



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 07:04 PM EDT

PDB ID : 3BG2
Title : Crystal structure of deoxyguanosinetriphosphate triphosphohydrolase from *Flavobacterium* sp. MED217
Authors : Fedorov, A.A.; Fedorov, E.V.; Toro, R.; Meyer, A.J.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2007-11-25
Resolution : 1.95 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	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

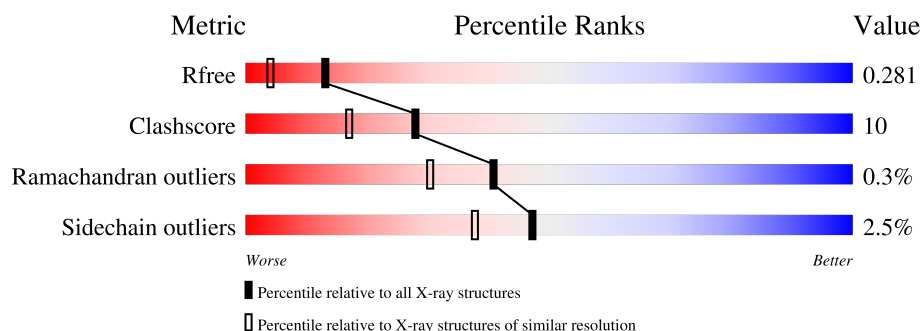
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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))
R_{free}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	444	 69% 18% • 11%
1	B	444	 70% 18% • 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6474 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 DGTP triphosphohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	S	0	0	0
			3178	2024	540	606	8			
1	B	397	Total	C	N	O	S	0	0	0
			3178	2024	540	606	8			

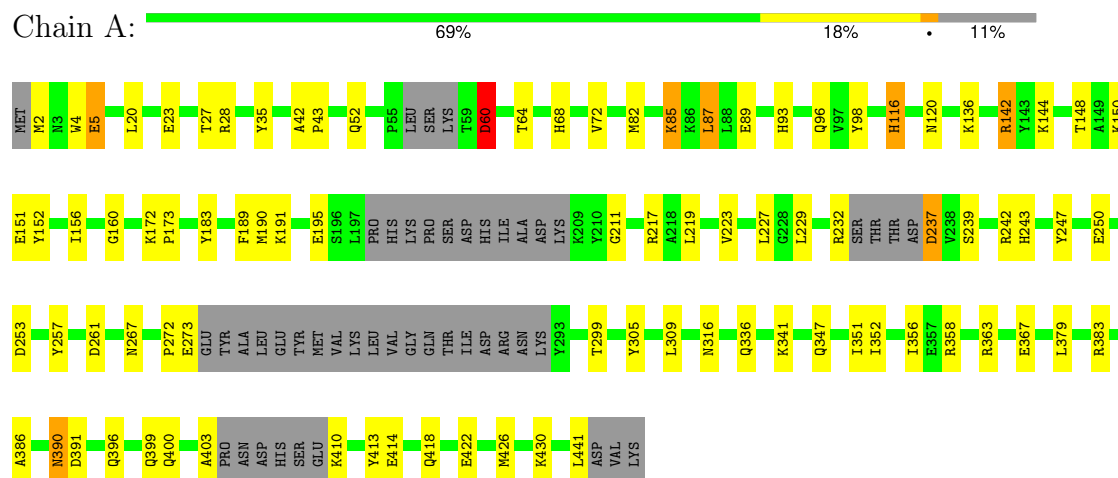
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	58	Total	O	0	0
			58	58		
2	B	60	Total	O	0	0
			60	60		

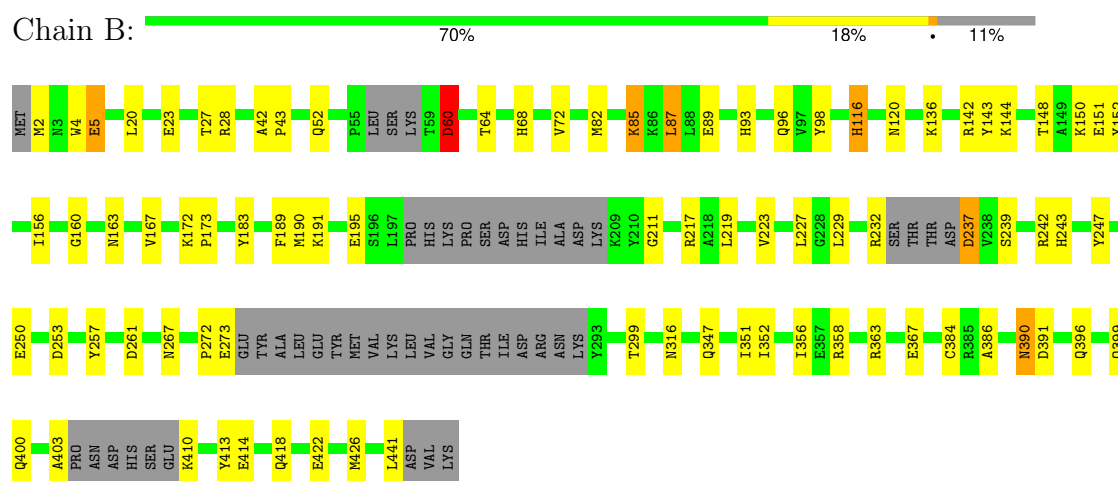
3 Residue-property plots [i](#)

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.

- Molecule 1: DGTP triphosphohydrolase



- Molecule 1: DGTP triphosphohydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	200.40Å 200.40Å 86.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.93 – 1.95 38.76 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.7 (24.93-1.95) 98.8 (38.76-1.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 1.95Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.268 , 0.285 0.265 , 0.281	Depositor DCC
R_{free} test set	4656 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	38.6	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 34.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.298 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6474	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.35	0/3232	0.55	1/4350 (0.0%)
1	B	0.35	0/3232	0.55	1/4350 (0.0%)
All	All	0.35	0/6464	0.55	2/8700 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	THR	N-CA-C	-5.16	97.08	111.00
1	B	64	THR	N-CA-C	-5.13	97.14	111.00

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	3178	0	3157	65	0
1	B	3178	0	3157	60	0
2	A	58	0	0	3	0
2	B	60	0	0	1	0
All	All	6474	0	6314	125	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 10.

All (125) 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:116:HIS:NE2	1:A:191:LYS:HE3	1.90	0.85
1:B:116:HIS:NE2	1:B:191:LYS:HE3	1.92	0.84
1:B:363:ARG:O	1:B:367:GLU:HG3	1.90	0.71
1:A:363:ARG:O	1:A:367:GLU:HG3	1.91	0.70
1:A:85:LYS:O	1:A:89:GLU:HG3	1.92	0.69
1:B:85:LYS:O	1:B:89:GLU:HG3	1.93	0.68
1:B:418:GLN:HG2	2:B:489:HOH:O	1.93	0.67
1:A:2:MET:HE2	1:A:229:LEU:HA	1.76	0.67
1:B:2:MET:HE2	1:B:229:LEU:HA	1.77	0.67
1:A:148:THR:OG1	1:A:151:GLU:HG3	1.96	0.66
1:B:148:THR:OG1	1:B:151:GLU:HG3	1.97	0.65
1:B:396:GLN:O	1:B:400:GLN:HG3	1.99	0.63
1:A:396:GLN:O	1:A:400:GLN:HG3	2.00	0.61
1:A:116:HIS:HD2	1:A:253:ASP:OD2	1.85	0.60
1:A:20:LEU:HB2	1:A:23:GLU:HG2	1.85	0.59
1:A:151:GLU:HB3	1:A:413:TYR:CD1	2.39	0.57
1:B:20:LEU:HB2	1:B:23:GLU:HG2	1.86	0.57
1:B:27:THR:O	1:B:28:ARG:HD2	2.05	0.57
1:B:232:ARG:HH11	1:B:232:ARG:HG3	1.70	0.57
1:A:232:ARG:HG3	1:A:232:ARG:HH11	1.69	0.56
1:B:390:ASN:C	1:B:390:ASN:HD22	2.08	0.56
1:A:27:THR:O	1:A:28:ARG:HD2	2.06	0.56
1:A:232:ARG:HB2	1:A:239:SER:OG	2.06	0.56
1:B:151:GLU:HB3	1:B:413:TYR:CD1	2.41	0.56
1:A:390:ASN:HD22	1:A:390:ASN:C	2.09	0.55
1:A:152:TYR:CZ	1:A:156:ILE:HD11	2.42	0.55
1:B:116:HIS:HD2	1:B:253:ASP:OD2	1.89	0.55
1:A:5:GLU:HG2	1:A:98:TYR:CE2	2.41	0.54
1:B:5:GLU:HG2	1:B:98:TYR:CE2	2.43	0.54
1:B:232:ARG:HB2	1:B:239:SER:OG	2.06	0.54
1:A:390:ASN:HD22	1:A:391:ASP:N	2.06	0.54
1:B:390:ASN:HD22	1:B:391:ASP:N	2.05	0.54
1:B:152:TYR:CZ	1:B:156:ILE:HD11	2.43	0.53
1:A:242:ARG:HD2	1:A:247:TYR:CZ	2.43	0.53
1:B:120:ASN:OD1	1:B:160:GLY:HA3	2.09	0.53
1:B:150:LYS:NZ	1:B:217:ARG:HH12	2.07	0.52
1:B:399:GLN:O	1:B:403:ALA:HB3	2.09	0.52
1:A:52:GLN:NE2	2:A:478:HOH:O	2.23	0.52
1:A:82:MET:HE3	1:A:316:ASN:ND2	2.24	0.52
1:A:120:ASN:OD1	1:A:160:GLY:HA3	2.08	0.52
1:A:399:GLN:O	1:A:403:ALA:HB3	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:LYS:HG2	1:B:152:TYR:CE2	2.44	0.52
1:A:150:LYS:NZ	1:A:217:ARG:HH12	2.07	0.52
1:B:52:GLN:HE22	1:B:68:HIS:CD2	2.28	0.51
1:A:195:GLU:OE1	1:A:237:ASP:HA	2.10	0.51
1:B:242:ARG:HD2	1:B:247:TYR:CZ	2.45	0.51
1:B:195:GLU:OE1	1:B:237:ASP:HA	2.11	0.50
1:A:183:TYR:CD2	1:A:223:VAL:HA	2.47	0.50
1:A:52:GLN:HE22	1:A:68:HIS:CD2	2.29	0.50
1:B:352:ILE:O	1:B:356:ILE:HG13	2.12	0.50
1:A:386:ALA:CB	1:A:399:GLN:HE21	2.25	0.50
1:B:4:TRP:CZ2	1:B:87:LEU:HD21	2.47	0.50
1:A:4:TRP:CZ2	1:A:87:LEU:HD21	2.47	0.49
1:A:144:LYS:HG2	1:A:152:TYR:CE2	2.47	0.49
1:B:183:TYR:CD2	1:B:223:VAL:HA	2.47	0.49
1:A:410:LYS:HB3	1:A:414:GLU:HB2	1.94	0.49
1:B:386:ALA:CB	1:B:399:GLN:HE21	2.24	0.49
1:B:410:LYS:HB3	1:B:414:GLU:HB2	1.95	0.49
1:A:142:ARG:HH11	1:A:142:ARG:HG3	1.78	0.48
1:A:352:ILE:O	1:A:356:ILE:HG13	2.14	0.48
1:A:190:MET:SD	1:A:211:GLY:HA3	2.54	0.48
1:B:144:LYS:HG2	1:B:152:TYR:CZ	2.49	0.48
1:A:150:LYS:NZ	1:A:217:ARG:NH1	2.61	0.48
1:B:257:TYR:O	1:B:261:ASP:HB2	2.14	0.48
1:B:227:LEU:HD13	1:B:243:HIS:HD2	1.79	0.47
1:B:20:LEU:HB2	1:B:23:GLU:CG	2.44	0.47
1:A:347:GLN:O	1:A:351:ILE:HG13	2.15	0.47
1:B:422:GLU:O	1:B:426:MET:HG3	2.14	0.47
1:A:142:ARG:HG3	1:A:142:ARG:NH1	2.30	0.46
1:A:172:LYS:CG	1:A:173:PRO:HD2	2.45	0.46
1:B:150:LYS:NZ	1:B:217:ARG:NH1	2.63	0.46
1:A:20:LEU:HB2	1:A:23:GLU:CG	2.46	0.46
1:A:68:HIS:O	1:A:72:VAL:HG23	2.15	0.46
1:B:82:MET:HE1	1:B:316:ASN:HD22	1.81	0.46
1:B:142:ARG:HH11	1:B:142:ARG:HG3	1.79	0.46
1:A:93:HIS:HA	1:A:96:GLN:HG2	1.97	0.46
1:B:191:LYS:HE2	1:B:250:GLU:HA	1.98	0.46
1:A:422:GLU:O	1:A:426:MET:HG3	2.14	0.46
1:B:93:HIS:HA	1:B:96:GLN:HG2	1.96	0.46
1:A:272:PRO:HD3	1:A:358:ARG:NH1	2.31	0.46
1:A:144:LYS:HG2	1:A:152:TYR:CZ	2.50	0.45
1:B:136:LYS:CA	1:B:156:ILE:HD12	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:MET:SD	1:B:211:GLY:HA3	2.56	0.45
1:B:172:LYS:CG	1:B:173:PRO:HD2	2.47	0.45
1:A:227:LEU:HD13	1:A:243:HIS:HD2	1.82	0.45
1:B:273:GLU:OE2	1:B:299:THR:HG22	2.16	0.45
1:A:257:TYR:O	1:A:261:ASP:HB2	2.16	0.45
1:B:272:PRO:HD3	1:B:358:ARG:NH1	2.31	0.45
1:B:142:ARG:HG3	1:B:142:ARG:NH1	2.32	0.45
1:A:232:ARG:HG3	1:A:232:ARG:NH1	2.33	0.44
1:A:441:LEU:N	1:A:441:LEU:HD12	2.33	0.44
1:A:82:MET:CE	1:A:316:ASN:HD22	2.31	0.44
1:B:136:LYS:HA	1:B:156:ILE:HD12	2.00	0.44
1:B:116:HIS:HE1	1:B:189:PHE:O	2.00	0.44
1:B:232:ARG:HG3	1:B:232:ARG:NH1	2.33	0.44
1:A:191:LYS:HE2	1:A:250:GLU:HA	2.00	0.44
1:A:136:LYS:CA	1:A:156:ILE:HD12	2.47	0.44
1:B:347:GLN:O	1:B:351:ILE:HG13	2.17	0.44
1:A:35:TYR:HB2	2:A:455:HOH:O	2.18	0.43
1:A:116:HIS:HE1	1:A:189:PHE:O	2.00	0.43
1:A:136:LYS:HA	1:A:156:ILE:HD12	1.99	0.43
1:B:60:ASP:CG	1:B:267:ASN:HB3	2.39	0.43
1:B:136:LYS:HB2	1:B:156:ILE:HG23	1.99	0.43
1:B:82:MET:HE3	1:B:316:ASN:ND2	2.33	0.43
1:B:42:ALA:N	1:B:43:PRO:HD2	2.34	0.43
1:A:60:ASP:CG	1:A:267:ASN:HB3	2.39	0.43
1:A:273:GLU:OE2	1:A:299:THR:HG22	2.18	0.42
1:B:441:LEU:HD12	1:B:441:LEU:N	2.33	0.42
1:A:136:LYS:HB2	1:A:156:ILE:HG23	2.01	0.42
1:B:82:MET:CE	1:B:316:ASN:HD22	2.31	0.42
1:B:386:ALA:HB3	1:B:399:GLN:HE21	1.84	0.42
1:B:68:HIS:O	1:B:72:VAL:HG23	2.19	0.42
1:A:386:ALA:HB3	1:A:399:GLN:HE21	1.84	0.42
1:A:430:LYS:HD2	2:A:494:HOH:O	2.20	0.42
1:A:316:ASN:HD22	1:A:316:ASN:HA	1.63	0.41
1:A:42:ALA:N	1:A:43:PRO:HD2	2.34	0.41
1:A:82:MET:CE	1:A:316:ASN:ND2	2.83	0.41
1:B:82:MET:CE	1:B:316:ASN:ND2	2.83	0.41
1:A:242:ARG:HD2	1:A:247:TYR:CE2	2.55	0.41
1:A:379:LEU:O	1:A:383:ARG:HG3	2.20	0.41
1:B:143:TYR:OH	1:B:384:CYS:HB3	2.20	0.41
1:A:305:TYR:CZ	1:A:309:LEU:HD11	2.56	0.41
1:A:336:GLN:CD	1:A:341:LYS:HE2	2.41	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:GLN:O	1:A:422:GLU:HG3	2.21	0.41
1:B:163:ASN:O	1:B:167:VAL:HG23	2.21	0.41

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	385/444 (87%)	377 (98%)	7 (2%)	1 (0%)	41	30
1	B	385/444 (87%)	377 (98%)	7 (2%)	1 (0%)	41	30
All	All	770/888 (87%)	754 (98%)	14 (2%)	2 (0%)	41	30

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	60	ASP
1	A	60	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	339/383 (88%)	330 (97%)	9 (3%)	44	34
1	B	339/383 (88%)	331 (98%)	8 (2%)	49	40

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	678/766 (88%)	661 (98%)	17 (2%)	47	38

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLU
1	A	60	ASP
1	A	85	LYS
1	A	87	LEU
1	A	116	HIS
1	A	142	ARG
1	A	219	LEU
1	A	237	ASP
1	A	390	ASN
1	B	5	GLU
1	B	60	ASP
1	B	85	LYS
1	B	87	LEU
1	B	116	HIS
1	B	219	LEU
1	B	237	ASP
1	B	390	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	96	GLN
1	A	116	HIS
1	A	214	GLN
1	A	267	ASN
1	A	294	ASN
1	A	297	GLN
1	A	316	ASN
1	A	353	ASN
1	A	390	ASN
1	A	399	GLN
1	A	400	GLN
1	A	415	ASN
1	A	418	GLN
1	B	68	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	96	GLN
1	B	116	HIS
1	B	176	GLN
1	B	267	ASN
1	B	294	ASN
1	B	297	GLN
1	B	316	ASN
1	B	353	ASN
1	B	390	ASN
1	B	399	GLN
1	B	400	GLN
1	B	415	ASN
1	B	418	GLN

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](#)

There are no ligands in this entry.

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](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.