wwPDB X-ray Structure Validation Summary Report (i)

Aug 15, 2023 – 06:43 PM EDT

PDB ID	:	1TW9
Title	:	Glutathione Transferase-2, apo form, from the nematode Heligmosomoides polygyrus
Authors	:	Schuller, D.J.; Liu, Q.; Kriksunov, I.A.; Campbell, A.M.; Barrett, J.; Brophy, P.M.; Hao, Q.
Deposited on	:	2004-06-30
Resolution	:	1.71 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (1)) were used in the production of this report:

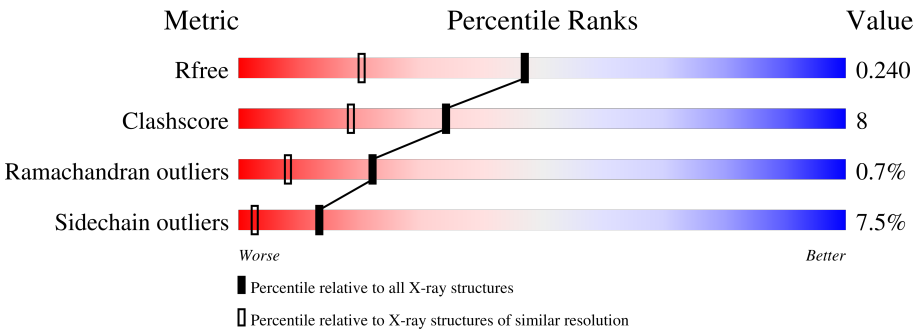
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.71 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	5722 (1.74-1.70)
Clashscore	141614	6152 (1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)

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%

Mol	Chain	Length	Quality of chain
1	A	206	75% 16% • 7%
1	B	206	74% 13% • • 9%
1	C	206	80% 13% • 6%
1	D	206	77% 15% • • 6%
1	E	206	73% 17% • • 6%
1	F	206	77% 18% •
1	G	206	75% 15% • 8%

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Mol	Chain	Length	Quality of chain
1	H	206	71% 16% 5% 7%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 14254 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 glutathione S-transferase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	191	1531	989	256	280	6	0	0	0
1	B	188	1507	974	252	275	6	0	0	0
1	C	194	1563	1013	260	284	6	0	0	0
1	D	194	1559	1008	260	285	6	0	0	0
1	E	193	1542	997	257	282	6	0	0	0
1	F	205	1645	1066	271	301	7	0	0	0
1	G	189	1516	980	254	276	6	0	0	0
1	H	191	1531	989	256	280	6	0	0	0

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	cloning artifact	UNP Q9NJQ6
A	2	VAL	-	cloning artifact	UNP Q9NJQ6
A	21	VAL	ILE	conflict	UNP Q9NJQ6
A	40	VAL	ALA	conflict	UNP Q9NJQ6
A	91	LEU	PRO	conflict	UNP Q9NJQ6
A	108	THR	MET	conflict	UNP Q9NJQ6
A	120	PRO	LEU	conflict	UNP Q9NJQ6
A	140	LEU	PRO	conflict	UNP Q9NJQ6
B	1	MET	-	cloning artifact	UNP Q9NJQ6
B	2	VAL	-	cloning artifact	UNP Q9NJQ6
B	21	VAL	ILE	conflict	UNP Q9NJQ6
B	40	VAL	ALA	conflict	UNP Q9NJQ6
B	91	LEU	PRO	conflict	UNP Q9NJQ6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	108	THR	MET	conflict	UNP Q9NJQ6
B	120	PRO	LEU	conflict	UNP Q9NJQ6
B	140	LEU	PRO	conflict	UNP Q9NJQ6
C	1	MET	-	cloning artifact	UNP Q9NJQ6
C	2	VAL	-	cloning artifact	UNP Q9NJQ6
C	21	VAL	ILE	conflict	UNP Q9NJQ6
C	40	VAL	ALA	conflict	UNP Q9NJQ6
C	91	LEU	PRO	conflict	UNP Q9NJQ6
C	108	THR	MET	conflict	UNP Q9NJQ6
C	120	PRO	LEU	conflict	UNP Q9NJQ6
C	140	LEU	PRO	conflict	UNP Q9NJQ6
D	1	MET	-	cloning artifact	UNP Q9NJQ6
D	2	VAL	-	cloning artifact	UNP Q9NJQ6
D	21	VAL	ILE	conflict	UNP Q9NJQ6
D	40	VAL	ALA	conflict	UNP Q9NJQ6
D	91	LEU	PRO	conflict	UNP Q9NJQ6
D	108	THR	MET	conflict	UNP Q9NJQ6
D	120	PRO	LEU	conflict	UNP Q9NJQ6
D	140	LEU	PRO	conflict	UNP Q9NJQ6
E	1	MET	-	cloning artifact	UNP Q9NJQ6
E	2	VAL	-	cloning artifact	UNP Q9NJQ6
E	21	VAL	ILE	conflict	UNP Q9NJQ6
E	40	VAL	ALA	conflict	UNP Q9NJQ6
E	91	LEU	PRO	conflict	UNP Q9NJQ6
E	108	THR	MET	conflict	UNP Q9NJQ6
E	120	PRO	LEU	conflict	UNP Q9NJQ6
E	140	LEU	PRO	conflict	UNP Q9NJQ6
F	1	MET	-	cloning artifact	UNP Q9NJQ6
F	2	VAL	-	cloning artifact	UNP Q9NJQ6
F	21	VAL	ILE	conflict	UNP Q9NJQ6
F	40	VAL	ALA	conflict	UNP Q9NJQ6
F	91	LEU	PRO	conflict	UNP Q9NJQ6
F	108	THR	MET	conflict	UNP Q9NJQ6
F	120	PRO	LEU	conflict	UNP Q9NJQ6
F	140	LEU	PRO	conflict	UNP Q9NJQ6
G	1	MET	-	cloning artifact	UNP Q9NJQ6
G	2	VAL	-	cloning artifact	UNP Q9NJQ6
G	21	VAL	ILE	conflict	UNP Q9NJQ6
G	40	VAL	ALA	conflict	UNP Q9NJQ6
G	91	LEU	PRO	conflict	UNP Q9NJQ6
G	108	THR	MET	conflict	UNP Q9NJQ6
G	120	PRO	LEU	conflict	UNP Q9NJQ6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	140	LEU	PRO	conflict	UNP Q9NJQ6
H	1	MET	-	cloning artifact	UNP Q9NJQ6
H	2	VAL	-	cloning artifact	UNP Q9NJQ6
H	21	VAL	ILE	conflict	UNP Q9NJQ6
H	40	VAL	ALA	conflict	UNP Q9NJQ6
H	91	LEU	PRO	conflict	UNP Q9NJQ6
H	108	THR	MET	conflict	UNP Q9NJQ6
H	120	PRO	LEU	conflict	UNP Q9NJQ6
H	140	LEU	PRO	conflict	UNP Q9NJQ6

- Molecule 2 is water.

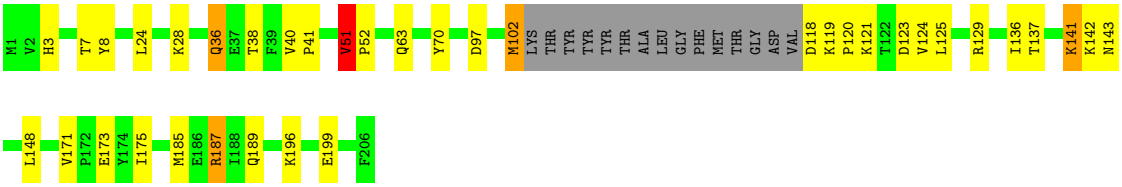
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	384	384	384	0	0
			Total	O		
2	B	220	220	220	0	0
			Total	O		
2	C	285	285	285	0	0
			Total	O		
2	D	251	251	251	0	0
			Total	O		
2	E	149	149	149	0	0
			Total	O		
2	F	186	186	186	0	0
			Total	O		
2	G	216	216	216	0	0
			Total	O		
2	H	169	169	169	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.

• Molecule 1: glutathione S-transferase 2

Chain A:

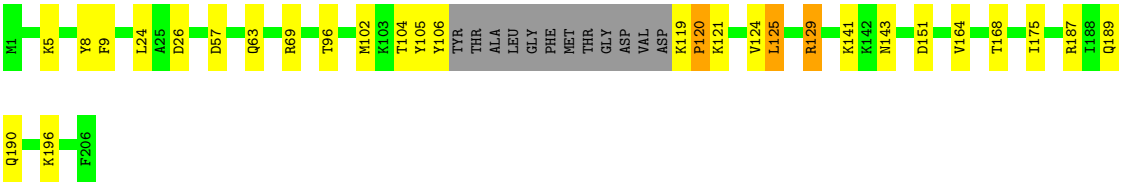


• Molecule 1: glutathione S-transferase 2

Chain B:

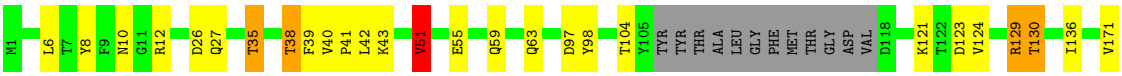
• Molecule 1: glutathione S-transferase 2

Chain C:



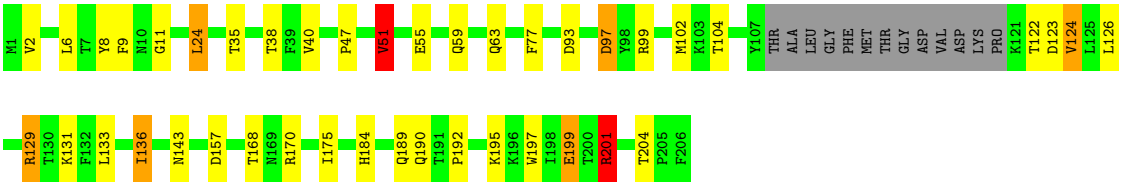
• Molecule 1: glutathione S-transferase 2

Chain D:



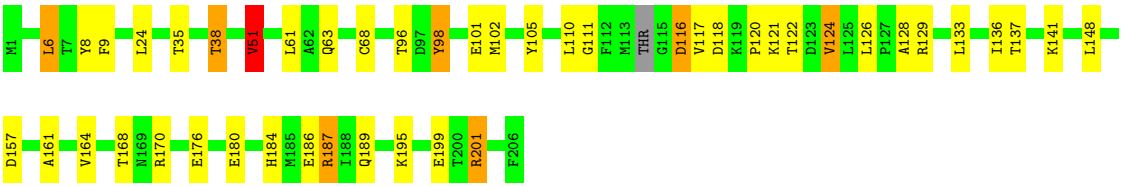
• Molecule 1: glutathione S-transferase 2

Chain E:



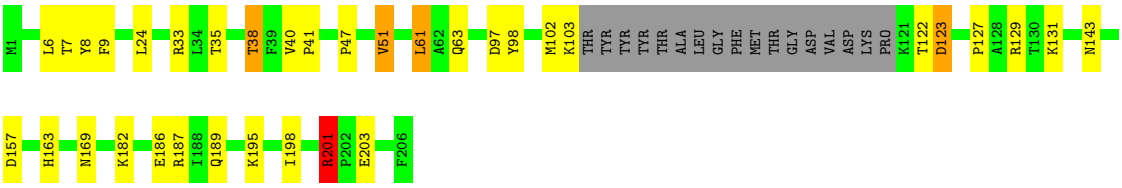
• Molecule 1: glutathione S-transferase 2

Chain F:



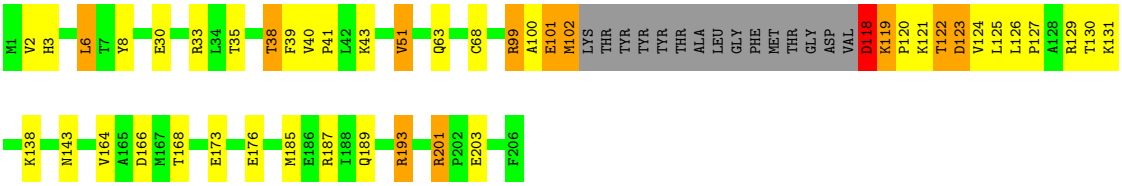
• Molecule 1: glutathione S-transferase 2

Chain G:



• Molecule 1: glutathione S-transferase 2

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	72.68Å 74.03Å 88.57Å 79.09° 80.08° 81.55°	Depositor
Resolution (Å)	25.00 – 1.71 24.26 – 1.71	Depositor EDS
% Data completeness (in resolution range)	95.2 (25.00-1.71) 95.2 (24.26-1.71)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 1.71Å)	Xtriage
Refinement program	REFMAC 5.1.9999	Depositor
R, R_{free}	0.180 , 0.232 0.189 , 0.240	Depositor DCC
R_{free} test set	4568 reflections (2.48%)	wwPDB-VP
Wilson B-factor (Å^2)	23.7	Xtriage
Anisotropy	0.495	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 39.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.009 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14254	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	1.05	2/1568 (0.1%)	1.11	6/2120 (0.3%)
1	B	0.88	0/1543	1.00	8/2086 (0.4%)
1	C	0.96	0/1602	1.01	6/2166 (0.3%)
1	D	0.95	0/1597	0.99	5/2159 (0.2%)
1	E	0.94	2/1579 (0.1%)	0.98	8/2136 (0.4%)
1	F	0.97	2/1686 (0.1%)	1.04	6/2280 (0.3%)
1	G	0.88	0/1552	1.06	8/2097 (0.4%)
1	H	0.87	1/1568 (0.1%)	1.02	7/2120 (0.3%)
All	All	0.94	7/12695 (0.1%)	1.03	54/17164 (0.3%)

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	B	0	1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	199	GLU	CD-OE2	17.71	1.45	1.25
1	E	199	GLU	CD-OE1	8.35	1.34	1.25
1	H	68	CYS	CB-SG	-5.76	1.72	1.81
1	A	70	TYR	CD2-CE2	-5.55	1.31	1.39
1	A	70	TYR	CD1-CE1	-5.39	1.31	1.39

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	201	ARG	NE-CZ-NH1	14.00	127.30	120.30
1	C	187	ARG	NE-CZ-NH1	13.65	127.13	120.30
1	B	201	ARG	NE-CZ-NH1	11.89	126.24	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	187	ARG	NE-CZ-NH1	11.70	126.15	120.30
1	F	201	ARG	NE-CZ-NH1	11.46	126.03	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	102	MET	Peptide

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	1531	0	1527	26	0
1	B	1507	0	1503	27	0
1	C	1563	0	1561	20	0
1	D	1559	0	1556	28	0
1	E	1542	0	1527	29	0
1	F	1645	0	1634	36	1
1	G	1516	0	1516	16	0
1	H	1531	0	1527	27	0
2	A	384	0	0	12	1
2	B	220	0	0	10	0
2	C	285	0	0	8	0
2	D	251	0	0	8	1
2	E	149	0	0	11	1
2	F	186	0	0	8	0
2	G	216	0	0	8	0
2	H	169	0	0	4	0
All	All	14254	0	12351	207	2

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.

The worst 5 of 207 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:G:195:LYS:NZ	2:G:268:HOH:O	1.73	1.18
1:E:2:VAL:HB	2:E:1781:HOH:O	0.96	1.12
1:C:106:TYR:C	2:C:1685:HOH:O	1.88	1.10
1:B:96:THR:HG22	2:B:337:HOH:O	1.52	1.08
1:E:143:ASN:CG	2:E:1376:HOH:O	1.95	1.03

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:240:HOH:O	2:E:1566:HOH:O[1_444]	1.76	0.44
1:F:180:GLU:OE1	2:D:367:HOH:O[1_665]	2.07	0.13

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	187/206 (91%)	184 (98%)	2 (1%)	1 (0%)	29	13
1	B	184/206 (89%)	180 (98%)	3 (2%)	1 (0%)	29	13
1	C	190/206 (92%)	186 (98%)	2 (1%)	2 (1%)	14	3
1	D	190/206 (92%)	187 (98%)	2 (1%)	1 (0%)	29	13
1	E	189/206 (92%)	185 (98%)	3 (2%)	1 (0%)	29	13
1	F	201/206 (98%)	197 (98%)	2 (1%)	2 (1%)	15	4
1	G	185/206 (90%)	181 (98%)	3 (2%)	1 (0%)	29	13
1	H	187/206 (91%)	180 (96%)	5 (3%)	2 (1%)	14	3
All	All	1513/1648 (92%)	1480 (98%)	22 (2%)	11 (1%)	22	8

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	111	GLY
1	H	63	GLN
1	B	63	GLN
1	C	63	GLN
1	E	63	GLN

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	162/174 (93%)	151 (93%)	11 (7%)	16	3
1	B	159/174 (91%)	147 (92%)	12 (8%)	13	3
1	C	165/174 (95%)	157 (95%)	8 (5%)	25	8
1	D	165/174 (95%)	153 (93%)	12 (7%)	14	3
1	E	161/174 (92%)	149 (92%)	12 (8%)	13	3
1	F	173/174 (99%)	161 (93%)	12 (7%)	15	3
1	G	160/174 (92%)	145 (91%)	15 (9%)	8	1
1	H	162/174 (93%)	146 (90%)	16 (10%)	8	1
All	All	1307/1392 (94%)	1209 (92%)	98 (8%)	13	3

5 of 98 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	38	THR
1	G	61	LEU
1	F	61	LEU
1	F	189	GLN
1	G	129	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	63	GLN

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Mol	Chain	Res	Type
1	F	63	GLN
1	H	143	ASN
1	E	190	GLN
1	F	184	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 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.