



# Full wwPDB X-ray Structure Validation Report i

Feb 28, 2014 – 09:42 AM GMT

PDB ID : 3UBL  
Title : Crystal structure of glutathione transferase (TARGET EFI-501770) from leptospira interrogans with gsh bound  
Authors : Patskovsky, Y.; Toro, R.; Bhosle, R.; Zencheck, W.D.; Hillerich, B.; Seidel, R.D.; Washington, E.; Scott Glenn, A.; Chowdhury, S.; Evans, B.; Hammonds, J.; Imker, H.J.; Armstrong, R.N.; Gerlt, J.A.; Almo, S.C.; (Efi), Enzyme Function Initiative  
Deposited on : 2011-10-24  
Resolution : 2.00 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

---

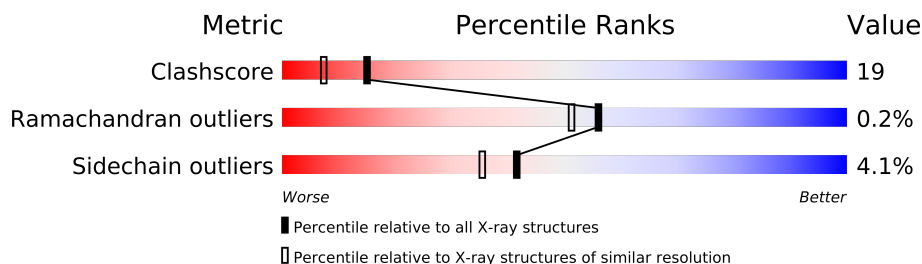
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	<b>FAILED</b>
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.00 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	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	242	
1	B	242	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3634 atoms, of which 0 are hydrogen and 0 are deuterium.

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 transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	2	0
			1700	1114	278	303	5			
1	B	207	Total	C	N	O	S	0	1	0
			1664	1087	272	300	5			

There are 48 discrepancies between the modelled and reference sequences:

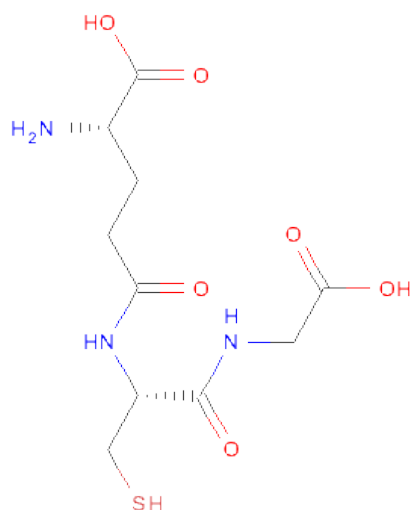
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	EXPRESSION TAG	UNP Q8F2Y8
A	0	VAL	-	EXPRESSION TAG	UNP Q8F2Y8
A	219	ALA	-	EXPRESSION TAG	UNP Q8F2Y8
A	220	GLU	-	EXPRESSION TAG	UNP Q8F2Y8
A	221	ASN	-	EXPRESSION TAG	UNP Q8F2Y8
A	222	LEU	-	EXPRESSION TAG	UNP Q8F2Y8
A	223	TYR	-	EXPRESSION TAG	UNP Q8F2Y8
A	224	PHE	-	EXPRESSION TAG	UNP Q8F2Y8
A	225	GLN	-	EXPRESSION TAG	UNP Q8F2Y8
A	226	SER	-	EXPRESSION TAG	UNP Q8F2Y8
A	227	HIS	-	EXPRESSION TAG	UNP Q8F2Y8
A	228	HIS	-	EXPRESSION TAG	UNP Q8F2Y8
A	229	HIS	-	EXPRESSION TAG	UNP Q8F2Y8
A	230	HIS	-	EXPRESSION TAG	UNP Q8F2Y8
A	231	HIS	-	EXPRESSION TAG	UNP Q8F2Y8
A	232	HIS	-	EXPRESSION TAG	UNP Q8F2Y8
A	233	TRP	-	EXPRESSION TAG	UNP Q8F2Y8
A	234	SER	-	EXPRESSION TAG	UNP Q8F2Y8
A	235	HIS	-	EXPRESSION TAG	UNP Q8F2Y8
A	236	PRO	-	EXPRESSION TAG	UNP Q8F2Y8
A	237	GLN	-	EXPRESSION TAG	UNP Q8F2Y8
A	238	PHE	-	EXPRESSION TAG	UNP Q8F2Y8
A	239	GLU	-	EXPRESSION TAG	UNP Q8F2Y8
A	240	LYS	-	EXPRESSION TAG	UNP Q8F2Y8
B	-1	MET	-	EXPRESSION TAG	UNP Q8F2Y8

*Continued on next page...*

Continued from previous page...

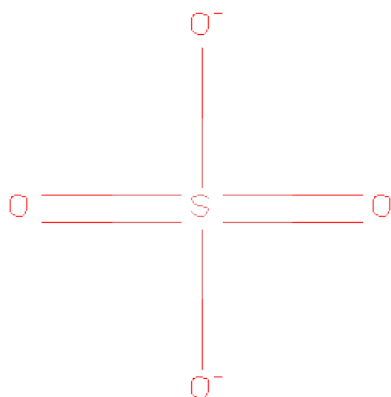
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	VAL	-	EXPRESSION TAG	UNP Q8F2Y8
B	219	ALA	-	EXPRESSION TAG	UNP Q8F2Y8
B	220	GLU	-	EXPRESSION TAG	UNP Q8F2Y8
B	221	ASN	-	EXPRESSION TAG	UNP Q8F2Y8
B	222	LEU	-	EXPRESSION TAG	UNP Q8F2Y8
B	223	TYR	-	EXPRESSION TAG	UNP Q8F2Y8
B	224	PHE	-	EXPRESSION TAG	UNP Q8F2Y8
B	225	GLN	-	EXPRESSION TAG	UNP Q8F2Y8
B	226	SER	-	EXPRESSION TAG	UNP Q8F2Y8
B	227	HIS	-	EXPRESSION TAG	UNP Q8F2Y8
B	228	HIS	-	EXPRESSION TAG	UNP Q8F2Y8
B	229	HIS	-	EXPRESSION TAG	UNP Q8F2Y8
B	230	HIS	-	EXPRESSION TAG	UNP Q8F2Y8
B	231	HIS	-	EXPRESSION TAG	UNP Q8F2Y8
B	232	HIS	-	EXPRESSION TAG	UNP Q8F2Y8
B	233	TRP	-	EXPRESSION TAG	UNP Q8F2Y8
B	234	SER	-	EXPRESSION TAG	UNP Q8F2Y8
B	235	HIS	-	EXPRESSION TAG	UNP Q8F2Y8
B	236	PRO	-	EXPRESSION TAG	UNP Q8F2Y8
B	237	GLN	-	EXPRESSION TAG	UNP Q8F2Y8
B	238	PHE	-	EXPRESSION TAG	UNP Q8F2Y8
B	239	GLU	-	EXPRESSION TAG	UNP Q8F2Y8
B	240	LYS	-	EXPRESSION TAG	UNP Q8F2Y8

- Molecule 2 is GLUTATHIONE (three-letter code: GSH) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>3</sub>O<sub>6</sub>S).



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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	0
			1	1		
5	A	1	Total	Cl	0	0
			1	1		

- Molecule 6 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	X	0	1
			1	1		
6	A	1	Total	X	0	1
			1	1		

- Molecule 7 is water.

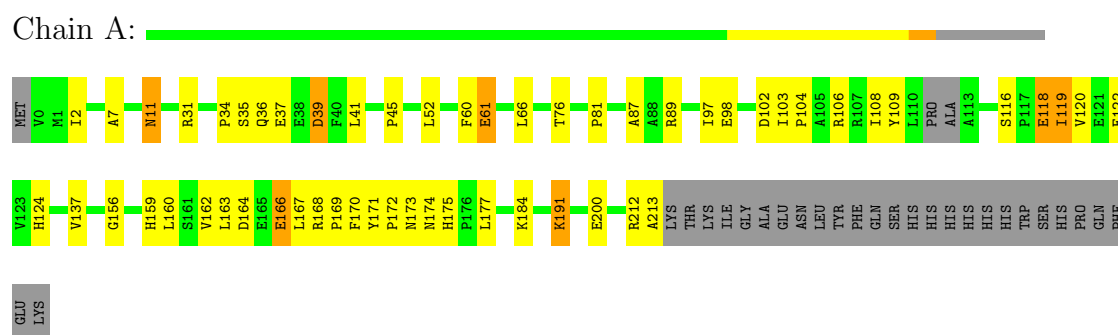
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	74	Total 74	O 74	0	0
7	B	68	Total 68	O 68	0	0

### 3 Residue-property plots

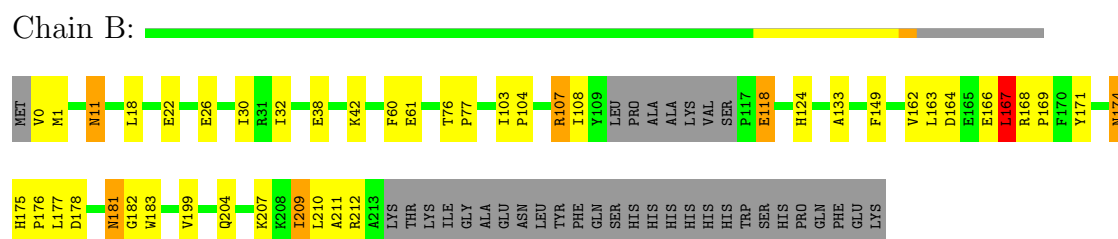
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

- Molecule 1: Glutathione transferase



- Molecule 1: Glutathione transferase





## 4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.59Å 82.59Å 175.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00	Depositor
% Data completeness (in resolution range)	97.3 (50.00-2.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.200 , 0.235	Depositor
Wilson B-factor (Å <sup>2</sup> )	41.6	Xtriage
Anisotropy	0.447	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 43293 reflections	Xtriage
Total number of atoms	3634	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: UNX, GOL, GSH, SO4, CL

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	0.54	0/1744	0.57	0/2361
1	B	0.50	0/1705	0.57	2/2306 (0.1%)
All	All	0.52	0/3449	0.57	2/4667 (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	B	209	ILE	CB-CA-C	-5.57	100.45	111.60
1	B	167	LEU	CA-CB-CG	-5.20	103.34	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1700	0	1765	75	0
1	B	1664	0	1711	60	0
2	A	40	0	29	2	0
2	B	40	0	30	0	0
3	A	15	0	0	3	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	5	0	0	0	0
4	A	18	0	24	0	0
4	B	6	0	8	0	0
5	A	1	0	0	0	0
5	B	1	0	0	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	74	0	0	0	0
7	B	68	0	0	1	0
All	All	3634	0	3567	134	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 19.

All (134) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:166:GLU:C	1:B:167:LEU:HD23	1.47	1.32
1:B:118:GLU:CD	1:B:118:GLU:O	1.80	1.18
1:B:0:VAL:HG21	1:B:26:GLU:HB3	1.30	1.13
1:B:167:LEU:HD23	1:B:167:LEU:N	1.58	1.04
1:B:0:VAL:CG2	1:B:26:GLU:HB3	1.87	1.03
1:A:124:HIS:HD2	1:A:171:TYR:CD1	1.78	1.01
1:B:166:GLU:O	1:B:167:LEU:HD23	1.60	1.00
1:A:171:TYR:HB3	1:A:174:ASN:HB3	1.52	0.92
1:A:11:ASN:H	1:A:11:ASN:HD22	1.19	0.90
1:B:171:TYR:HB3	1:B:174:ASN:HB3	1.53	0.90
1:B:11:ASN:HD22	1:B:11:ASN:H	0.90	0.89
1:B:11:ASN:H	1:B:11:ASN:ND2	1.70	0.89
1:B:0:VAL:HG21	1:B:26:GLU:CB	2.04	0.88
1:A:108:ILE:CG2	1:A:170:PHE:CE2	2.56	0.88
1:A:60:PHE:O	1:A:61:GLU:HB2	1.71	0.88
1:A:166:GLU:HA	1:A:166:GLU:OE1	1.70	0.88
1:A:118:GLU:HG3	1:A:119:ILE:N	1.88	0.87
1:A:124:HIS:CD2	1:A:171:TYR:CD1	2.63	0.85
1:A:124:HIS:HD2	1:A:171:TYR:CE1	1.94	0.85
1:A:159:HIS:O	1:A:163:LEU:HG	1.75	0.85
1:B:11:ASN:N	1:B:11:ASN:HD22	1.70	0.84
1:B:209:ILE:HG22	1:B:210:LEU:N	1.92	0.84
1:A:124:HIS:CD2	1:A:171:TYR:CE1	2.67	0.83
1:B:164:ASP:HB2	1:B:177:LEU:CD2	2.09	0.82
1:B:168:ARG:N	1:B:169:PRO:HD2	1.95	0.81
1:B:164:ASP:HB2	1:B:177:LEU:HD23	1.59	0.81

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:167:LEU:HB2	1:A:175:HIS:CE1	2.17	0.80
1:B:166:GLU:O	1:B:167:LEU:CD2	2.30	0.79
1:A:166:GLU:CA	1:A:166:GLU:OE1	2.30	0.79
5:B:244:CL:CL	7:B:312:HOH:O	2.37	0.79
1:A:118:GLU:HG3	1:A:119:ILE:H	1.48	0.79
1:A:167:LEU:N	1:A:167:LEU:HD23	1.96	0.78
1:A:103:ILE:HB	1:A:104:PRO:HD3	1.67	0.77
1:A:116:SER:HB2	1:A:119:ILE:HB	1.65	0.77
1:A:108:ILE:HG23	1:A:170:PHE:CZ	2.21	0.76
1:A:116:SER:HB2	1:A:119:ILE:H	1.49	0.76
1:B:103:ILE:HB	1:B:104:PRO:HD3	1.68	0.75
1:A:172:PRO:O	1:A:173:ASN:HB2	1.86	0.74
1:B:118:GLU:O	1:B:118:GLU:OE1	2.05	0.74
1:A:168:ARG:N	1:A:169:PRO:CD	2.52	0.72
1:A:124:HIS:HB2	1:A:171:TYR:HE1	1.54	0.72
1:A:164:ASP:C	1:A:164:ASP:OD1	2.29	0.71
1:B:118:GLU:C	1:B:118:GLU:CD	2.50	0.71
1:B:164:ASP:OD1	1:B:164:ASP:C	2.29	0.70
1:B:118:GLU:O	1:B:118:GLU:CG	2.40	0.69
1:A:166:GLU:C	1:A:167:LEU:HD23	2.13	0.69
1:B:0:VAL:HG12	1:B:1:MET:N	2.09	0.68
1:A:37:GLU:OE1	1:A:39:ASP:HB2	1.94	0.66
1:A:191:LYS:HE3	1:A:200:GLU:HG3	1.78	0.66
1:B:0:VAL:HG12	1:B:1:MET:H	1.60	0.65
1:B:168:ARG:N	1:B:169:PRO:CD	2.59	0.65
1:A:119:ILE:HG22	1:A:120:VAL:N	2.12	0.64
1:B:108:ILE:CG2	1:B:108:ILE:O	2.45	0.63
1:A:11:ASN:HD22	1:A:11:ASN:N	1.91	0.61
1:B:207:LYS:O	1:B:211:ALA:HB2	2.01	0.61
1:A:124:HIS:HB2	1:A:171:TYR:CE1	2.35	0.60
1:B:107:ARG:O	1:B:108:ILE:HD12	2.02	0.59
1:B:0:VAL:HG23	1:B:26:GLU:HB3	1.83	0.59
1:B:30:ILE:HG22	1:B:32:ILE:HG23	1.84	0.59
1:A:11:ASN:H	1:A:11:ASN:ND2	1.97	0.59
1:B:181:ASN:C	1:B:181:ASN:HD22	2.05	0.58
1:B:166:GLU:C	1:B:167:LEU:CD2	2.43	0.58
1:A:76[A]:THR:HG23	3:A:243:SO4:O3	2.04	0.57
1:A:168:ARG:N	1:A:169:PRO:HD3	2.20	0.56
1:B:60:PHE:O	1:B:61:GLU:HB2	2.05	0.56
1:B:181:ASN:HD22	1:B:182:GLY:N	2.05	0.55
1:B:0:VAL:HG12	1:B:1:MET:HG3	1.89	0.54
1:A:108:ILE:HG22	1:A:109:TYR:N	2.22	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:34:PRO:HB3	2:A:241[A]:GSH:HA31	1.88	0.54
1:A:36:GLN:HA	1:A:41:LEU:HD21	1.91	0.53
1:A:164:ASP:HB2	1:A:177:LEU:CD1	2.39	0.52
1:A:172:PRO:C	1:A:174:ASN:H	2.13	0.52
1:B:175:HIS:HB3	1:B:178:ASP:OD2	2.10	0.52
1:A:166:GLU:O	1:A:169:PRO:HD2	2.10	0.52
1:A:162:VAL:O	1:A:166:GLU:HG2	2.11	0.51
1:A:98:GLU:O	1:A:103:ILE:HG12	2.11	0.51
1:A:7:ALA:HB2	1:A:31:ARG:HG3	1.92	0.51
1:A:164:ASP:HB2	1:A:177:LEU:HD12	1.91	0.51
1:A:108:ILE:CG2	1:A:170:PHE:CZ	2.85	0.51
1:A:34:PRO:HB3	2:A:241[B]:GSH:HA31	1.93	0.51
1:A:108:ILE:HG21	1:A:170:PHE:CE2	2.44	0.50
1:A:108:ILE:HG22	1:A:170:PHE:CE2	2.43	0.50
1:B:124:HIS:HB2	1:B:171:TYR:CE1	2.47	0.50
1:A:212:ARG:O	1:A:213:ALA:C	2.50	0.49
1:B:211:ALA:C	1:B:212:ARG:HG3	2.33	0.49
1:B:0:VAL:CG2	1:B:26:GLU:CB	2.72	0.48
1:A:184:LYS:HB2	3:A:244:SO4:S	2.53	0.48
1:B:118:GLU:OE2	1:B:118:GLU:C	2.52	0.48
1:B:107:ARG:C	1:B:108:ILE:HD12	2.34	0.48
1:A:60:PHE:O	1:A:61:GLU:CB	2.50	0.47
1:A:31:ARG:CB	1:A:31:ARG:CZ	2.92	0.47
1:B:108:ILE:HG23	1:B:108:ILE:O	2.13	0.47
1:B:167:LEU:N	1:B:167:LEU:CD2	2.38	0.47
1:B:118:GLU:OE2	1:B:118:GLU:O	2.30	0.47
1:B:22:GLU:HG3	1:B:77:PRO:HG3	1.97	0.46
1:A:116:SER:CB	1:A:119:ILE:HB	2.40	0.46
1:B:38:GLU:O	1:B:42:LYS:HG2	2.16	0.46
1:A:166:GLU:N	1:A:166:GLU:OE1	2.49	0.46
1:A:108:ILE:HG21	1:A:170:PHE:CD2	2.50	0.46
1:A:118:GLU:O	1:A:122:GLU:HG3	2.15	0.46
1:B:0:VAL:CG1	1:B:1:MET:H	2.25	0.45
1:B:103:ILE:CB	1:B:104:PRO:HD3	2.44	0.45
1:A:7:ALA:CB	1:A:31:ARG:HG3	2.46	0.45
1:B:171:TYR:CB	1:B:174:ASN:HB3	2.37	0.45
1:A:102:ASP:O	1:A:106:ARG:HG3	2.17	0.45
1:A:171:TYR:CB	1:A:174:ASN:HB3	2.37	0.45
1:B:162:VAL:HG13	1:B:166:GLU:HG3	2.00	0.44
1:A:160:LEU:HD23	1:A:163:LEU:HD12	1.98	0.44
1:A:11:ASN:N	1:A:11:ASN:ND2	2.60	0.44
1:A:97:ILE:HD13	1:A:156:GLY:HA2	1.99	0.44

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:31:ARG:HB3	1:A:31:ARG:CZ	2.48	0.44
1:A:31:ARG:HB2	1:A:31:ARG:NH1	2.33	0.44
1:B:22:GLU:HG2	1:B:149:PHE:CD1	2.52	0.44
1:B:76:THR:CG2	1:B:77:PRO:HA	2.48	0.44
1:A:184:LYS:HB2	3:A:244:SO4:O1	2.17	0.43
1:A:2:ILE:HG23	1:A:52:LEU:HD11	2.00	0.43
1:A:66:LEU:HA	1:A:66:LEU:HD23	1.91	0.43
1:A:81:PRO:HD2	1:A:87:ALA:HA	2.00	0.43
1:B:11:ASN:N	1:B:11:ASN:ND2	2.40	0.43
1:A:45:PRO:CB	1:B:133:ALA:HB1	2.49	0.43
1:A:116:SER:HB3	1:A:118:GLU:HG2	2.01	0.42
1:B:18:LEU:HG	1:B:199:VAL:HG21	2.02	0.42
1:A:103:ILE:N	1:A:104:PRO:CD	2.82	0.41
1:B:76:THR:HG23	1:B:77:PRO:HA	2.01	0.41
1:B:38:GLU:OE2	1:B:42:LYS:HE2	2.20	0.41
1:B:108:ILE:HG22	1:B:108:ILE:O	2.18	0.41
1:A:172:PRO:C	1:A:174:ASN:N	2.73	0.41
1:A:167:LEU:C	1:A:169:PRO:HD2	2.41	0.41
1:B:177:LEU:HD21	1:B:183:TRP:NE1	2.36	0.41
1:A:164:ASP:OD1	1:A:164:ASP:O	2.38	0.41
1:A:103:ILE:HB	1:A:104:PRO:CD	2.45	0.40
1:A:89:ARG:NH1	1:A:137:VAL:O	2.48	0.40
1:B:175:HIS:HA	1:B:176:PRO:HD3	1.83	0.40
1:A:45:PRO:HB2	1:B:133:ALA:HB1	2.04	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	210/242 (87%)	201 (96%)	8 (4%)	1 (0%)	38	29
1	B	204/242 (84%)	200 (98%)	4 (2%)	0	100	100
All	All	414/484 (86%)	401 (97%)	12 (3%)	1 (0%)	56	51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	GLU

### 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	186/213 (87%)	179 (96%)	7 (4%)	44	39
1	B	182/213 (85%)	174 (96%)	8 (4%)	39	32
All	All	368/426 (86%)	353 (96%)	15 (4%)	41	35

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	35	SER
1	A	39	ASP
1	A	118	GLU
1	A	119	ILE
1	A	166	GLU
1	A	191	LYS
1	B	11	ASN
1	B	107	ARG
1	B	118	GLU
1	B	163	LEU
1	B	167	LEU
1	B	174	ASN
1	B	181	ASN
1	B	204	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	124	HIS
1	A	175	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	11	ASN
1	B	174	ASN
1	B	181	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 2 are unknown and 2 are monoatomic - leaving 12 for Mogul analysis.

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	GSH	A	241[A]	-	19,19,19	2.57	3 (15%)	24,24,24	1.29	2 (8%)
2	GSH	A	241[B]	-	19,19,19	2.57	3 (15%)	24,24,24	1.34	3 (12%)
3	SO4	A	242	-	4,4,4	0.12	0	6,6,6	0.12	0
3	SO4	A	243	-	4,4,4	0.30	0	6,6,6	0.22	0
3	SO4	A	244	-	4,4,4	1.02	0	6,6,6	0.64	0
4	GOL	A	245	-	5,5,5	0.70	0	5,5,5	0.30	0
4	GOL	A	247	-	5,5,5	0.58	0	5,5,5	0.46	0
4	GOL	A	248	-	5,5,5	0.40	0	5,5,5	0.38	0
2	GSH	B	241[A]	-	19,19,19	2.53	3 (15%)	24,24,24	1.28	6 (25%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GSH	B	241[B]	-	19,19,19	2.69	4 (21%)	24,24,24	1.90	8 (33%)
3	SO4	B	242	-	4,4,4	0.24	0	6,6,6	0.16	0
4	GOL	B	243	-	5,5,5	0.60	0	5,5,5	0.66	0

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	GSH	A	241[A]	-	-	0/24/24/24	0/0/0/0
2	GSH	A	241[B]	-	-	0/24/24/24	0/0/0/0
3	SO4	A	242	-	-	0/0/0/0	0/0/0/0
3	SO4	A	243	-	-	0/0/0/0	0/0/0/0
3	SO4	A	244	-	-	0/0/0/0	0/0/0/0
4	GOL	A	245	-	-	0/4/4/4	0/0/0/0
4	GOL	A	247	-	-	0/4/4/4	0/0/0/0
4	GOL	A	248	-	-	0/4/4/4	0/0/0/0
2	GSH	B	241[A]	-	-	0/24/24/24	0/0/0/0
2	GSH	B	241[B]	-	-	0/24/24/24	0/0/0/0
3	SO4	B	242	-	-	0/0/0/0	0/0/0/0
4	GOL	B	243	-	-	0/4/4/4	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	241[A]	GSH	OE1-CD1	7.52	1.39	1.23
2	B	241[B]	GSH	OE1-CD1	7.51	1.39	1.23
2	A	241[B]	GSH	OE1-CD1	7.48	1.39	1.23
2	A	241[A]	GSH	OE1-CD1	7.40	1.39	1.23
2	B	241[B]	GSH	O2-C2	7.34	1.38	1.23
2	A	241[B]	GSH	O2-C2	7.24	1.37	1.23
2	A	241[A]	GSH	O2-C2	7.11	1.37	1.23
2	B	241[A]	GSH	O2-C2	6.76	1.36	1.23
2	B	241[B]	GSH	CB2-CA2	2.87	1.56	1.53
2	A	241[B]	GSH	O12-C1	-2.39	1.21	1.30
2	A	241[A]	GSH	O12-C1	-2.39	1.21	1.30
2	B	241[B]	GSH	O12-C1	-2.30	1.22	1.30
2	B	241[A]	GSH	O12-C1	-2.27	1.22	1.30

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	241[B]	GSH	CB2-CA2-C2	5.06	120.70	109.70
2	B	241[B]	GSH	O2-C2-N3	-3.13	116.70	123.05
2	A	241[B]	GSH	CB2-CA2-C2	2.89	115.98	109.70
2	B	241[B]	GSH	O32-C3-O31	-2.79	116.19	123.30
2	A	241[A]	GSH	O12-C1-O11	-2.70	117.98	124.07
2	A	241[B]	GSH	O12-C1-O11	-2.66	118.05	124.07
2	A	241[A]	GSH	CG1-CB1-CA1	-2.64	109.50	114.43
2	B	241[B]	GSH	O32-C3-CA3	2.63	122.55	112.98
2	B	241[B]	GSH	C2-CA2-N2	-2.53	104.16	111.28
2	B	241[A]	GSH	O32-C3-CA3	2.50	122.07	112.98
2	B	241[A]	GSH	O32-C3-O31	-2.43	117.11	123.30
2	B	241[A]	GSH	O12-C1-O11	-2.39	118.68	124.07
2	B	241[B]	GSH	O12-C1-O11	-2.32	118.83	124.07
2	B	241[B]	GSH	CA2-C2-N3	2.14	120.91	116.72
2	B	241[A]	GSH	O12-C1-CA1	2.12	121.63	116.88
2	B	241[A]	GSH	CG1-CB1-CA1	-2.11	110.50	114.43
2	A	241[B]	GSH	CG1-CB1-CA1	-2.10	110.51	114.43
2	B	241[A]	GSH	CB2-CA2-C2	2.10	114.26	109.70
2	B	241[B]	GSH	O12-C1-CA1	2.06	121.50	116.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.