



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 06:56 am GMT

PDB ID : 1U88  
Title : Crystal Structure Of The 26 Kda Glutathione S-Transferase Y7F mutant From Schistosoma Japonicum Complexed With S-Octyl Glutathione  
Authors : Smith, A.W.; Camara-Artigas, A.  
Deposited on : 2004-08-05  
Resolution : 3.50 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

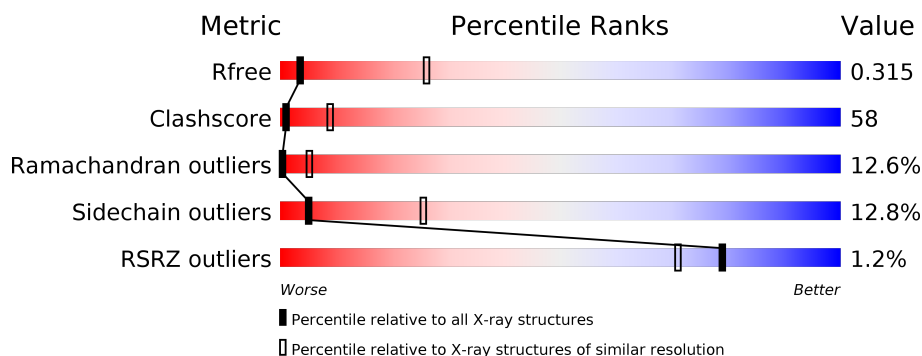
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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))
$R_{free}$	100719	1195 (3.60-3.40)
Clashscore	112137	1322 (3.60-3.40)
Ramachandran outliers	110173	1283 (3.60-3.40)
Sidechain outliers	110143	1284 (3.60-3.40)
RSRZ outliers	101464	1226 (3.60-3.40)

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  $\geq 3$ , 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.

Mol	Chain	Length	Quality of chain
1	A	218	
1	B	218	

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3486 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.

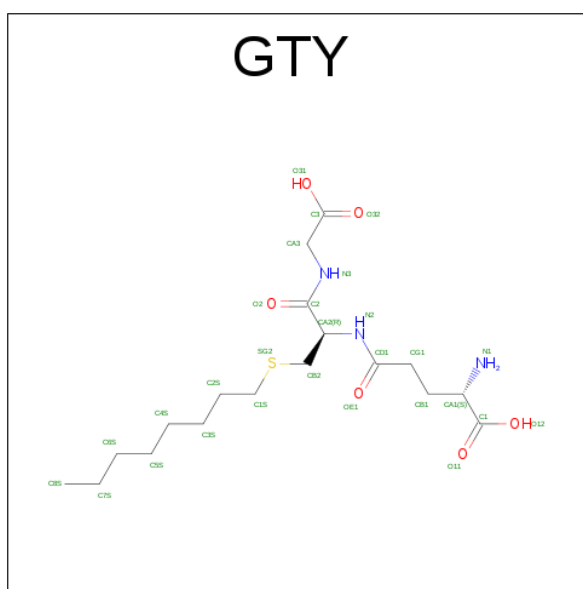
- Molecule 1 is a protein called Glutathione S-transferase 26 kDa.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	0	0
			1729	1128	279	309	13			
1	B	209	Total	C	N	O	S	0	0	0
			1729	1128	279	309	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	PHE	TYR	ENGINEERED	UNP P08515
B	7	PHE	TYR	ENGINEERED	UNP P08515

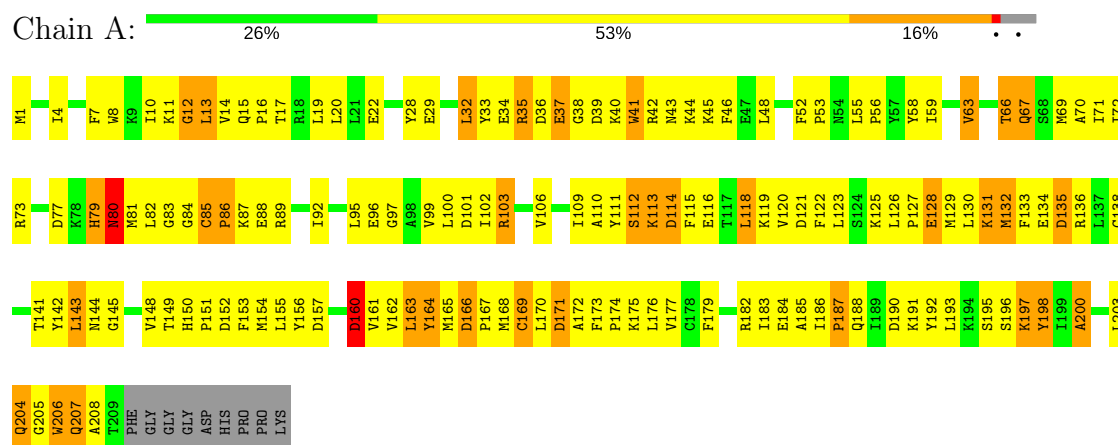
- Molecule 2 is L-GAMMA-GLUTAMYL-S-OCTYL-D-CYSTEINYLGLYCINE (three-letter code: GTY) (formula: C<sub>18</sub>H<sub>33</sub>N<sub>3</sub>O<sub>6</sub>S).



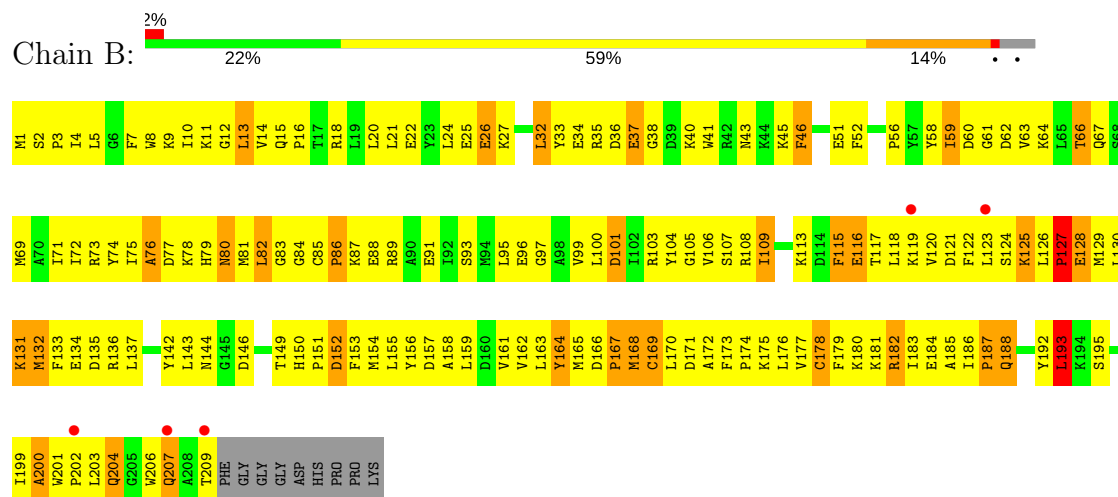
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

#### • Molecule 1: Glutathione S-transferase 26 kDa



#### • Molecule 1: Glutathione S-transferase 26 kDa



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.10Å 116.10Å 73.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.73 – 3.50 19.73 – 3.50	Depositor EDS
% Data completeness (in resolution range)	87.7 (19.73-3.50) 87.7 (19.73-3.50)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.25 (at 3.52Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.220 , 0.317 0.221 , 0.315	Depositor DCC
$R_{free}$ test set	354 reflections (5.64%)	DCC
Wilson B-factor (Å <sup>2</sup> )	65.5	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 20.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.197 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	3486	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTY

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	0.46	0/1774	0.76	0/2393
1	B	0.50	0/1774	0.75	0/2393
All	All	0.48	0/3548	0.75	0/4786

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	1729	0	1740	192	0
1	B	1729	0	1740	227	0
2	A	28	0	31	2	0
All	All	3486	0	3511	408	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 58.

All (408) 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:161:VAL:HG22	1:A:203:LEU:HD22	1.31	1.11
1:B:149:THR:OG1	1:B:151:PRO:HD2	1.66	0.94
1:A:163:LEU:HD21	1:A:170:LEU:HD12	1.49	0.94
1:B:120:VAL:HA	1:B:123:LEU:HB2	1.49	0.90
1:A:170:LEU:HB3	1:A:177:VAL:HG22	1.57	0.87
1:B:163:LEU:HD21	1:B:170:LEU:HD12	1.58	0.85
1:A:173:PHE:O	1:A:177:VAL:HG23	1.79	0.83
1:A:161:VAL:HG13	1:A:203:LEU:HD13	1.58	0.83
1:B:18:ARG:HH22	1:B:199:ILE:CD1	1.92	0.83
1:A:149:THR:OG1	1:A:151:PRO:HD2	1.79	0.83
1:B:13:LEU:HD12	1:B:13:LEU:H	1.44	0.82
1:B:120:VAL:HA	1:B:123:LEU:CB	2.10	0.82
1:B:11:LYS:HZ1	1:B:203:LEU:HD22	1.43	0.81
1:B:18:ARG:HH22	1:B:199:ILE:HD11	1.45	0.81
1:A:15:GLN:HB3	1:A:16:PRO:HD3	1.63	0.81
1:B:174:PRO:O	1:B:178:CYS:HB2	1.80	0.81
1:A:13:LEU:H	1:A:13:LEU:HD12	1.46	0.80
1:B:122:PHE:C	1:B:124:SER:H	1.81	0.80
1:A:17:THR:HG23	1:A:72:ILE:HG13	1.63	0.80
1:B:35:ARG:HB2	1:B:206:TRP:CE3	2.17	0.79
1:B:18:ARG:O	1:B:22:GLU:HG2	1.82	0.79
1:A:125:LYS:O	1:A:129:MET:HG3	1.82	0.78
1:B:109:ILE:HG22	1:B:118:LEU:HB3	1.66	0.78
1:B:66:THR:O	1:B:67:GLN:HB2	1.83	0.77
1:B:122:PHE:HA	1:B:125:LYS:CE	2.16	0.76
1:A:168:MET:O	1:A:170:LEU:N	2.19	0.75
1:B:158:ALA:O	1:B:162:VAL:HG23	1.86	0.75
1:A:125:LYS:HA	1:A:128:GLU:OE2	1.86	0.75
1:B:106:VAL:HA	1:B:109:ILE:HD11	1.69	0.75
1:A:102:ILE:HD11	1:A:133:PHE:HE2	1.52	0.74
1:A:11:LYS:HE3	1:A:200:ALA:O	1.87	0.74
1:B:73:ARG:HH22	1:B:82:LEU:HD21	1.51	0.74
1:B:2:SER:HB3	1:B:27:LYS:HE3	1.69	0.74
1:B:115:PHE:HE1	1:B:119:LYS:HA	1.53	0.73
1:B:171:ASP:C	1:B:173:PHE:H	1.89	0.73
1:B:182:ARG:HH21	1:B:182:ARG:HB2	1.53	0.73
1:B:1:MET:HG2	1:B:2:SER:H	1.53	0.73
1:B:15:GLN:HB3	1:B:16:PRO:HD3	1.71	0.72
1:A:161:VAL:O	1:A:164:TYR:HB2	1.88	0.72
1:A:44:LYS:HD3	1:A:48:LEU:HD21	1.71	0.72
1:A:70:ALA:HB2	1:B:93:SER:O	1.89	0.72
1:A:162:VAL:C	1:A:164:TYR:H	1.93	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:LYS:HB2	1:B:203:LEU:O	1.90	0.72
1:A:92:ILE:HA	1:A:95:LEU:HD12	1.70	0.71
1:B:11:LYS:NZ	1:B:203:LEU:HD22	2.05	0.70
1:B:149:THR:HG1	1:B:151:PRO:HD2	1.57	0.70
1:A:111:TYR:O	1:A:113:LYS:N	2.24	0.70
1:B:21:LEU:CD2	1:B:75:ILE:HD13	2.21	0.70
1:B:120:VAL:HA	1:B:123:LEU:CG	2.22	0.69
1:B:122:PHE:C	1:B:124:SER:N	2.43	0.69
1:B:45:LYS:HB3	1:B:46:PHE:CE1	2.27	0.69
1:B:74:TYR:OH	1:B:78:LYS:HE3	1.91	0.69
1:A:69:MET:HE1	1:A:96:GLU:HG2	1.74	0.69
1:A:45:LYS:HE2	1:A:53:PRO:HB2	1.74	0.69
1:B:179:PHE:HA	1:B:182:ARG:NH2	2.08	0.69
1:A:161:VAL:HG22	1:A:203:LEU:CD2	2.16	0.68
1:A:174:PRO:HG2	1:A:175:LYS:H	1.58	0.68
1:B:52:PHE:O	1:B:66:THR:HG21	1.93	0.68
1:B:182:ARG:HH21	1:B:182:ARG:CB	2.06	0.68
1:A:119:LYS:HE2	1:A:123:LEU:CD1	2.24	0.68
1:B:122:PHE:HD1	1:B:125:LYS:HE3	1.59	0.68
1:A:19:LEU:HA	1:A:22:GLU:HB2	1.77	0.67
1:A:41:TRP:HE1	2:A:220:GTU:HA31	1.59	0.67
1:B:159:LEU:HD22	1:B:170:LEU:HD11	1.76	0.67
1:A:13:LEU:HD12	1:A:13:LEU:N	2.10	0.67
1:B:182:ARG:NH2	1:B:182:ARG:HB2	2.09	0.67
1:B:24:LEU:HD13	1:B:79:HIS:CD2	2.30	0.67
1:B:122:PHE:HA	1:B:125:LYS:NZ	2.10	0.66
1:A:77:ASP:HB2	1:A:82:LEU:HD12	1.76	0.66
1:B:40:LYS:O	1:B:43:ASN:HB2	1.95	0.66
1:A:79:HIS:O	1:A:81:MET:HG3	1.95	0.66
1:B:156:TYR:CE1	1:B:180:LYS:HG3	2.30	0.66
1:B:46:PHE:CD1	1:B:46:PHE:N	2.63	0.66
1:B:73:ARG:NH2	1:B:82:LEU:HD11	2.11	0.65
1:B:183:ILE:C	1:B:185:ALA:H	2.00	0.65
1:A:126:LEU:HG	1:A:130:LEU:HD12	1.78	0.65
1:A:77:ASP:CB	1:A:82:LEU:HD12	2.27	0.65
1:B:115:PHE:CE1	1:B:119:LYS:HA	2.31	0.65
1:B:63:VAL:C	1:B:64:LYS:HD3	2.16	0.65
1:B:201:TRP:HB2	1:B:202:PRO:HA	1.78	0.65
1:A:138:CYS:HA	1:A:175:LYS:NZ	2.11	0.65
1:A:207:GLN:HE21	1:A:207:GLN:N	1.95	0.64
1:B:179:PHE:HA	1:B:182:ARG:HH22	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:GLN:O	1:A:71:ILE:HG13	1.97	0.64
1:A:138:CYS:HA	1:A:175:LYS:HE2	1.81	0.63
1:A:41:TRP:C	1:A:43:ASN:H	2.01	0.63
1:B:20:LEU:O	1:B:24:LEU:HG	1.98	0.63
1:B:96:GLU:OE2	1:B:150:HIS:NE2	2.29	0.63
1:A:41:TRP:CZ2	1:A:55:LEU:HG	2.34	0.63
1:A:7:PHE:CD1	1:A:56:PRO:HB3	2.33	0.63
1:B:3:PRO:HB3	1:B:60:ASP:HB2	1.79	0.63
1:A:39:ASP:OD1	1:A:40:LYS:N	2.32	0.63
1:B:115:PHE:HB2	1:B:209:THR:HB	1.81	0.63
1:B:156:TYR:HE1	1:B:180:LYS:HG3	1.63	0.63
1:B:131:LYS:O	1:B:133:PHE:N	2.32	0.62
1:A:110:ALA:HB1	1:A:204:GLN:HG2	1.82	0.62
1:B:171:ASP:C	1:B:173:PHE:N	2.53	0.62
1:B:13:LEU:N	1:B:13:LEU:HD12	2.13	0.61
1:B:122:PHE:CD1	1:B:125:LYS:HE3	2.36	0.61
1:A:83:GLY:O	1:A:89:ARG:HG2	2.01	0.61
1:B:125:LYS:O	1:B:128:GLU:OE1	2.20	0.60
1:B:116:GLU:HA	1:B:119:LYS:HG3	1.83	0.60
1:B:11:LYS:HD2	1:B:203:LEU:HA	1.82	0.60
1:A:134:GLU:OE1	1:A:173:PHE:HA	2.01	0.60
1:B:106:VAL:CA	1:B:109:ILE:HD11	2.30	0.60
1:B:120:VAL:CG2	1:B:123:LEU:HD12	2.31	0.60
1:B:176:LEU:O	1:B:179:PHE:N	2.34	0.60
1:B:9:LYS:HG3	1:B:32:LEU:HD12	1.83	0.60
1:B:124:SER:O	1:B:127:PRO:HD2	2.01	0.60
1:B:21:LEU:HD21	1:B:75:ILE:HD13	1.84	0.60
1:A:73:ARG:NH1	1:A:96:GLU:OE2	2.34	0.60
1:B:73:ARG:O	1:B:77:ASP:HB2	2.02	0.60
1:A:109:ILE:HA	1:A:112:SER:HB3	1.84	0.59
1:A:183:ILE:C	1:A:185:ALA:H	2.04	0.59
1:B:128:GLU:O	1:B:132:MET:HG3	2.00	0.59
1:A:40:LYS:O	1:A:43:ASN:HB3	2.01	0.59
1:B:131:LYS:O	1:B:134:GLU:N	2.35	0.59
1:A:197:LYS:O	1:A:198:TYR:C	2.41	0.59
1:A:197:LYS:O	1:A:198:TYR:O	2.21	0.59
1:A:114:ASP:O	1:A:118:LEU:HG	2.03	0.59
1:B:173:PHE:HB3	1:B:176:LEU:HD12	1.85	0.59
1:A:138:CYS:HA	1:A:175:LYS:CE	2.33	0.59
1:B:134:GLU:OE1	1:B:173:PHE:HB3	2.02	0.59
1:B:120:VAL:CA	1:B:123:LEU:HB2	2.28	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:TRP:O	1:A:43:ASN:N	2.36	0.59
1:A:121:ASP:O	1:A:125:LYS:HE3	2.03	0.58
1:A:183:ILE:O	1:A:186:ILE:HG13	2.03	0.58
1:A:77:ASP:HB2	1:A:82:LEU:CD1	2.33	0.58
1:A:41:TRP:C	1:A:43:ASN:N	2.57	0.58
1:A:171:ASP:C	1:A:173:PHE:H	2.08	0.58
1:B:116:GLU:HA	1:B:119:LYS:HD2	1.86	0.57
1:B:127:PRO:O	1:B:128:GLU:C	2.43	0.57
1:A:10:ILE:HD12	1:A:204:GLN:O	2.03	0.57
1:A:22:GLU:OE1	1:A:22:GLU:HA	2.04	0.57
1:B:18:ARG:HH22	1:B:199:ILE:HD12	1.70	0.57
1:A:171:ASP:O	1:A:173:PHE:N	2.38	0.57
1:B:124:SER:OG	1:B:125:LYS:N	2.38	0.57
1:A:7:PHE:CE1	1:A:56:PRO:HD3	2.40	0.56
1:A:20:LEU:CD2	1:A:72:ILE:HG12	2.35	0.56
1:A:205:GLY:C	1:A:207:GLN:H	2.07	0.56
1:A:207:GLN:HE21	1:A:207:GLN:H	1.52	0.56
1:A:129:MET:HA	1:A:132:MET:HE3	1.88	0.56
1:B:143:LEU:HD13	1:B:152:ASP:HA	1.88	0.56
1:A:156:TYR:CD2	1:A:156:TYR:C	2.78	0.56
1:A:79:HIS:O	1:A:80:ASN:C	2.44	0.56
1:B:182:ARG:O	1:B:185:ALA:HB3	2.06	0.56
1:B:109:ILE:HD12	1:B:115:PHE:CZ	2.41	0.55
1:B:181:LYS:O	1:B:185:ALA:HB2	2.06	0.55
1:B:126:LEU:N	1:B:127:PRO:CD	2.70	0.55
1:B:126:LEU:HB3	1:B:127:PRO:HD3	1.87	0.55
1:B:183:ILE:HG22	1:B:184:GLU:N	2.21	0.54
1:B:32:LEU:H	1:B:32:LEU:HD23	1.71	0.54
1:B:32:LEU:N	1:B:32:LEU:HD23	2.23	0.54
1:A:85:CYS:SG	1:A:88:GLU:HB3	2.47	0.54
1:B:120:VAL:HG22	1:B:123:LEU:HD12	1.89	0.54
1:B:179:PHE:O	1:B:182:ARG:N	2.40	0.54
1:A:176:LEU:O	1:A:179:PHE:HB3	2.08	0.54
1:A:11:LYS:HB3	1:A:15:GLN:HB2	1.90	0.54
1:A:150:HIS:N	1:A:151:PRO:CD	2.71	0.53
1:B:41:TRP:C	1:B:43:ASN:N	2.61	0.53
1:A:126:LEU:N	1:A:127:PRO:CD	2.71	0.53
1:A:171:ASP:C	1:A:173:PHE:N	2.60	0.53
1:A:85:CYS:HG	1:A:88:GLU:HB3	1.72	0.53
1:A:41:TRP:CZ3	1:A:45:LYS:HA	2.43	0.53
1:B:202:PRO:HG3	1:B:206:TRP:CD1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:GLU:N	1:B:37:GLU:OE1	2.42	0.53
1:A:182:ARG:O	1:A:185:ALA:HB3	2.08	0.53
1:B:125:LYS:H	1:B:125:LYS:HE2	1.73	0.53
1:A:84:GLY:O	1:A:85:CYS:HB3	2.09	0.53
1:A:132:MET:HA	1:A:135:ASP:OD2	2.09	0.53
1:B:18:ARG:NH2	1:B:199:ILE:HD11	2.21	0.53
1:A:131:LYS:O	1:A:133:PHE:N	2.42	0.53
1:A:103:ARG:HD2	1:A:103:ARG:O	2.08	0.52
1:A:151:PRO:HA	1:A:154:MET:SD	2.48	0.52
1:B:125:LYS:HA	1:B:128:GLU:OE2	2.10	0.52
1:B:66:THR:O	1:B:67:GLN:CB	2.53	0.52
1:A:142:TYR:O	1:A:144:ASN:N	2.43	0.52
1:B:120:VAL:HA	1:B:123:LEU:HG	1.90	0.52
1:B:73:ARG:NH1	1:B:150:HIS:HE2	2.07	0.52
1:A:70:ALA:HB2	1:B:93:SER:C	2.29	0.52
1:B:116:GLU:HA	1:B:119:LYS:CD	2.39	0.52
1:B:176:LEU:O	1:B:179:PHE:HB3	2.10	0.52
1:A:188:GLN:OE1	1:A:188:GLN:N	2.33	0.52
1:B:109:ILE:HD12	1:B:115:PHE:HZ	1.73	0.51
1:A:69:MET:CE	1:A:96:GLU:HG2	2.40	0.51
1:A:119:LYS:HE2	1:A:123:LEU:HD12	1.90	0.51
1:B:153:PHE:O	1:B:154:MET:C	2.46	0.51
1:A:99:VAL:HG11	1:A:154:MET:C	2.30	0.51
1:A:11:LYS:HG2	1:A:15:GLN:OE1	2.11	0.51
1:B:171:ASP:O	1:B:173:PHE:N	2.44	0.51
1:B:83:GLY:O	1:B:89:ARG:HG3	2.10	0.51
1:A:69:MET:HE2	1:A:100:LEU:HD11	1.93	0.51
1:A:136:ARG:NH1	1:B:51:GLU:OE1	2.43	0.51
1:A:13:LEU:HD11	2:A:220:GTY:H1S2	1.93	0.51
1:B:21:LEU:HD21	1:B:75:ILE:CD1	2.41	0.51
1:A:183:ILE:C	1:A:185:ALA:N	2.64	0.51
1:B:159:LEU:HD22	1:B:170:LEU:CD1	2.41	0.51
1:B:204:GLN:HA	1:B:204:GLN:HE21	1.76	0.51
1:B:115:PHE:CD1	1:B:119:LYS:HG2	2.45	0.51
1:B:192:TYR:O	1:B:195:SER:N	2.40	0.51
1:A:20:LEU:HD23	1:A:72:ILE:HG12	1.92	0.51
1:A:192:TYR:O	1:A:195:SER:N	2.43	0.50
1:B:41:TRP:C	1:B:43:ASN:H	2.13	0.50
1:A:87:LYS:HG3	1:B:63:VAL:HG12	1.93	0.50
1:B:120:VAL:C	1:B:122:PHE:N	2.65	0.50
1:A:129:MET:HA	1:A:132:MET:CE	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:TYR:HB2	1:A:71:ILE:CG2	2.40	0.50
1:B:157:ASP:O	1:B:158:ALA:C	2.48	0.50
1:B:3:PRO:C	1:B:4:ILE:HD12	2.32	0.50
1:B:8:TRP:HH2	1:B:38:GLY:HA2	1.75	0.50
1:A:92:ILE:HG23	1:A:151:PRO:HG2	1.92	0.50
1:A:131:LYS:O	1:A:134:GLU:N	2.41	0.50
1:B:38:GLY:O	1:B:41:TRP:HB3	2.12	0.50
1:A:126:LEU:HB3	1:A:127:PRO:HD3	1.93	0.50
1:A:34:GLU:O	1:A:36:ASP:N	2.45	0.50
1:A:7:PHE:HD1	1:A:56:PRO:HB3	1.76	0.50
1:B:134:GLU:OE2	1:B:175:LYS:HB2	2.12	0.50
1:A:174:PRO:HG2	1:A:175:LYS:N	2.26	0.49
1:B:120:VAL:O	1:B:124:SER:N	2.45	0.49
1:B:193:LEU:H	1:B:193:LEU:HD23	1.77	0.49
1:A:113:LYS:O	1:A:115:PHE:N	2.44	0.49
1:A:162:VAL:O	1:A:164:TYR:N	2.43	0.49
1:A:99:VAL:O	1:A:99:VAL:HG12	2.12	0.49
1:B:108:ARG:H	1:B:109:ILE:HG12	1.77	0.49
1:B:8:TRP:CE3	1:B:33:TYR:HB2	2.47	0.49
1:A:162:VAL:C	1:A:164:TYR:N	2.60	0.49
1:A:36:ASP:C	1:A:38:GLY:H	2.16	0.49
1:B:11:LYS:CE	1:B:203:LEU:HD22	2.41	0.49
1:B:20:LEU:HD23	1:B:72:ILE:HG13	1.93	0.49
1:A:165:MET:O	1:A:166:ASP:HB2	2.12	0.49
1:A:207:GLN:NE2	1:A:207:GLN:N	2.60	0.49
1:A:73:ARG:HH11	1:A:73:ARG:HG2	1.77	0.49
1:B:35:ARG:HB2	1:B:206:TRP:CZ3	2.48	0.49
1:A:36:ASP:O	1:A:38:GLY:N	2.45	0.49
1:B:76:ALA:O	1:B:77:ASP:C	2.51	0.49
1:A:45:LYS:HD3	1:A:46:PHE:CZ	2.48	0.49
1:A:97:GLY:HA3	1:B:67:GLN:OE1	2.13	0.49
1:B:101:ASP:O	1:B:129:MET:HE1	2.13	0.49
1:B:159:LEU:CD2	1:B:170:LEU:HD11	2.41	0.49
1:B:79:HIS:O	1:B:80:ASN:HB2	2.12	0.49
1:A:151:PRO:C	1:A:153:PHE:H	2.16	0.48
1:A:190:ASP:O	1:A:191:LYS:C	2.51	0.48
1:B:91:GLU:O	1:B:95:LEU:HG	2.13	0.48
1:A:150:HIS:H	1:A:151:PRO:HD3	1.78	0.48
1:B:133:PHE:O	1:B:136:ARG:N	2.45	0.48
1:A:160:ASP:O	1:A:160:ASP:OD1	2.31	0.48
1:B:166:ASP:O	1:B:169:CYS:SG	2.63	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:THR:HG22	1:B:117:THR:O	2.13	0.48
1:A:138:CYS:HA	1:A:175:LYS:HZ3	1.78	0.48
1:A:142:TYR:O	1:A:145:GLY:N	2.47	0.48
1:A:99:VAL:O	1:A:103:ARG:HB2	2.13	0.48
1:B:130:LEU:O	1:B:131:LYS:C	2.51	0.48
1:B:207:GLN:HE21	1:B:207:GLN:N	2.12	0.48
1:A:161:VAL:CG2	1:A:203:LEU:HD22	2.23	0.48
1:A:155:LEU:C	1:A:157:ASP:N	2.66	0.48
1:A:58:TYR:HB2	1:A:71:ILE:HG23	1.95	0.48
1:A:103:ARG:CD	1:A:103:ARG:O	2.62	0.47
1:B:10:ILE:O	1:B:199:ILE:HD12	2.13	0.47
1:A:102:ILE:HD11	1:A:133:PHE:CE2	2.42	0.47
1:A:45:LYS:HG2	1:A:53:PRO:HB3	1.95	0.47
1:A:63:VAL:HG13	1:B:87:LYS:HD2	1.96	0.47
1:A:118:LEU:O	1:A:119:LYS:C	2.52	0.47
1:B:120:VAL:O	1:B:122:PHE:N	2.47	0.47
1:B:7:PHE:HB2	1:B:56:PRO:HB3	1.96	0.47
1:B:69:MET:O	1:B:73:ARG:HG3	2.15	0.47
1:B:73:ARG:NH1	1:B:96:GLU:OE2	2.47	0.47
1:B:3:PRO:CB	1:B:60:ASP:HB2	2.44	0.47
1:B:99:VAL:HG11	1:B:155:LEU:N	2.29	0.47
1:B:10:ILE:HD12	1:B:204:GLN:O	2.15	0.47
1:A:52:PHE:HA	1:B:132:MET:HE2	1.96	0.47
1:A:120:VAL:O	1:A:121:ASP:C	2.53	0.47
1:B:116:GLU:HA	1:B:119:LYS:CG	2.44	0.47
1:B:120:VAL:O	1:B:123:LEU:N	2.48	0.47
1:B:7:PHE:CG	1:B:8:TRP:N	2.83	0.46
1:A:109:ILE:C	1:A:111:TYR:N	2.69	0.46
1:A:119:LYS:HE2	1:A:123:LEU:HD11	1.95	0.46
1:A:32:LEU:N	1:A:32:LEU:HD12	2.30	0.46
1:A:4:ILE:HD12	1:A:4:ILE:N	2.31	0.46
1:A:66:THR:O	1:A:67:GLN:HB2	2.15	0.46
1:A:69:MET:O	1:A:71:ILE:N	2.48	0.46
1:B:99:VAL:HG11	1:B:154:MET:HB3	1.98	0.46
1:B:176:LEU:O	1:B:177:VAL:C	2.53	0.46
1:A:155:LEU:O	1:A:157:ASP:N	2.48	0.46
1:A:67:GLN:OE1	1:B:97:GLY:HA3	2.16	0.46
1:B:179:PHE:O	1:B:180:LYS:C	2.54	0.46
1:B:18:ARG:NH2	1:B:199:ILE:CD1	2.71	0.46
1:B:85:CYS:SG	1:B:86:PRO:HD2	2.55	0.46
1:B:25:GLU:OE2	1:B:188:GLN:NE2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:PHE:O	1:B:124:SER:N	2.49	0.46
1:B:155:LEU:O	1:B:156:TYR:C	2.54	0.46
1:B:1:MET:HG2	1:B:2:SER:N	2.25	0.46
1:A:156:TYR:O	1:A:156:TYR:CD2	2.69	0.45
1:B:203:LEU:HD23	1:B:203:LEU:N	2.32	0.45
1:B:20:LEU:CD2	1:B:72:ILE:HG13	2.47	0.45
1:B:34:GLU:HG3	1:B:37:GLU:OE1	2.17	0.45
1:A:148:VAL:HG12	1:A:149:THR:O	2.15	0.45
1:B:88:GLU:CG	1:B:88:GLU:O	2.65	0.45
1:A:41:TRP:CE2	1:A:55:LEU:HG	2.51	0.45
1:A:187:PRO:HB2	1:A:188:GLN:OE1	2.17	0.45
1:A:192:TYR:O	1:A:195:SER:HB3	2.16	0.45
1:B:40:LYS:C	1:B:43:ASN:HB2	2.37	0.45
1:A:133:PHE:HB3	1:A:176:LEU:HD21	1.99	0.44
1:A:192:TYR:O	1:A:195:SER:CB	2.65	0.44
1:A:7:PHE:HB2	1:A:56:PRO:HB3	1.99	0.44
1:B:26:GLU:CD	1:B:27:LYS:H	2.20	0.44
1:A:52:PHE:CA	1:B:132:MET:HE2	2.47	0.44
1:A:99:VAL:HG11	1:A:155:LEU:N	2.33	0.44
1:A:35:ARG:HB3	1:A:206:TRP:CD2	2.52	0.44
1:B:116:GLU:HG2	1:B:119:LYS:HD2	1.99	0.44
1:B:11:LYS:HE3	1:B:200:ALA:O	2.17	0.44
1:B:134:GLU:OE1	1:B:176:LEU:HG	2.18	0.44
1:A:22:GLU:OE2	1:A:192:TYR:CD1	2.70	0.44
1:B:88:GLU:HG2	1:B:88:GLU:O	2.16	0.44
1:A:183:ILE:O	1:A:185:ALA:N	2.51	0.44
1:B:168:MET:O	1:B:170:LEU:N	2.50	0.44
1:B:58:TYR:HB2	1:B:71:ILE:HD13	1.99	0.44
1:B:99:VAL:HG13	1:B:155:LEU:HA	1.99	0.44
1:A:106:VAL:O	1:A:110:ALA:HB2	2.17	0.44
1:A:165:MET:HG2	1:A:165:MET:O	2.18	0.44
1:B:133:PHE:O	1:B:134:GLU:C	2.57	0.44
1:B:193:LEU:H	1:B:193:LEU:CD2	2.31	0.44
1:B:204:GLN:NE2	1:B:204:GLN:HA	2.33	0.44
1:B:134:GLU:OE2	1:B:175:LYS:CB	2.67	0.43
1:B:74:TYR:O	1:B:75:ILE:C	2.56	0.43
1:A:66:THR:O	1:A:67:GLN:CB	2.66	0.43
1:B:183:ILE:C	1:B:185:ALA:N	2.69	0.43
1:B:11:LYS:CD	1:B:203:LEU:HA	2.48	0.43
1:B:51:GLU:HB2	1:B:52:PHE:CD1	2.52	0.43
1:A:113:LYS:CD	1:A:114:ASP:N	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ASP:OD2	1:A:118:LEU:HD21	2.19	0.43
1:B:161:VAL:O	1:B:164:TYR:HB3	2.18	0.43
1:A:113:LYS:CD	1:A:114:ASP:H	2.31	0.43
1:A:69:MET:C	1:A:71:ILE:N	2.69	0.43
1:B:109:ILE:HB	1:B:115:PHE:CZ	2.53	0.43
1:B:192:TYR:O	1:B:193:LEU:C	2.56	0.43
1:A:126:LEU:O	1:A:129:MET:HB2	2.18	0.43
1:A:69:MET:C	1:A:71:ILE:H	2.22	0.43
1:A:89:ARG:NH1	1:B:77:ASP:OD1	2.52	0.43
1:A:113:LYS:HD2	1:A:114:ASP:H	1.84	0.43
1:A:205:GLY:C	1:A:207:GLN:N	2.71	0.43
1:B:14:VAL:O	1:B:15:GLN:C	2.57	0.43
1:A:141:THR:HG22	1:A:182:ARG:HD3	2.00	0.43
1:A:204:GLN:HB3	1:A:205:GLY:H	1.63	0.43
1:B:11:LYS:HB3	1:B:15:GLN:HB2	2.00	0.43
1:B:126:LEU:O	1:B:129:MET:HB2	2.19	0.43
1:B:156:TYR:CE1	1:B:180:LYS:HE2	2.54	0.43
1:B:36:ASP:OD1	1:B:37:GLU:N	2.51	0.43
1:A:113:LYS:O	1:A:114:ASP:C	2.57	0.43
1:A:127:PRO:C	1:A:129:MET:N	2.71	0.43
1:B:73:ARG:HH22	1:B:82:LEU:CD2	2.27	0.43
1:A:182:ARG:CB	1:A:182:ARG:HH21	2.32	0.42
1:B:100:LEU:HD23	1:B:100:LEU:HA	1.79	0.42
1:B:105:GLY:C	1:B:109:ILE:HD11	2.39	0.42
1:A:195:SER:OG	1:A:196:SER:N	2.52	0.42
1:A:69:MET:HE2	1:A:100:LEU:CD1	2.49	0.42
1:B:106:VAL:HA	1:B:109:ILE:CD1	2.42	0.42
1:B:76:ALA:O	1:B:79:HIS:N	2.45	0.42
1:B:115:PHE:O	1:B:117:THR:N	2.52	0.42
1:B:59:ILE:HG23	1:B:64:LYS:HA	2.02	0.42
1:B:183:ILE:O	1:B:186:ILE:HG13	2.20	0.42
1:A:150:HIS:N	1:A:151:PRO:HD3	2.34	0.42
1:A:36:ASP:OD1	1:A:37:GLU:N	2.53	0.42
1:B:186:ILE:O	1:B:187:PRO:C	2.57	0.42
1:B:41:TRP:O	1:B:43:ASN:N	2.53	0.42
1:B:152:ASP:O	1:B:153:PHE:C	2.58	0.42
1:B:51:GLU:HB2	1:B:52:PHE:HD1	1.85	0.42
1:A:155:LEU:O	1:A:156:TYR:C	2.57	0.42
1:A:85:CYS:O	1:A:85:CYS:SG	2.78	0.42
1:A:14:VAL:O	1:A:15:GLN:C	2.57	0.41
1:B:124:SER:OG	1:B:125:LYS:HE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:GLY:O	1:B:109:ILE:HD11	2.21	0.41
1:B:14:VAL:HG13	1:B:15:GLN:N	2.33	0.41
1:B:64:LYS:HD3	1:B:64:LYS:N	2.34	0.41
1:A:73:ARG:CZ	1:A:82:LEU:HD21	2.50	0.41
1:B:168:MET:O	1:B:169:CYS:C	2.58	0.41
1:B:11:LYS:HD2	1:B:203:LEU:HB3	2.01	0.41
1:A:29:GLU:OE1	1:A:29:GLU:HA	2.20	0.41
1:B:182:ARG:NH2	1:B:182:ARG:CB	2.77	0.41
1:B:201:TRP:CB	1:B:202:PRO:HA	2.48	0.41
1:A:11:LYS:O	1:A:12:GLY:C	2.57	0.41
1:A:32:LEU:C	1:A:33:TYR:CD1	2.94	0.41
1:A:205:GLY:O	1:A:207:GLN:N	2.53	0.41
1:B:36:ASP:O	1:B:38:GLY:N	2.54	0.41
1:B:36:ASP:C	1:B:38:GLY:H	2.24	0.41
1:A:63:VAL:CG1	1:B:87:LYS:HG3	2.50	0.41
1:A:142:TYR:O	1:A:143:LEU:C	2.59	0.41
1:A:73:ARG:NH1	1:A:73:ARG:HG2	2.36	0.41
1:B:115:PHE:O	1:B:119:LYS:HG3	2.21	0.41
1:B:151:PRO:O	1:B:154:MET:HB2	2.21	0.41
1:B:109:ILE:HG21	1:B:118:LEU:O	2.20	0.41
1:B:133:PHE:C	1:B:135:ASP:N	2.73	0.41
1:B:201:TRP:HE3	1:B:202:PRO:HA	1.85	0.41
1:B:63:VAL:O	1:B:64:LYS:HD3	2.20	0.41
1:A:127:PRO:O	1:A:131:LYS:HB2	2.21	0.41
1:B:73:ARG:NH1	1:B:150:HIS:NE2	2.69	0.41
1:A:44:LYS:O	1:A:45:LYS:C	2.59	0.41
1:A:4:ILE:HD12	1:A:59:ILE:O	2.22	0.40
1:A:73:ARG:NH1	1:A:82:LEU:HD21	2.35	0.40
1:B:142:TYR:O	1:B:144:ASN:N	2.54	0.40
1:A:119:LYS:O	1:A:122:PHE:HB3	2.21	0.40
1:A:170:LEU:O	1:A:173:PHE:N	2.43	0.40
1:B:150:HIS:N	1:B:151:PRO:CD	2.84	0.40
1:B:137:LEU:HD12	1:B:176:LEU:HD23	2.04	0.40
1:A:77:ASP:CG	1:A:82:LEU:HD12	2.41	0.40
1:B:11:LYS:O	1:B:12:GLY:C	2.60	0.40
1:A:99:VAL:HG13	1:A:155:LEU:HA	2.03	0.40
1:B:125:LYS:HB2	1:B:128:GLU:OE1	2.22	0.40
1:B:84:GLY:HA2	1:B:89:ARG:NH1	2.36	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	207/218 (95%)	129 (62%)	48 (23%)	30 (14%)	0	3
1	B	207/218 (95%)	124 (60%)	61 (30%)	22 (11%)	0	7
All	All	414/436 (95%)	253 (61%)	109 (26%)	52 (13%)	0	5

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	TRP
1	A	35	ARG
1	A	37	GLU
1	A	67	GLN
1	A	80	ASN
1	A	86	PRO
1	A	112	SER
1	A	114	ASP
1	A	132	MET
1	A	143	LEU
1	A	169	CYS
1	A	198	TYR
1	A	200	ALA
1	A	208	ALA
1	B	61	GLY
1	B	113	LYS
1	B	132	MET
1	B	169	CYS
1	B	204	GLN
1	A	85	CYS
1	A	152	ASP
1	A	163	LEU
1	A	171	ASP
1	B	37	GLU
1	B	81	MET

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Mol	Chain	Res	Type
1	B	167	PRO
1	B	200	ALA
1	A	42	ARG
1	A	131	LYS
1	A	167	PRO
1	A	184	GLU
1	A	206	TRP
1	B	116	GLU
1	B	152	ASP
1	B	193	LEU
1	A	12	GLY
1	A	113	LYS
1	A	160	ASP
1	A	166	ASP
1	A	193	LEU
1	B	76	ALA
1	B	121	ASP
1	B	127	PRO
1	B	172	ALA
1	A	172	ALA
1	A	197	LYS
1	B	86	PRO
1	B	107	SER
1	B	131	LYS
1	B	164	TYR
1	B	168	MET
1	B	187	PRO

### 5.3.2 Protein sidechains ⓘ

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	188/194 (97%)	166 (88%)	22 (12%)	6	29
1	B	188/194 (97%)	162 (86%)	26 (14%)	4	23
All	All	376/388 (97%)	328 (87%)	48 (13%)	5	25

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	13	LEU
1	A	28	TYR
1	A	32	LEU
1	A	41	TRP
1	A	63	VAL
1	A	66	THR
1	A	79	HIS
1	A	80	ASN
1	A	86	PRO
1	A	101	ASP
1	A	103	ARG
1	A	116	GLU
1	A	118	LEU
1	A	128	GLU
1	A	135	ASP
1	A	160	ASP
1	A	164	TYR
1	A	169	CYS
1	A	187	PRO
1	A	204	GLN
1	A	207	GLN
1	B	5	LEU
1	B	13	LEU
1	B	26	GLU
1	B	32	LEU
1	B	46	PHE
1	B	59	ILE
1	B	62	ASP
1	B	66	THR
1	B	80	ASN
1	B	82	LEU
1	B	101	ASP
1	B	103	ARG
1	B	104	TYR
1	B	109	ILE
1	B	115	PHE
1	B	125	LYS
1	B	127	PRO
1	B	128	GLU
1	B	146	ASP
1	B	165	MET

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Mol	Chain	Res	Type
1	B	167	PRO
1	B	178	CYS
1	B	182	ARG
1	B	188	GLN
1	B	193	LEU
1	B	207	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	207	GLN
1	B	204	GLN
1	B	207	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](#)

1 ligand is 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	GTY	A	220	-	19,27,27	1.01	1 (5%)	22,32,32	1.14	2 (9%)

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	GTY	A	220	-	-	0/26/32/32	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	220	GTY	CA2-N2	2.44	1.51	1.45

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	220	GTY	CA2-N2-CD1	2.57	128.42	121.62
2	A	220	GTY	CG1-CB1-CA1	2.77	120.30	113.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	220	GTY	2	0

## 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](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	209/218 (95%)	-0.41	0 <b>100</b> <b>100</b>	18, 30, 53, 62	1 (0%)
1	B	209/218 (95%)	-0.34	5 (2%) 59 50	18, 27, 72, 83	1 (0%)
All	All	418/436 (95%)	-0.37	5 (1%) 79 71	18, 29, 63, 83	2 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	119	LYS	3.5
1	B	209	THR	2.9
1	B	202	PRO	2.6
1	B	123	LEU	2.3
1	B	207	GLN	2.3

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GTY	A	220	28/28	0.94	0.32	0.97	17,30,34,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.