413 (93%)	29 (7%)	21	17

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	8	LEU
1	A	13	PHE
1	A	102	VAL
1	A	124	LEU
1	A	151	ASP
1	A	185	PRO
1	A	201	THR
1	A	215	THR
1	A	243	VAL
1	A	249	ASN
1	A	253	ILE
1	A	282	GLN
1	A	286	ARG
1	C	307	VAL
1	C	308	LEU
1	C	313	PHE
1	C	316	HIS
1	C	337	LYS
1	C	419	LYS
1	C	423	LEU
1	C	451	ASP
1	C	485	PRO
1	C	501	THR
1	C	515	THR
1	C	543	VAL
1	C	563	LYS
1	C	582	GLN
1	C	590	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	84	HIS
1	A	216	HIS
1	A	224	GLN
1	A	249	ASN
1	C	312	ASN
1	C	375	ASN
1	C	387	ASN
1	C	401	HIS
1	C	478	HIS

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Mol	Chain	Res	Type
1	C	516	HIS
1	C	524	GLN
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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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 will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.