



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 05:59 am GMT

PDB ID : 3FR3  
Title : Tetramerization and Cooperativity in Plasmodium falciparum glutathione transferase are mediated by the atypic loop 113-118  
Authors : Perbandt, M.; Liebau, E.; Ricci, G.  
Deposited on : 2009-01-08  
Resolution : 1.90 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](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

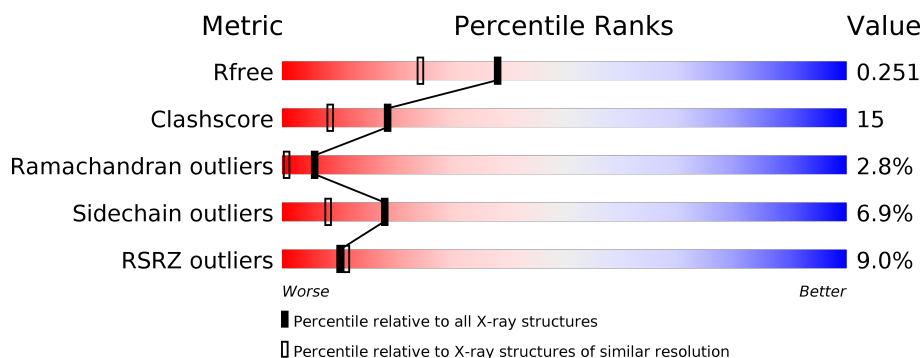
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
$R_{free}$	100719	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

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  $\geq 3$ , 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	208	<div> <div>6%</div> <div> <div></div> <div>72%</div> <div>18%</div> <div>5% • •</div> </div> </div>
1	B	208	<div> <div>12%</div> <div> <div></div> <div>71%</div> <div>20%</div> <div>• • 5%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3585 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.

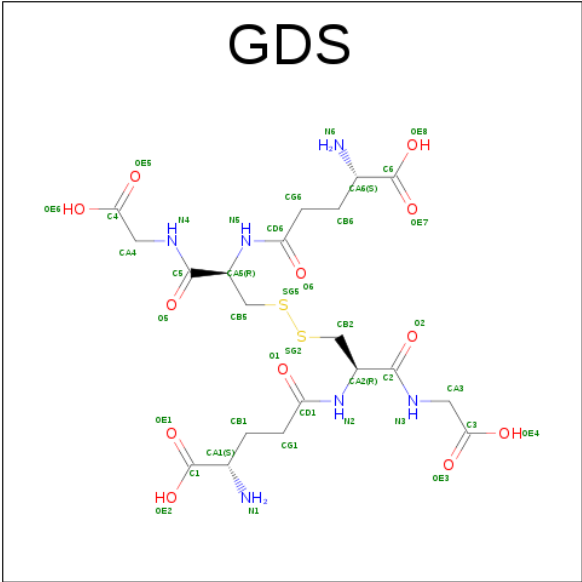
- Molecule 1 is a protein called Glutathione S-transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	201	Total	C	N	O	S	0	3	0
			1667	1084	271	309	3			
1	B	198	Total	C	N	O	S	0	2	0
			1626	1062	263	298	3			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASN	DELETION	UNP Q8MU52
A	?	-	LEU	DELETION	UNP Q8MU52
A	?	-	PHE	DELETION	UNP Q8MU52
A	?	-	LYS	DELETION	UNP Q8MU52
A	?	-	GLN	DELETION	UNP Q8MU52
A	114	ALA	-	INSERTION	UNP Q8MU52
A	115	ALA	-	INSERTION	UNP Q8MU52
B	?	-	ASN	DELETION	UNP Q8MU52
B	?	-	LEU	DELETION	UNP Q8MU52
B	?	-	PHE	DELETION	UNP Q8MU52
B	?	-	LYS	DELETION	UNP Q8MU52
B	?	-	GLN	DELETION	UNP Q8MU52
B	114	ALA	-	INSERTION	UNP Q8MU52
B	115	ALA	-	INSERTION	UNP Q8MU52

- Molecule 2 is OXIDIZED GLUTATHIONE DISULFIDE (three-letter code: GDS) (formula:  $C_{20}H_{32}N_6O_{12}S_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			40	20	6	12	2		
2	B	1	Total	C	N	O	S	0	0
			40	20	6	12	2		

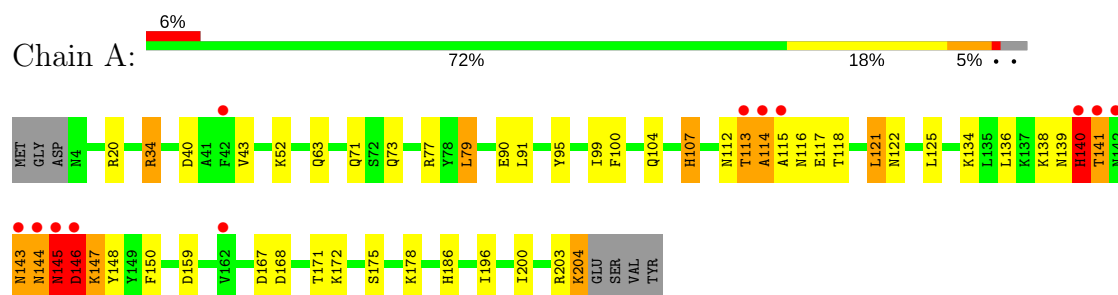
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	132	Total	O	0	0
			132	132		
3	B	80	Total	O	0	0
			80	80		

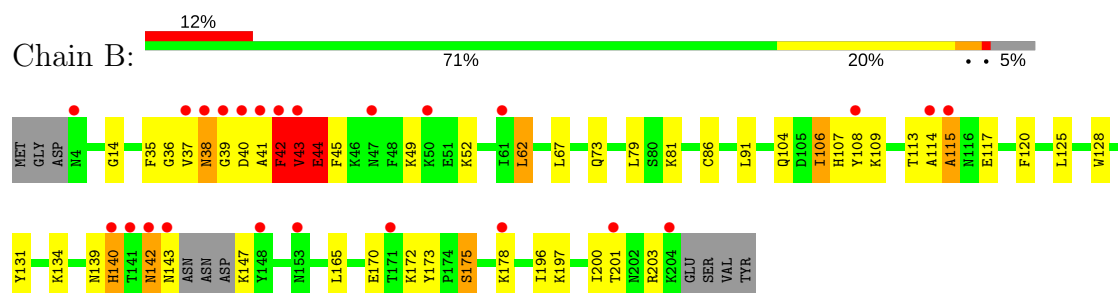
### 3 Residue-property plots [i](#)

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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.89Å 87.06Å 74.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 19.77 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.6 (20.00-1.90) 97.6 (19.77-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.74 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.211 , 0.252 0.210 , 0.251	Depositor DCC
$R_{free}$ test set	1591 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.9	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 59.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3585	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.45% 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: GDS

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	0.96	0/1714	0.96	9/2318 (0.4%)
1	B	0.81	0/1668	0.86	2/2252 (0.1%)
All	All	0.89	0/3382	0.92	11/4570 (0.2%)

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	7
1	B	0	1
All	All	0	8

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	ARG	NE-CZ-NH2	-7.51	116.55	120.30
1	A	147	LYS	N-CA-C	-6.71	92.87	111.00
1	A	79	LEU	CB-CG-CD2	6.52	122.08	111.00
1	A	34	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	B	62	LEU	CA-CB-CG	6.18	129.51	115.30
1	A	140	HIS	N-CA-C	5.76	126.55	111.00
1	B	62	LEU	CB-CG-CD2	5.43	120.23	111.00
1	A	79	LEU	CA-CB-CG	5.39	127.70	115.30
1	A	79	LEU	CB-CG-CD1	5.22	119.88	111.00
1	A	145	ASN	N-CA-C	5.11	124.80	111.00
1	A	146	ASP	N-CA-C	-5.09	97.25	111.00

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	ASN	Peptide
1	A	114	ALA	Peptide
1	A	140	HIS	Peptide
1	A	143	ASN	Peptide
1	A	146	ASP	Peptide
1	A	147	LYS	Peptide
1	A	203	ARG	Peptide
1	B	115	ALA	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	1667	0	1622	51	0
1	B	1626	0	1580	47	1
2	A	40	0	28	1	0
2	B	40	0	28	1	0
3	A	132	0	0	5	0
3	B	80	0	0	1	0
All	All	3585	0	3258	98	1

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 15.

All (98) 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:B:41:ALA:N	1:B:42:PHE:HB2	1.52	1.23
1:B:37:VAL:HB	1:B:38:ASN:HB2	1.24	1.17
1:B:41:ALA:H	1:B:42:PHE:HB2	0.91	1.04
1:B:42:PHE:HB3	1:B:43:VAL:HG12	1.35	1.03
1:A:113:THR:HA	1:A:114:ALA:HB3	1.42	1.02
1:B:40:ASP:HB2	1:B:41:ALA:HB2	1.42	1.00
1:B:37:VAL:CB	1:B:38:ASN:HB2	1.93	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:ALA:H	1:B:42:PHE:CB	1.78	0.94
1:A:118[B]:THR:HG23	1:A:122:ASN:ND2	1.91	0.86
1:B:109:LYS:O	1:B:113:THR:HB	1.77	0.83
1:A:52:LYS:NZ	1:A:63:GLN:HE22	1.80	0.80
1:A:204:LYS:CE	1:A:204:LYS:HA	2.11	0.79
1:A:144:ASN:HB2	1:A:145:ASN:HB2	1.65	0.79
1:A:144:ASN:CB	1:A:145:ASN:HB2	2.14	0.77
1:A:144:ASN:CA	1:A:145:ASN:HB2	2.16	0.76
1:B:36:GLY:HA2	1:B:39:GLY:HA2	1.67	0.75
1:B:35:PHE:HB3	1:B:41:ALA:O	1.86	0.74
1:B:42:PHE:HB3	1:B:43:VAL:CG1	2.13	0.74
1:B:139:ASN:O	1:B:140:HIS:HB2	1.87	0.73
1:A:204:LYS:HE2	1:A:204:LYS:CA	2.18	0.72
1:A:204:LYS:HE2	1:A:204:LYS:HA	1.71	0.72
1:B:37:VAL:CA	1:B:38:ASN:HB2	2.18	0.71
1:B:43:VAL:O	1:B:44:GLU:HB2	1.91	0.70
1:A:118[B]:THR:HG23	1:A:122:ASN:HD21	1.57	0.69
1:A:145:ASN:H	1:A:146:ASP:HB2	1.58	0.69
1:B:142:ASN:CA	1:B:147:LYS:O	2.43	0.67
1:B:40:ASP:CB	1:B:41:ALA:HB2	2.20	0.66
1:B:41:ALA:HB3	1:B:42:PHE:HD1	1.61	0.66
1:B:117[A]:GLU:OE1	3:B:266:HOH:O	2.14	0.65
1:A:204:LYS:O	3:A:331:HOH:O	2.15	0.65
1:A:113:THR:HA	1:A:114:ALA:CB	2.20	0.64
1:B:42:PHE:CB	1:B:43:VAL:HG12	2.21	0.64
1:A:196:ILE:HG22	1:A:200:ILE:HD12	1.80	0.63
1:B:37:VAL:HB	1:B:38:ASN:CB	2.16	0.62
1:A:52:LYS:HZ1	1:A:63:GLN:HE22	1.49	0.60
1:B:113:THR:OG1	1:B:120:PHE:HB2	2.01	0.60
1:B:36:GLY:HA2	1:B:40:ASP:HA	1.84	0.60
1:A:73:GLN:HE21	1:A:77:ARG:HH12	1.49	0.59
1:A:204:LYS:HA	1:A:204:LYS:NZ	2.16	0.59
1:B:106:ILE:HD13	1:B:165:LEU:HD21	1.82	0.59
1:A:91:LEU:HG	1:A:95:TYR:CE2	2.39	0.58
1:B:38:ASN:N	1:B:39:GLY:HA3	2.19	0.58
1:B:41:ALA:HB3	1:B:42:PHE:CD1	2.38	0.57
1:B:41:ALA:CA	1:B:42:PHE:HB2	2.32	0.57
3:A:282:HOH:O	1:B:42:PHE:HE2	1.87	0.56
1:A:100:PHE:CE1	1:A:104[B]:GLN:NE2	2.72	0.56
1:A:113:THR:HB	1:A:114:ALA:C	2.25	0.56
1:A:34:ARG:NH2	3:A:276:HOH:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:TRP:HA	1:B:131:TYR:CD2	2.43	0.54
1:A:107:HIS:HD2	3:A:257:HOH:O	1.91	0.54
1:A:175:SER:O	1:A:178:LYS:HG2	2.09	0.53
1:A:144:ASN:HB2	1:A:145:ASN:CB	2.39	0.52
1:B:113:THR:O	1:B:117[A]:GLU:HB2	2.09	0.52
1:A:139:ASN:O	1:A:141:THR:O	2.28	0.52
1:A:113:THR:HB	1:A:115:ALA:N	2.25	0.51
1:A:144:ASN:N	1:A:145:ASN:HB2	2.24	0.51
1:A:145:ASN:N	1:A:146:ASP:HB2	2.26	0.50
1:A:118[B]:THR:CG2	1:A:122:ASN:ND2	2.71	0.50
1:A:159:ASP:OD1	1:A:186:HIS:HE1	1.93	0.50
1:A:167:ASP:O	1:A:171:THR:HG23	2.12	0.50
2:A:400:GDS:HB52	1:B:115:ALA:HB3	1.94	0.50
1:A:52:LYS:HZ2	1:A:63:GLN:HE22	1.59	0.49
1:B:42:PHE:H	1:B:45:PHE:H	1.61	0.49
1:A:114:ALA:O	3:A:321:HOH:O	2.20	0.49
1:B:113:THR:O	1:B:117[B]:GLU:HB3	2.13	0.49
1:A:140:HIS:N	1:A:141:THR:HB	2.28	0.49
1:A:144:ASN:CB	1:A:145:ASN:CB	2.90	0.48
1:A:148:TYR:CD2	1:A:148:TYR:N	2.81	0.48
1:B:106:ILE:HG12	1:B:128:TRP:HB3	1.95	0.48
1:A:145:ASN:H	1:A:146:ASP:CB	2.24	0.47
1:A:144:ASN:HB3	1:A:145:ASN:ND2	2.28	0.47
1:B:200:ILE:HD12	1:B:203:ARG:NH2	2.30	0.47
1:A:73:GLN:OE1	1:A:104[A]:GLN:OE1	2.33	0.47
1:B:172:LYS:HG2	1:B:173:TYR:CZ	2.50	0.47
1:A:145:ASN:N	1:A:146:ASP:CB	2.78	0.47
1:B:45:PHE:CE1	1:B:49:LYS:NZ	2.81	0.46
1:A:118[B]:THR:HG23	1:A:122:ASN:HD22	1.75	0.45
1:B:114:ALA:HA	1:B:115:ALA:HA	1.69	0.45
1:B:197:LYS:O	1:B:201:THR:HG23	2.17	0.45
1:A:143:ASN:O	1:A:144:ASN:HB2	2.17	0.45
1:B:175:SER:HB3	1:B:178:LYS:HE2	1.99	0.44
1:B:36:GLY:HA2	1:B:39:GLY:CA	2.43	0.44
1:B:81:LYS:HA	1:B:86:CYS:SG	2.57	0.44
1:A:40:ASP:HB3	1:A:43:VAL:HB	2.00	0.44
1:A:107:HIS:HE1	1:A:168:ASP:OD2	2.01	0.43
1:A:117:GLU:HB2	1:A:121:LEU:HD22	1.99	0.43
1:A:118[B]:THR:CG2	1:A:122:ASN:HD22	2.29	0.43
1:B:196[A]:ILE:O	1:B:200:ILE:HG12	2.19	0.43
1:B:39:GLY:HA2	1:B:40:ASP:HA	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:LYS:NZ	1:A:138:LYS:NZ	2.67	0.42
1:B:40:ASP:HB2	1:B:41:ALA:CB	2.31	0.41
1:B:37:VAL:H	1:B:38:ASN:CB	2.33	0.41
1:B:14:GLY:CA	2:B:401:GDS:HA6	2.51	0.41
1:A:136:LEU:HG	1:A:150:PHE:CE2	2.56	0.41
1:B:73:GLN:NE2	1:B:104:GLN:HG3	2.36	0.41
1:A:113:THR:CB	1:A:115:ALA:N	2.84	0.41
1:A:99:ILE:HD13	1:A:150:PHE:HB3	2.02	0.41
1:A:20:ARG:HD2	1:A:20:ARG:HH11	1.70	0.40

All (1) 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)
1:B:108:TYR:OH	1:B:108:TYR:OH[2_555]	2.15	0.05

## 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	202/208 (97%)	187 (93%)	11 (5%)	4 (2%)	9	2
1	B	196/208 (94%)	178 (91%)	11 (6%)	7 (4%)	4	0
All	All	398/416 (96%)	365 (92%)	22 (6%)	11 (3%)	6	1

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	ASP
1	B	42	PHE
1	B	43	VAL
1	B	44	GLU

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Mol	Chain	Res	Type
1	A	144	ASN
1	A	145	ASN
1	B	38	ASN
1	B	140	HIS
1	B	170	GLU
1	A	71	GLN
1	B	142	ASN

### 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	179/186 (96%)	169 (94%)	10 (6%)	25	13
1	B	172/186 (92%)	158 (92%)	14 (8%)	14	5
All	All	351/372 (94%)	327 (93%)	24 (7%)	18	8

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	LEU
1	A	90	GLU
1	A	107	HIS
1	A	113	THR
1	A	116	ASN
1	A	121	LEU
1	A	125	LEU
1	A	141	THR
1	A	172	LYS
1	A	204	LYS
1	B	42	PHE
1	B	43	VAL
1	B	44	GLU
1	B	52	LYS
1	B	62	LEU
1	B	67	LEU

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Mol	Chain	Res	Type
1	B	79	LEU
1	B	91	LEU
1	B	106	ILE
1	B	107	HIS
1	B	125	LEU
1	B	134	LYS
1	B	143	ASN
1	B	175	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	71	GLN
1	A	73	GLN
1	A	92	ASN
1	A	107	HIS
1	A	122	ASN
1	A	145	ASN
1	A	154	ASN
1	A	186	HIS
1	A	192	ASN
1	A	195	ASN
1	B	47	ASN
1	B	58	GLN
1	B	71	GLN
1	B	92	ASN
1	B	107	HIS
1	B	122	ASN
1	B	143	ASN
1	B	192	ASN
1	B	195	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are 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	GDS	A	400	-	23,39,39	0.91	0	30,50,50	2.20	7 (23%)
2	GDS	B	401	-	23,39,39	0.81	1 (4%)	30,50,50	1.70	5 (16%)

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	GDS	A	400	-	-	0/39/51/51	0/0/0/0
2	GDS	B	401	-	-	0/39/51/51	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	GDS	CA2-C2	-2.01	1.47	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	GDS	CB2-SG2-SG5	-6.09	91.99	103.83
2	B	401	GDS	CB2-SG2-SG5	-4.22	95.63	103.83
2	A	400	GDS	O6-CD6-CG6	-2.79	116.77	122.01
2	B	401	GDS	O6-CD6-CG6	-2.77	116.81	122.01
2	B	401	GDS	CG1-CB1-CA1	-2.72	107.49	113.84
2	A	400	GDS	C2-CA2-N2	-2.67	103.85	111.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	GDS	CB6-CG6-CD6	2.23	118.22	113.18
2	B	401	GDS	CA4-N4-C5	2.48	125.75	122.39
2	A	400	GDS	CG6-CD6-N5	3.52	122.02	115.82
2	A	400	GDS	CB5-SG5-SG2	4.43	112.45	103.83
2	B	401	GDS	CB5-SG5-SG2	4.63	112.84	103.83
2	A	400	GDS	CG6-CB6-CA6	5.83	127.45	113.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	GDS	1	0
2	B	401	GDS	1	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	201/208 (96%)	0.43	12 (5%) 23 26	15, 27, 47, 69	0
1	B	198/208 (95%)	0.79	24 (12%) 5 5	23, 38, 63, 76	0
All	All	399/416 (95%)	0.61	36 (9%) 10 11	15, 32, 58, 76	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	141	THR	6.7
1	B	143	ASN	5.9
1	B	38	ASN	5.7
1	A	144	ASN	5.6
1	A	143	ASN	4.9
1	B	141	THR	4.7
1	A	145	ASN	4.7
1	B	50	LYS	4.3
1	B	142	ASN	4.0
1	B	40	ASP	3.9
1	A	140	HIS	3.8
1	B	115	ALA	3.8
1	A	142	ASN	3.7
1	B	41	ALA	3.7
1	B	42	PHE	3.5
1	A	146	ASP	3.4
1	B	39	GLY	3.4
1	B	43	VAL	3.4
1	B	4	ASN	3.4
1	A	115	ALA	3.3
1	B	201	THR	3.0
1	B	171	THR	2.9
1	B	204	LYS	2.9
1	B	140	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	178	LYS	2.8
1	B	108	TYR	2.8
1	B	61	ILE	2.6
1	B	37	VAL	2.6
1	B	148	TYR	2.4
1	A	114	ALA	2.4
1	A	113	THR	2.4
1	B	114	ALA	2.3
1	A	42	PHE	2.3
1	B	47	ASN	2.3
1	B	153	ASN	2.3
1	A	162	VAL	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(Å <sup>2</sup> )	Q<0.9
2	GDS	B	401	40/40	0.88	0.15	0.14	28,38,52,54	0
2	GDS	A	400	40/40	0.92	0.13	-0.16	17,36,52,56	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.