



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:41 PM GMT

PDB ID : 1GUK
Title : CRYSTAL STRUCTURE OF MURINE ALPHA-CLASS GSTA4-4
Authors : Krengel, U.; Schroter, K.H.; Hoier, H.; Dijkstra, B.W.
Deposited on : 1997-12-11
Resolution : 2.90 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
<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

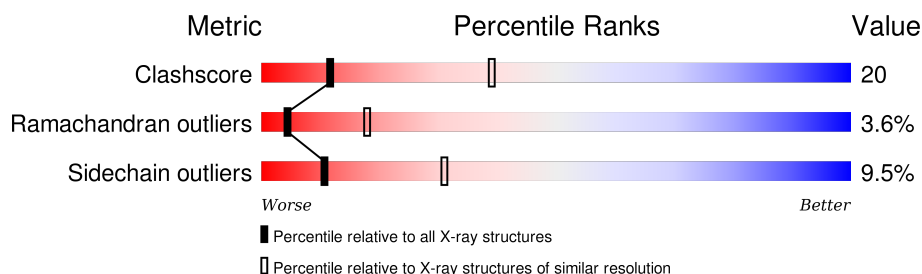
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)

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 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 $\leq 5\%$. 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	222	 54% 36% 6% . .
1	B	222	 54% 35% 5% 6%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3438 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 A4-4.

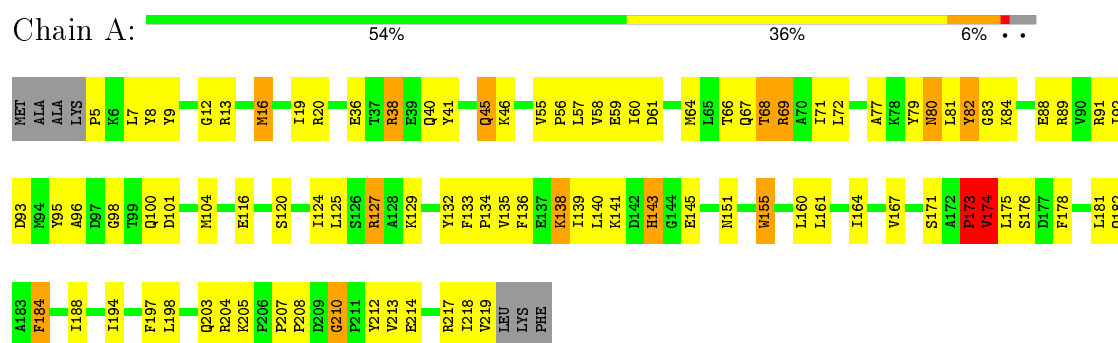
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1745	1133	287	316	9			
1	B	209	Total	C	N	O	S	0	0	0
			1693	1101	279	304	9			

3 Residue-property plots

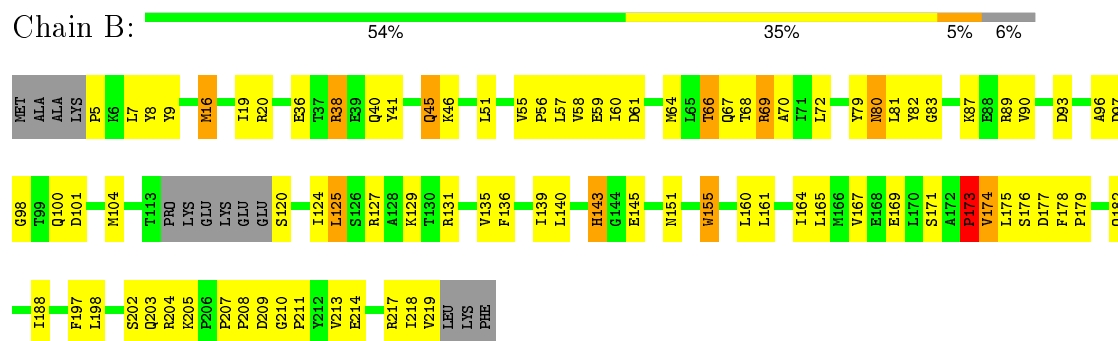
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: GLUTATHIONE S-TRANSFERASE A4-4



• Molecule 1: GLUTATHIONE S-TRANSFERASE A4-4



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	114.30 Å 95.90 Å 50.80 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.90	Depositor
% Data completeness (in resolution range)	77.8 (10.00-2.90)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.234 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3438	wwPDB-VP
Average B, all atoms (Å ²)	42.0	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	0.53	0/1784	0.74	0/2407
1	B	0.49	0/1730	0.73	0/2334
All	All	0.51	0/3514	0.73	0/4741

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	5
1	B	0	2
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	173	PRO	Mainchain
1	A	174	VAL	Peptide
1	A	178	PHE	Sidechain
1	A	184	PHE	Sidechain
1	A	212	TYR	Sidechain
1	B	173	PRO	Mainchain
1	B	211	PRO	Peptide

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	1745	0	1779	73	0
1	B	1693	0	1727	72	0
All	All	3438	0	3506	141	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 20.

All (141) 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:174:VAL:HG13	1:A:175:LEU:HB2	1.41	1.02
1:B:174:VAL:HG13	1:B:175:LEU:HB2	1.54	0.89
1:A:161:LEU:HD22	1:A:188:ILE:HG22	1.54	0.88
1:B:161:LEU:HD22	1:B:188:ILE:HG22	1.58	0.84
1:A:197:PHE:CE1	1:A:204:ARG:HB2	2.15	0.81
1:B:36:GLU:H	1:B:40:GLN:HE22	1.30	0.78
1:A:36:GLU:H	1:A:40:GLN:HE22	1.32	0.76
1:B:36:GLU:H	1:B:40:GLN:NE2	1.84	0.75
1:A:36:GLU:H	1:A:40:GLN:NE2	1.88	0.72
1:A:210:GLY:O	1:A:213:VAL:HB	1.91	0.71
1:B:16:MET:HE3	1:B:19:ILE:HD12	1.73	0.71
1:B:165:LEU:O	1:B:169:GLU:HG3	1.91	0.70
1:B:135:VAL:HG12	1:B:139:ILE:HD11	1.75	0.68
1:B:176:SER:HA	1:B:182:GLN:NE2	2.09	0.67
1:A:69:ARG:HG2	1:A:69:ARG:HH11	1.60	0.67
1:A:197:PHE:CZ	1:A:204:ARG:HB2	2.30	0.67
1:A:16:MET:HE3	1:A:19:ILE:HD12	1.76	0.67
1:A:160:LEU:O	1:A:164:ILE:HG12	1.95	0.67
1:B:51:LEU:HB2	1:B:66:THR:HG21	1.78	0.66
1:A:135:VAL:O	1:A:139:ILE:HG13	1.97	0.65
1:B:9:TYR:HB2	1:B:16:MET:HG3	1.79	0.64
1:A:7:LEU:HB3	1:A:16:MET:SD	2.38	0.64
1:A:96:ALA:O	1:A:100:GLN:HB2	1.96	0.64
1:A:136:PHE:HA	1:A:139:ILE:HD12	1.80	0.64
1:B:7:LEU:HD13	1:B:16:MET:CE	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:LEU:HB3	1:B:16:MET:SD	2.39	0.63
1:A:89:ARG:NH2	1:B:89:ARG:NH2	2.47	0.62
1:A:181:LEU:O	1:A:184:PHE:HB3	1.99	0.62
1:B:60:ILE:HG12	1:B:61:ASP:OD1	1.99	0.62
1:B:160:LEU:O	1:B:164:ILE:HG12	2.00	0.61
1:A:161:LEU:HD22	1:A:188:ILE:CG2	2.27	0.60
1:A:9:TYR:HB2	1:A:16:MET:HG3	1.82	0.60
1:B:96:ALA:O	1:B:100:GLN:HB2	1.99	0.60
1:B:218:ILE:O	1:B:219:VAL:HB	2.02	0.60
1:B:213:VAL:O	1:B:217:ARG:HG3	2.02	0.60
1:A:218:ILE:O	1:A:219:VAL:HB	2.02	0.60
1:A:173:PRO:O	1:A:175:LEU:N	2.35	0.59
1:B:87:LYS:O	1:B:90:VAL:HG12	2.02	0.59
1:B:9:TYR:CB	1:B:16:MET:HG3	2.33	0.58
1:B:67:GLN:O	1:B:70:ALA:HB3	2.03	0.58
1:B:161:LEU:HD22	1:B:188:ILE:CG2	2.30	0.58
1:B:98:GLY:O	1:B:101:ASP:HB2	2.03	0.58
1:A:120:SER:O	1:A:124:ILE:HG13	2.04	0.58
1:A:9:TYR:CB	1:A:16:MET:HG3	2.34	0.57
1:A:176:SER:HA	1:A:182:GLN:NE2	2.18	0.57
1:A:72:LEU:HD13	1:A:155:TRP:CH2	2.39	0.57
1:A:82:TYR:CE2	1:A:89:ARG:NH2	2.72	0.57
1:A:38:ARG:HH21	1:A:218:ILE:HA	1.69	0.57
1:B:214:GLU:O	1:B:218:ILE:HD13	2.05	0.57
1:A:174:VAL:HG13	1:A:175:LEU:CB	2.27	0.56
1:A:140:LEU:HA	1:A:143:HIS:CE1	2.41	0.56
1:B:72:LEU:HD13	1:B:155:TRP:CH2	2.40	0.56
1:A:98:GLY:O	1:A:101:ASP:HB2	2.06	0.56
1:B:173:PRO:O	1:B:175:LEU:N	2.39	0.56
1:B:171:SER:O	1:B:174:VAL:HB	2.05	0.55
1:A:7:LEU:HD13	1:A:16:MET:CE	2.36	0.55
1:B:136:PHE:HA	1:B:139:ILE:HD12	1.88	0.55
1:B:7:LEU:N	1:B:7:LEU:HD23	2.22	0.54
1:B:7:LEU:HD13	1:B:16:MET:HE2	1.88	0.54
1:B:38:ARG:HH21	1:B:218:ILE:HA	1.73	0.53
1:B:69:ARG:HH11	1:B:69:ARG:HG2	1.74	0.53
1:B:198:LEU:HD23	1:B:204:ARG:HH11	1.72	0.53
1:A:7:LEU:HD13	1:A:16:MET:HE2	1.91	0.53
1:B:120:SER:O	1:B:124:ILE:HG13	2.09	0.52
1:A:8:TYR:O	1:A:9:TYR:HB2	2.10	0.52
1:B:135:VAL:O	1:B:139:ILE:HG13	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:LEU:HD23	1:A:7:LEU:N	2.25	0.51
1:A:198:LEU:HD23	1:A:204:ARG:HH11	1.75	0.50
1:A:171:SER:O	1:A:174:VAL:HB	2.12	0.50
1:B:20:ARG:NH2	1:B:205:LYS:HG3	2.27	0.50
1:B:140:LEU:HA	1:B:143:HIS:CE1	2.47	0.50
1:A:67:GLN:O	1:A:71:ILE:HG13	2.12	0.50
1:A:140:LEU:HA	1:A:143:HIS:HE1	1.78	0.49
1:B:8:TYR:O	1:B:9:TYR:HB2	2.12	0.49
1:B:177:ASP:O	1:B:179:PRO:HD3	2.12	0.49
1:A:77:ALA:HB2	1:A:82:TYR:HD2	1.78	0.48
1:A:194:ILE:O	1:A:198:LEU:HD12	2.12	0.48
1:A:138:LYS:HA	1:A:141:LYS:HB3	1.95	0.48
1:A:60:ILE:HG12	1:A:61:ASP:OD1	2.13	0.48
1:A:69:ARG:HG2	1:A:69:ARG:NH1	2.25	0.48
1:B:58:VAL:HG12	1:B:58:VAL:O	2.14	0.48
1:B:55:VAL:HA	1:B:56:PRO:O	2.13	0.47
1:B:9:TYR:CG	1:B:16:MET:HG3	2.50	0.47
1:B:197:PHE:CZ	1:B:204:ARG:HB2	2.50	0.47
1:B:176:SER:HA	1:B:182:GLN:HE21	1.78	0.47
1:A:55:VAL:HA	1:A:56:PRO:O	2.14	0.47
1:B:140:LEU:HA	1:B:143:HIS:HE1	1.80	0.46
1:A:9:TYR:CG	1:A:16:MET:HG3	2.51	0.46
1:A:91:ARG:O	1:A:95:TYR:CD2	2.69	0.46
1:B:69:ARG:NH1	1:B:69:ARG:HG2	2.30	0.45
1:A:213:VAL:O	1:A:217:ARG:HG3	2.16	0.45
1:B:16:MET:HE3	1:B:19:ILE:CD1	2.44	0.45
1:A:92:ILE:O	1:A:95:TYR:N	2.49	0.45
1:A:41:TYR:CZ	1:A:45:GLN:NE2	2.85	0.45
1:B:167:VAL:HG12	1:B:174:VAL:HG21	1.97	0.45
1:B:8:TYR:HB2	1:B:57:LEU:HB3	1.99	0.45
1:B:20:ARG:CZ	1:B:205:LYS:HG3	2.47	0.45
1:A:207:PRO:HA	1:A:208:PRO:HD2	1.82	0.45
1:A:139:ILE:O	1:A:143:HIS:ND1	2.50	0.44
1:B:41:TYR:CZ	1:B:45:GLN:NE2	2.85	0.44
1:B:7:LEU:HD22	1:B:58:VAL:HG22	2.00	0.44
1:A:5:PRO:HA	1:A:59:GLU:O	2.18	0.44
1:B:57:LEU:HD11	1:B:64:MET:HB3	1.99	0.44
1:A:138:LYS:HE3	1:A:138:LYS:HB3	1.80	0.44
1:B:97:ASP:O	1:B:100:GLN:HB3	2.18	0.43
1:A:45:GLN:OE1	1:A:46:LYS:NZ	2.51	0.43
1:A:79:TYR:O	1:A:81:LEU:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:ILE:O	1:B:219:VAL:CB	2.65	0.43
1:B:45:GLN:OE1	1:B:46:LYS:NZ	2.52	0.42
1:A:13:ARG:NE	1:A:205:LYS:O	2.51	0.42
1:B:55:VAL:HA	1:B:56:PRO:C	2.39	0.42
1:A:127:ARG:HG2	1:A:132:TYR:HE1	1.84	0.42
1:B:79:TYR:O	1:B:81:LEU:N	2.52	0.42
1:B:5:PRO:HA	1:B:59:GLU:O	2.20	0.42
1:B:16:MET:CE	1:B:19:ILE:HB	2.49	0.42
1:A:57:LEU:HD11	1:A:64:MET:HB3	2.01	0.42
1:B:38:ARG:NH2	1:B:218:ILE:HA	2.33	0.42
1:A:167:VAL:HG12	1:A:174:VAL:HG21	2.01	0.42
1:A:8:TYR:HB2	1:A:57:LEU:HB3	2.01	0.42
1:B:41:TYR:CE2	1:B:45:GLN:NE2	2.88	0.42
1:A:84:LYS:NZ	1:A:88:GLU:OE2	2.52	0.42
1:B:207:PRO:HA	1:B:208:PRO:HD2	1.82	0.42
1:B:174:VAL:HG13	1:B:175:LEU:CB	2.37	0.41
1:A:41:TYR:CE2	1:A:45:GLN:NE2	2.88	0.41
1:A:12:GLY:O	1:A:20:ARG:NH2	2.42	0.41
1:A:135:VAL:HG12	1:A:139:ILE:HD11	2.02	0.41
1:A:58:VAL:O	1:A:58:VAL:HG12	2.19	0.41
1:B:125:LEU:HD12	1:B:125:LEU:HA	1.86	0.41
1:B:173:PRO:HB2	1:B:174:VAL:H	1.74	0.41
1:A:16:MET:CE	1:A:19:ILE:HB	2.51	0.41
1:A:16:MET:HE3	1:A:19:ILE:CD1	2.49	0.41
1:B:175:LEU:HA	1:B:178:PHE:HD2	1.85	0.41
1:A:214:GLU:O	1:A:218:ILE:HD13	2.20	0.41
1:A:7:LEU:HD22	1:A:58:VAL:HG22	2.02	0.41
1:A:89:ARG:CZ	1:B:89:ARG:NH2	2.84	0.41
1:A:55:VAL:HA	1:A:56:PRO:C	2.41	0.41
1:B:209:ASP:CG	1:B:210:GLY:H	2.24	0.41
1:A:89:ARG:NH2	1:B:89:ARG:CZ	2.84	0.41
1:A:69:ARG:HD3	1:B:69:ARG:HD3	2.03	0.40
1:B:38:ARG:HA	1:B:219:VAL:HB	2.03	0.40
1:A:133:PHE:HB2	1:A:134:PRO:HD3	2.04	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	213/222 (96%)	185 (87%)	20 (9%)	8 (4%)	4	16
1	B	205/222 (92%)	175 (85%)	23 (11%)	7 (3%)	5	19
All	All	418/444 (94%)	360 (86%)	43 (10%)	15 (4%)	4	18

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	80	ASN
1	A	145	GLU
1	A	174	VAL
1	A	210	GLY
1	B	38	ARG
1	B	80	ASN
1	B	145	GLU
1	B	174	VAL
1	B	83	GLY
1	A	68	THR
1	A	173	PRO
1	B	173	PRO
1	B	68	THR
1	A	83	GLY

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	188/193 (97%)	170 (90%)	18 (10%)	10	31
1	B	182/193 (94%)	165 (91%)	17 (9%)	11	32
All	All	370/386 (96%)	335 (90%)	35 (10%)	11	31

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	MET
1	A	45	GLN
1	A	66	THR
1	A	68	THR
1	A	69	ARG
1	A	80	ASN
1	A	82	TYR
1	A	93	ASP
1	A	104	MET
1	A	116	GLU
1	A	125	LEU
1	A	127	ARG
1	A	129	LYS
1	A	138	LYS
1	A	143	HIS
1	A	151	ASN
1	A	155	TRP
1	A	203	GLN
1	B	16	MET
1	B	45	GLN
1	B	66	THR
1	B	69	ARG
1	B	80	ASN
1	B	82	TYR
1	B	93	ASP
1	B	104	MET
1	B	125	LEU
1	B	127	ARG
1	B	129	LYS
1	B	131	ARG
1	B	143	HIS
1	B	151	ASN
1	B	155	TRP
1	B	202	SER
1	B	203	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	151	ASN
1	A	203	GLN
1	B	40	GLN
1	B	54	GLN
1	B	67	GLN
1	B	151	ASN
1	B	159	GLN
1	B	203	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 carbohydrates 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 ⓘ

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.