wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 09:26 PM GMT

PDB ID	:	1OYJ
Title	:	Crystal structure solution of Rice GST1 (OsGSTU1) in complex with glutathione.
Authors	:	Dixon, D.P.; McEwen, A.G.; Lapthorn, A.J.; Edwards, R.
Deposited on	:	2003-04-04
Resolution	:	1.95 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

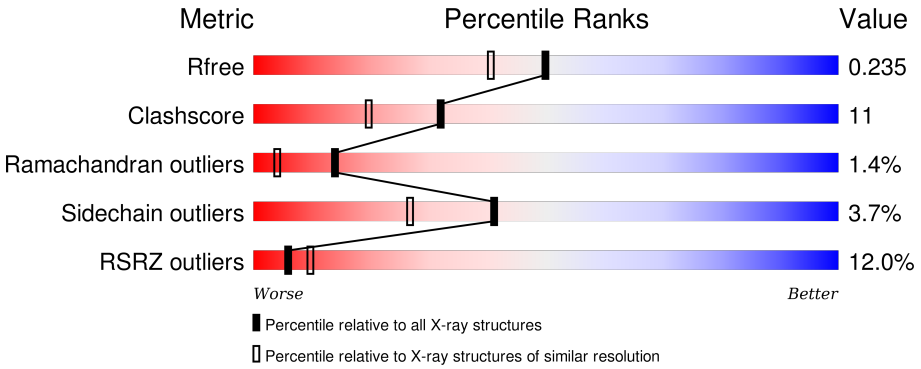
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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 <=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	231	6% 82% 14%
1	B	231	13% 77% 15%
1	C	231	9% 85% 10%
1	D	231	18% 74% 19%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	B	831	-	-	X	-
3	CL	B	835	-	-	-	X
4	GSH	A	800	X	-	-	-
4	GSH	B	801	X	-	-	-
4	GSH	C	802	X	-	-	-
4	GSH	C	803	X	-	-	-
4	GSH	C	804	X	-	-	X
4	GSH	D	805	X	-	-	-
5	GOL	A	811	-	-	-	X
5	GOL	A	814	-	-	X	X
5	GOL	B	806	-	-	-	X
5	GOL	C	810	-	-	-	X
5	GOL	C	812	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7954 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	228	Total	C	N	O	S	0	3	0
			1807	1156	319	326	6			
1	B	224	Total	C	N	O	S	2	4	0
			1778	1140	314	318	6			
1	C	227	Total	C	N	O	S	2	0	0
			1784	1143	317	318	6			
1	D	223	Total	C	N	O	S	0	3	0
			1757	1127	309	315	6			

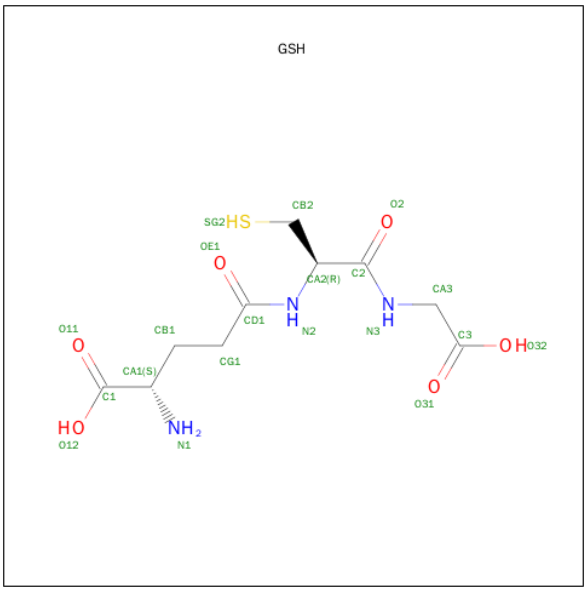
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

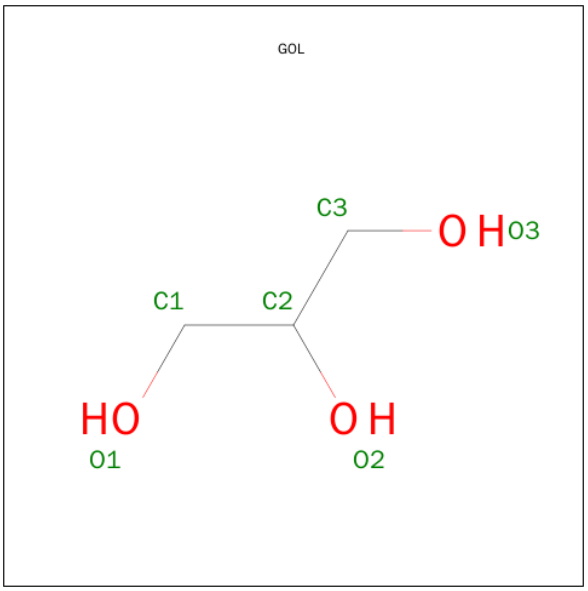
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Cl	0	0
			3	3		
3	A	7	Total	Cl	0	0
			7	7		
3	D	4	Total	Cl	0	0
			4	4		
3	C	6	Total	Cl	0	0
			6	6		

- Molecule 4 is GLUTATHIONE (three-letter code: GSH) (formula: $C_{10}H_{17}N_3O_6S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
4	A	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
4	B	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
4	C	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
4	C	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
4	C	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
4	D	1	Total	C	N	O	S	0	0
			20	10	3	6	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	140	Total O 140 140	0	0
6	B	109	Total O 109 109	0	0
6	C	224	Total O 224 224	0	0

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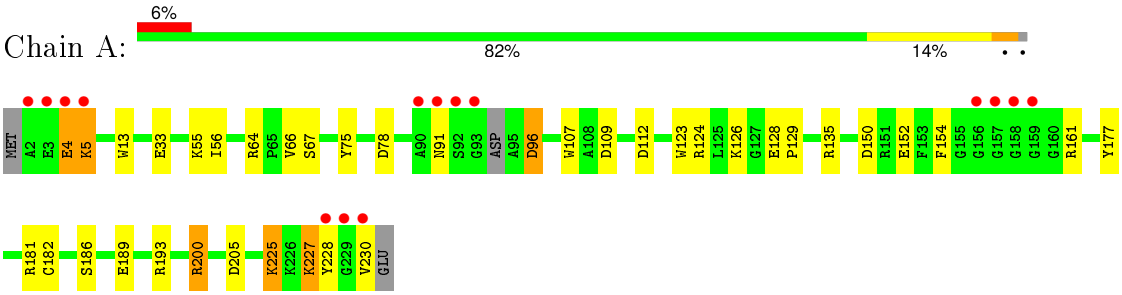
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	138	Total	O	0	0
			138	138		

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 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.

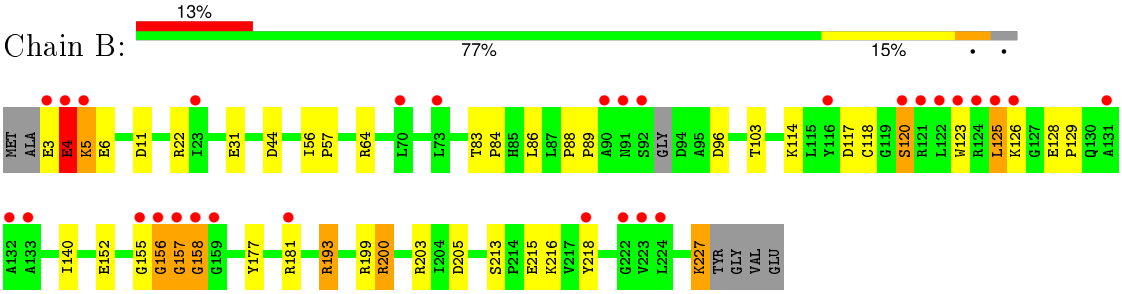
- Molecule 1: glutathione s-transferase

Chain A:



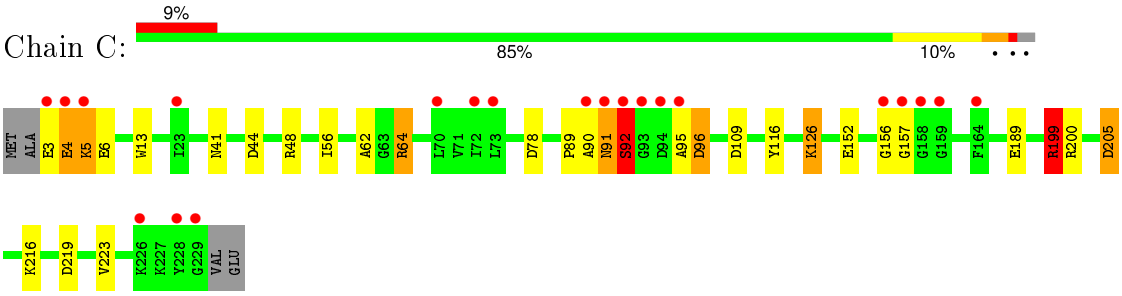
- Molecule 1: glutathione s-transferase

Chain B:



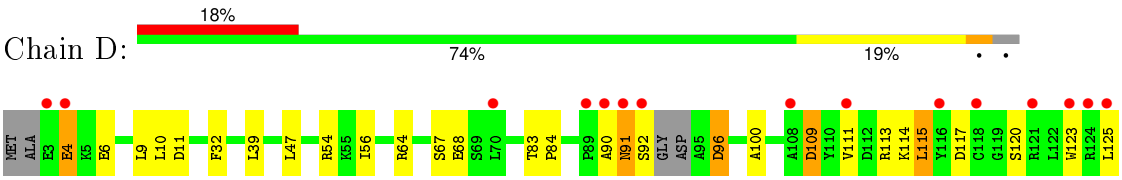
- Molecule 1: glutathione s-transferase

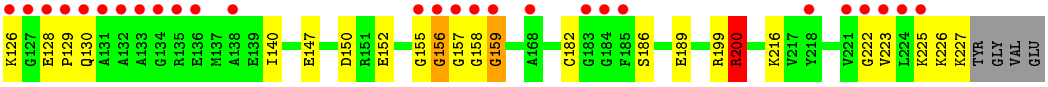
Chain C:



- Molecule 1: glutathione s-transferase

Chain D:




K126
G127
E128
P129
Q130
A131
A132
A133
G134
R135
E136
M137
A138
E139
T140
E147
D150
R151
E152
G155
G156
G157
G158
G159
A168
C182
G183
G184
F185
S186
E189
R199
K200
K216
V217
Y218
V221
G222
V223
L224
K225
K226
K227
TYR
GLY
VAL
GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	76.83Å 91.13Å 165.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.95 35.40 – 1.95	Depositor EDS
% Data completeness (in resolution range)	84.5 (40.00-1.95) 84.5 (35.40-1.95)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.61 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.178 , 0.227 0.190 , 0.235	Depositor DCC
R_{free} test set	3635 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	33.7	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 52.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	2 of 71925 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7954	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.87 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.3776e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, MG, CL, GSH

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	1.21	4/1868 (0.2%)	1.07	9/2528 (0.4%)
1	B	1.15	1/1843 (0.1%)	1.13	12/2494 (0.5%)
1	C	1.15	3/1830 (0.2%)	1.22	11/2476 (0.4%)
1	D	1.00	1/1819 (0.1%)	1.05	7/2463 (0.3%)
All	All	1.13	9/7360 (0.1%)	1.12	39/9961 (0.4%)

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	C	0	1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	216	LYS	CD-CE	16.32	1.92	1.51
1	A	123	TRP	CB-CG	-5.83	1.39	1.50
1	D	200	ARG	CG-CD	5.65	1.66	1.51
1	A	13	TRP	CG-CD1	-5.54	1.28	1.36
1	C	200	ARG	CG-CD	5.40	1.65	1.51

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	199	ARG	NE-CZ-NH1	-23.81	108.39	120.30
1	C	199	ARG	NE-CZ-NH2	15.74	128.17	120.30
1	A	205	ASP	CB-CG-OD2	10.40	127.66	118.30
1	B	200	ARG	NE-CZ-NH1	9.73	125.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	199	ARG	NE-CZ-NH2	8.93	124.76	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	199	ARG	Sidechain

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	1807	0	1765	28	0
1	B	1778	0	1743	41	0
1	C	1784	0	1753	39	0
1	D	1757	0	1709	50	0
2	A	2	0	0	0	0
2	C	1	0	0	0	0
3	A	7	0	0	2	0
3	B	3	0	0	3	0
3	C	6	0	0	0	0
3	D	4	0	0	1	0
4	A	40	0	29	2	0
4	B	20	0	15	0	0
4	C	60	0	41	3	0
4	D	20	0	15	2	0
5	A	12	0	16	5	0
5	B	6	0	8	1	0
5	C	24	0	32	5	0
5	D	12	0	16	1	0
6	A	140	0	0	7	0
6	B	109	0	0	5	1
6	C	224	0	0	11	1
6	D	138	0	0	7	0
All	All	7954	0	7142	154	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 11.

The worst 5 of 154 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:157:GLY:HA2	3:B:831:CL:CL	1.85	1.12
1:A:66:VAL:HA	5:A:814:GOL:H31	1.16	1.12
1:B:157:GLY:CA	3:B:831:CL:CL	2.40	1.06
1:A:182:CYS:SG	6:A:975:HOH:O	2.13	1.05
1:C:6:GLU:HA	1:C:6:GLU:OE1	1.56	1.02

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)
6:B:858:HOH:O	6:C:1032:HOH:O[4_456]	1.98	0.22

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	227/231 (98%)	220 (97%)	5 (2%)	2 (1%)	21 9
1	B	224/231 (97%)	218 (97%)	3 (1%)	3 (1%)	15 4
1	C	225/231 (97%)	215 (96%)	7 (3%)	3 (1%)	15 4
1	D	222/231 (96%)	210 (95%)	7 (3%)	5 (2%)	8 1
All	All	898/924 (97%)	863 (96%)	22 (2%)	13 (1%)	14 4

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	156	GLY
1	C	4	GLU

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Mol	Chain	Res	Type
1	C	92	SER
1	D	156	GLY
1	D	158	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	183/185 (99%)	176 (96%)	7 (4%)	40	25
1	B	180/185 (97%)	170 (94%)	10 (6%)	26	11
1	C	179/185 (97%)	174 (97%)	5 (3%)	51	39
1	D	177/185 (96%)	168 (95%)	9 (5%)	29	13
All	All	719/740 (97%)	688 (96%)	31 (4%)	41	20

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	126	LYS
1	C	41	ASN
1	D	200	ARG
1	B	193	ARG
1	C	91	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

Of 39 ligands modelled in this entry, 23 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
4	GSH	A	799	-	13,19,19	0.77	0	15,24,24	3.28	9 (60%)
4	GSH	A	800	2	13,19,19	0.92	0	15,24,24	1.65	3 (20%)
5	GOL	A	811	-	5,5,5	0.31	0	5,5,5	0.33	0
5	GOL	A	814	-	5,5,5	0.29	0	5,5,5	0.79	0
4	GSH	B	801	-	13,19,19	1.03	1 (7%)	15,24,24	2.11	3 (20%)
5	GOL	B	806	-	5,5,5	0.43	0	5,5,5	0.77	0
4	GSH	C	802	-	13,19,19	0.90	0	15,24,24	1.41	1 (6%)
4	GSH	C	803	2	13,19,19	1.01	1 (7%)	15,24,24	1.12	0
4	GSH	C	804	-	13,19,19	0.97	1 (7%)	15,24,24	5.92	11 (73%)
5	GOL	C	808	-	5,5,5	0.46	0	5,5,5	0.83	0
5	GOL	C	810	-	5,5,5	0.43	0	5,5,5	1.03	0
5	GOL	C	812	-	5,5,5	0.49	0	5,5,5	1.13	0
5	GOL	C	813	-	5,5,5	0.36	0	5,5,5	1.03	0
4	GSH	D	805	-	13,19,19	1.12	2 (15%)	15,24,24	3.91	6 (40%)
5	GOL	D	807	-	5,5,5	0.66	0	5,5,5	1.41	1 (20%)
5	GOL	D	809	-	5,5,5	0.41	0	5,5,5	0.60	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
4	GSH	A	799	-	-	0/18/24/24	0/0/0/0
4	GSH	A	800	2	1/1/6/8	0/18/24/24	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	811	-	-	0/4/4/4	0/0/0/0
5	GOL	A	814	-	-	0/4/4/4	0/0/0/0
4	GSH	B	801	-	1/1/6/8	0/18/24/24	0/0/0/0
5	GOL	B	806	-	-	0/4/4/4	0/0/0/0
4	GSH	C	802	-	1/1/6/8	0/18/24/24	0/0/0/0
4	GSH	C	803	2	1/1/6/8	0/18/24/24	0/0/0/0
4	GSH	C	804	-	1/1/6/8	1/18/24/24	0/0/0/0
5	GOL	C	808	-	-	0/4/4/4	0/0/0/0
5	GOL	C	810	-	-	0/4/4/4	0/0/0/0
5	GOL	C	812	-	-	0/4/4/4	0/0/0/0
5	GOL	C	813	-	-	0/4/4/4	0/0/0/0
4	GSH	D	805	-	1/1/6/8	0/18/24/24	0/0/0/0
5	GOL	D	807	-	-	0/4/4/4	0/0/0/0
5	GOL	D	809	-	-	0/4/4/4	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	805	GSH	O2-C2	-2.83	1.17	1.23
4	C	803	GSH	CB2-CA2	-2.44	1.50	1.53
4	B	801	GSH	CB2-CA2	2.05	1.55	1.53
4	C	804	GSH	CA2-N2	2.10	1.50	1.45
4	D	805	GSH	CG1-CD1	2.42	1.56	1.51

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	805	GSH	CA3-N3-C2	-12.52	105.13	122.34
4	C	804	GSH	CA3-N3-C2	-10.36	108.09	122.34
4	C	804	GSH	CB2-CA2-C2	-9.95	87.20	109.66
4	A	799	GSH	CA3-N3-C2	-8.75	110.31	122.34
4	C	804	GSH	CA2-N2-CD1	-5.68	107.09	121.58

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	C	802	GSH	CA1
4	C	803	GSH	CA1
4	B	801	GSH	CA1
4	A	800	GSH	CA1
4	C	804	GSH	CA1

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	804	GSH	OE1-CD1-N2-CA2

There are no ring outliers.

9 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	799	GSH	2	0
5	A	814	GOL	5	0
5	B	806	GOL	1	0
4	C	802	GSH	2	0
4	C	803	GSH	1	0
5	C	810	GOL	1	0
5	C	812	GOL	4	0
4	D	805	GSH	2	0
5	D	807	GOL	1	0

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

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^{th} 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^2)	Q<0.9
1	A	228/231 (98%)	0.40	15 (6%) 22 31	16, 23, 55, 84	0
1	B	224/231 (96%)	0.61	30 (13%) 4 7	20, 28, 56, 66	1 (0%)
1	C	227/231 (98%)	0.44	21 (9%) 11 17	19, 25, 53, 76	1 (0%)
1	D	223/231 (96%)	0.89	42 (18%) 2 2	23, 33, 66, 75	0
All	All	902/924 (97%)	0.59	108 (11%) 6 10	16, 27, 61, 84	2 (0%)

The worst 5 of 108 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	230	VAL	12.4
1	A	229	GLY	10.5
1	A	2	ALA	10.1
1	D	156	GLY	9.3
1	B	158	GLY	8.9

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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^{th} 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^2)	Q<0.9
3	CL	B	835	1/1	0.92	0.27	14.06	68,68,68,68	0
5	GOL	A	811	6/6	0.74	0.23	8.48	73,80,80,81	0
5	GOL	A	814	6/6	0.77	0.32	8.24	69,72,74,78	0
5	GOL	B	806	6/6	0.86	0.25	6.36	65,75,77,78	0
5	GOL	C	810	6/6	0.75	0.21	4.36	48,53,56,63	0
4	GSH	C	804	20/20	0.78	0.30	3.77	46,73,81,81	20
5	GOL	D	809	6/6	0.88	0.15	1.51	52,61,62,64	0
3	CL	C	830	1/1	0.97	0.18	1.36	65,65,65,65	0
5	GOL	D	807	6/6	0.94	0.18	1.10	40,55,58,59	0
4	GSH	C	803	20/20	0.92	0.12	0.74	32,37,68,69	0
3	CL	D	832	1/1	0.93	0.34	0.62	79,79,79,79	0
3	CL	A	823	1/1	0.95	0.20	0.32	58,58,58,58	0
4	GSH	A	800	20/20	0.94	0.13	0.28	33,39,69,73	0
5	GOL	C	813	6/6	0.89	0.11	0.23	48,64,67,69	0
5	GOL	C	808	6/6	0.93	0.13	-0.20	43,54,56,57	0
4	GSH	C	802	20/20	0.90	0.12	-0.27	32,39,51,53	0
3	CL	C	822	1/1	0.98	0.10	-0.30	52,52,52,52	0
4	GSH	A	799	20/20	0.91	0.12	-0.37	29,33,54,56	0
3	CL	B	831	1/1	0.77	0.18	-0.64	70,70,70,70	0
4	GSH	D	805	20/20	0.92	0.13	-0.65	35,43,57,58	0
4	GSH	B	801	20/20	0.94	0.11	-0.65	29,39,57,58	0
3	CL	A	827	1/1	0.90	0.09	-0.84	62,62,62,62	0
3	CL	D	821	1/1	0.98	0.04	-3.04	51,51,51,51	0
3	CL	C	824	1/1	0.99	0.03	-	54,54,54,54	0
3	CL	A	838	1/1	0.30	0.16	-	93,93,93,93	0
2	MG	C	816	1/1	0.96	0.08	-	41,41,41,41	0
3	CL	C	828	1/1	0.83	0.17	-	67,67,67,67	0
3	CL	A	837	1/1	0.95	0.23	-	72,72,72,72	0
5	GOL	C	812	6/6	0.68	0.23	-	63,67,69,69	0
3	CL	A	825	1/1	0.87	0.26	-	65,65,65,65	0
3	CL	D	819	1/1	0.96	0.15	-	55,55,55,55	0
3	CL	A	826	1/1	0.85	0.30	-	73,73,73,73	0
3	CL	B	820	1/1	0.95	0.09	-	65,65,65,65	0
3	CL	C	833	1/1	0.98	0.07	-	52,52,52,52	0
3	CL	A	836	1/1	0.94	0.17	-	61,61,61,61	0
2	MG	A	817	1/1	0.90	0.18	-	60,60,60,60	0
3	CL	C	829	1/1	0.95	0.10	-	74,74,74,74	0
2	MG	A	815	1/1	0.98	0.04	-	38,38,38,38	0
3	CL	D	834	1/1	0.91	0.09	-	58,58,58,58	0

6.5 Other polymers (i)

There are no such residues in this entry.