



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:38 PM GMT

PDB ID : 4IVF
Title : Crystal structure of glutathione transferase homolog from *Lodderomyces elongisporus*, target EFI-501753, with two GSH per subunit
Authors : Vetting, M.W.; Toro, R.; Bhosle, R.; Al Obaidi, N.F.; Morisco, L.L.; Wasserman, S.R.; Sojitra, S.; Washington, E.; Scott Glenn, A.; Chowdhury, S.; Evans, B.; Hammonds, J.; Hillerich, B.; Love, J.; Seidel, R.D.; Imker, H.J.; Armstrong, R.N.; Gerlt, J.A.; Almo, S.C.; Enzyme Function Initiative (EFI)
Deposited on : 2013-01-22
Resolution : 2.20 Å(reported)

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

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 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

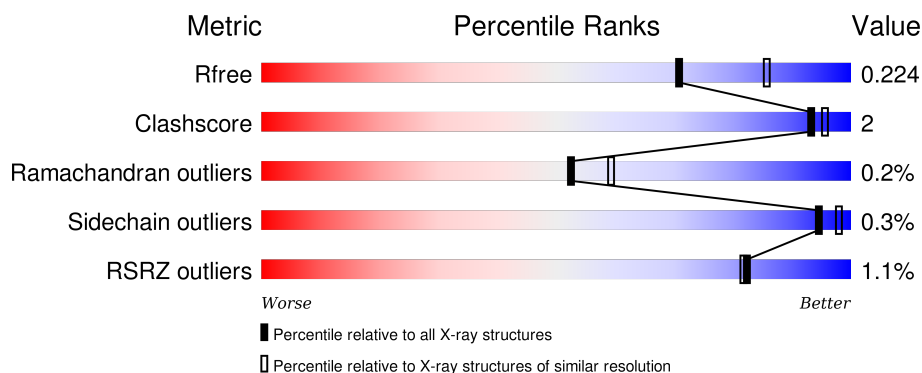
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	231	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>6%</div> <div>.</div> </div> </div>
1	B	231	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>10%</div> <div>6%</div> </div> </div>
1	C	231	<div> <div>%</div> <div> <div></div> <div>94%</div> <div>.</div> <div>.</div> </div> </div>
1	D	231	<div> <div></div> <div> <div>90%</div> <div>5%</div> <div>5%</div> </div> </div>
1	E	231	<div> <div>%</div> <div> <div></div> <div>95%</div> <div>.</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	231	<div><div></div><div>94%</div><div></div></div>
1	G	231	<div><div></div><div>94%</div><div></div></div>
1	H	231	<div><div>3%</div><div></div><div>89%</div><div>5%</div><div>6%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16087 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 Putative uncharacterized protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	0	0	0
			1792	1172	291	329			
1	B	218	Total	C	N	O	0	0	0
			1770	1159	286	325			
1	C	226	Total	C	N	O	0	0	0
			1840	1205	297	338			
1	D	219	Total	C	N	O	0	0	0
			1779	1165	288	326			
1	E	226	Total	C	N	O	0	0	0
			1840	1205	297	338			
1	F	227	Total	C	N	O	0	0	0
			1850	1210	299	341			
1	G	226	Total	C	N	O	0	0	0
			1840	1205	297	338			
1	H	218	Total	C	N	O	0	0	0
			1770	1159	286	325			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP A5E437
A	2	VAL	-	EXPRESSION TAG	UNP A5E437
A	225	ALA	-	EXPRESSION TAG	UNP A5E437
A	226	GLU	-	EXPRESSION TAG	UNP A5E437
A	227	ASN	-	EXPRESSION TAG	UNP A5E437
A	228	LEU	-	EXPRESSION TAG	UNP A5E437
A	229	TYR	-	EXPRESSION TAG	UNP A5E437
A	230	PHE	-	EXPRESSION TAG	UNP A5E437
A	231	GLN	-	EXPRESSION TAG	UNP A5E437
B	1	MET	-	EXPRESSION TAG	UNP A5E437
B	2	VAL	-	EXPRESSION TAG	UNP A5E437
B	225	ALA	-	EXPRESSION TAG	UNP A5E437
B	226	GLU	-	EXPRESSION TAG	UNP A5E437

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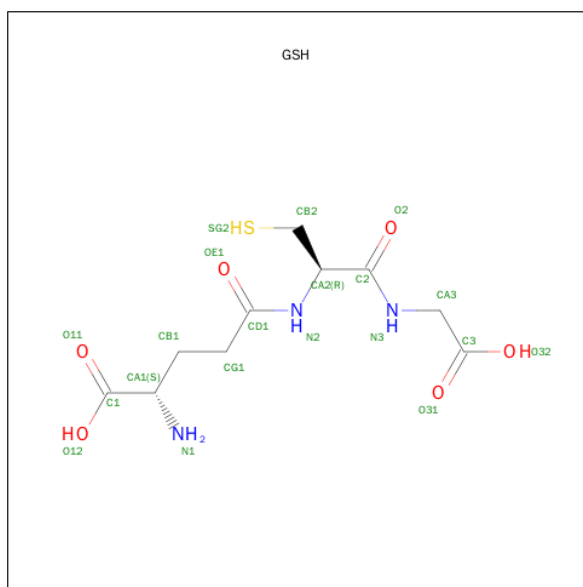
Chain	Residue	Modelled	Actual	Comment	Reference
B	227	ASN	-	EXPRESSION TAG	UNP A5E437
B	228	LEU	-	EXPRESSION TAG	UNP A5E437
B	229	TYR	-	EXPRESSION TAG	UNP A5E437
B	230	PHE	-	EXPRESSION TAG	UNP A5E437
B	231	GLN	-	EXPRESSION TAG	UNP A5E437
C	1	MET	-	EXPRESSION TAG	UNP A5E437
C	2	VAL	-	EXPRESSION TAG	UNP A5E437
C	225	ALA	-	EXPRESSION TAG	UNP A5E437
C	226	GLU	-	EXPRESSION TAG	UNP A5E437
C	227	ASN	-	EXPRESSION TAG	UNP A5E437
C	228	LEU	-	EXPRESSION TAG	UNP A5E437
C	229	TYR	-	EXPRESSION TAG	UNP A5E437
C	230	PHE	-	EXPRESSION TAG	UNP A5E437
C	231	GLN	-	EXPRESSION TAG	UNP A5E437
D	1	MET	-	EXPRESSION TAG	UNP A5E437
D	2	VAL	-	EXPRESSION TAG	UNP A5E437
D	225	ALA	-	EXPRESSION TAG	UNP A5E437
D	226	GLU	-	EXPRESSION TAG	UNP A5E437
D	227	ASN	-	EXPRESSION TAG	UNP A5E437
D	228	LEU	-	EXPRESSION TAG	UNP A5E437
D	229	TYR	-	EXPRESSION TAG	UNP A5E437
D	230	PHE	-	EXPRESSION TAG	UNP A5E437
D	231	GLN	-	EXPRESSION TAG	UNP A5E437
E	1	MET	-	EXPRESSION TAG	UNP A5E437
E	2	VAL	-	EXPRESSION TAG	UNP A5E437
E	225	ALA	-	EXPRESSION TAG	UNP A5E437
E	226	GLU	-	EXPRESSION TAG	UNP A5E437
E	227	ASN	-	EXPRESSION TAG	UNP A5E437
E	228	LEU	-	EXPRESSION TAG	UNP A5E437
E	229	TYR	-	EXPRESSION TAG	UNP A5E437
E	230	PHE	-	EXPRESSION TAG	UNP A5E437
E	231	GLN	-	EXPRESSION TAG	UNP A5E437
F	1	MET	-	EXPRESSION TAG	UNP A5E437
F	2	VAL	-	EXPRESSION TAG	UNP A5E437
F	225	ALA	-	EXPRESSION TAG	UNP A5E437
F	226	GLU	-	EXPRESSION TAG	UNP A5E437
F	227	ASN	-	EXPRESSION TAG	UNP A5E437
F	228	LEU	-	EXPRESSION TAG	UNP A5E437
F	229	TYR	-	EXPRESSION TAG	UNP A5E437
F	230	PHE	-	EXPRESSION TAG	UNP A5E437
F	231	GLN	-	EXPRESSION TAG	UNP A5E437
G	1	MET	-	EXPRESSION TAG	UNP A5E437

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Chain	Residue	Modelled	Actual	Comment	Reference
G	2	VAL	-	EXPRESSION TAG	UNP A5E437
G	225	ALA	-	EXPRESSION TAG	UNP A5E437
G	226	GLU	-	EXPRESSION TAG	UNP A5E437
G	227	ASN	-	EXPRESSION TAG	UNP A5E437
G	228	LEU	-	EXPRESSION TAG	UNP A5E437
G	229	TYR	-	EXPRESSION TAG	UNP A5E437
G	230	PHE	-	EXPRESSION TAG	UNP A5E437
G	231	GLN	-	EXPRESSION TAG	UNP A5E437
H	1	MET	-	EXPRESSION TAG	UNP A5E437
H	2	VAL	-	EXPRESSION TAG	UNP A5E437
H	225	ALA	-	EXPRESSION TAG	UNP A5E437
H	226	GLU	-	EXPRESSION TAG	UNP A5E437
H	227	ASN	-	EXPRESSION TAG	UNP A5E437
H	228	LEU	-	EXPRESSION TAG	UNP A5E437
H	229	TYR	-	EXPRESSION TAG	UNP A5E437
H	230	PHE	-	EXPRESSION TAG	UNP A5E437
H	231	GLN	-	EXPRESSION TAG	UNP A5E437

- Molecule 2 is GLUTATHIONE (three-letter code: GSH) (formula: C₁₀H₁₇N₃O₆S).



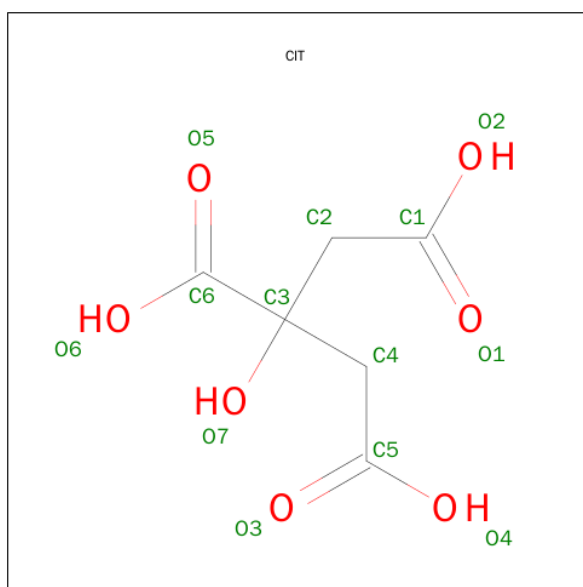
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	A	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	B	1	Total	C	N	O	S	0	0
			20	10	3	6	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	C	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	C	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	D	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	D	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	E	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	E	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	F	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	F	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	G	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	G	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	H	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	H	1	Total	C	N	O	S	0	0
			20	10	3	6	1		

- Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	163	Total	O	0	0
			163	163		
4	B	132	Total	O	0	0
			132	132		
4	C	133	Total	O	0	0
			133	133		
4	D	167	Total	O	0	2
			169	169		
4	E	181	Total	O	0	0
			181	181		
4	F	163	Total	O	0	0
			163	163		
4	G	170	Total	O	0	0
			170	170		
4	H	162	Total	O	0	0
			162	162		

- Molecule 1: Putative uncharacterized protein



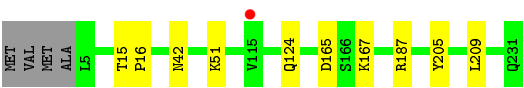
-
- | Amino Acid | Mutations |
|------------|-----------|
| MET | 0 |
| VAL | 11 |
| MET | 11 |
| ALA | 11 |
| LEU | 11 |
| PHE | 11 |
| GLN | 11 |

-
- Relative abundance of amino acids in the protein. The chart shows the relative abundance of various amino acids, with MET, VAL, MET, MET, ALA, and GLN being the most abundant (grey bars). Other amino acids (yellow and green bars) show lower relative abundance. Red dots above the bars indicate specific modifications: a red dot above K67 and another above V115.
- | Amino Acid | Relative Abundance (approx.) | Modification |
|------------|------------------------------|--------------|
| MET | 0.95 | No |
| VAL | 0.95 | No |
| MET | 0.95 | No |
| MET | 0.95 | No |
| ALA | 0.95 | No |
| L5 | 0.85 | No |
| T12 | 0.85 | No |
| A13 | 0.85 | No |
| P16 | 0.85 | No |
| P64 | 0.85 | No |
| K67 | 0.85 | Yes |
| G72 | 0.85 | No |
| E92 | 0.85 | No |
| H93 | 0.85 | No |
| K94 | 0.85 | No |
| V115 | 0.85 | Yes |
| P120 | 0.85 | No |
| Q124 | 0.85 | No |
| R187 | 0.85 | No |
| M227 | 0.85 | No |
| F230 | 0.85 | No |
| GLN | 0.95 | No |

-
- | Amino Acid | Count (approx.) |
|------------|-----------------|
| MET | 100 |
| VAL | 100 |
| MET | 100 |
| MET | 100 |
| ALA | 100 |
| L5 | 100 |
| K9 | 100 |
| P16 | 100 |
| N53 | 100 |
| R57 | 100 |
| N62 | 100 |
| L73 | 100 |
| P120 | 100 |
| Q124 | 100 |
| K133 | 100 |
| K167 | 100 |
| R187 | 100 |
| K210 | 100 |
| K223 | 100 |
| ASN | 100 |
| ALA | 100 |
| GLU | 100 |
| ASN | 100 |
| LEU | 100 |
| TYR | 100 |
| PHE | 100 |
| PIN | 100 |

- MET VAL MET ALA L5 I58 P59 Q77 L108 I112 V115 E155 D165 F230 GLN

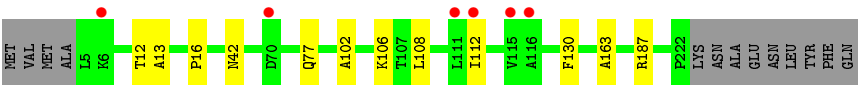
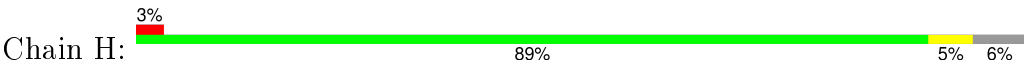
● Molecule 1: Putative uncharacterized protein



● Molecule 1: Putative uncharacterized protein



● Molecule 1: Putative uncharacterized protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.60 Å 112.48 Å 194.38 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.13 – 2.20 40.02 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.2 (37.13-2.20) 98.2 (40.02-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.20 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.156 , 0.223 0.164 , 0.224	Depositor DCC
R_{free} test set	4986 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	25.6	Xtriage
Anisotropy	0.761	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 99611 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16087	wwPDB-VP
Average B, all atoms (Å ²)	24.0	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 20.70 % 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 8.2033e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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: GSH, CIT

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	0.40	0/1841	0.50	0/2501
1	B	0.35	0/1819	0.49	0/2472
1	C	0.34	0/1891	0.48	0/2569
1	D	0.37	0/1828	0.50	0/2483
1	E	0.40	0/1891	0.51	0/2569
1	F	0.39	0/1901	0.52	0/2581
1	G	0.38	0/1891	0.49	0/2569
1	H	0.38	0/1819	0.50	0/2472
All	All	0.38	0/14881	0.50	0/20216

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 [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 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	1792	0	1783	8	0
1	B	1770	0	1759	14	0
1	C	1840	0	1824	5	0
1	D	1779	0	1772	7	0
1	E	1840	0	1824	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1850	0	1832	6	0
1	G	1840	0	1824	6	0
1	H	1770	0	1759	5	0
2	A	40	0	30	1	0
2	B	40	0	30	3	0
2	C	40	0	30	0	0
2	D	40	0	30	2	0
2	E	40	0	30	0	0
2	F	40	0	30	0	0
2	G	40	0	30	0	0
2	H	40	0	30	0	0
3	E	13	0	5	0	0
4	A	163	0	0	0	0
4	B	132	0	0	1	0
4	C	133	0	0	0	0
4	D	169	0	0	2	0
4	E	181	0	0	1	0
4	F	163	0	0	1	0
4	G	170	0	0	0	0
4	H	162	0	0	1	0
All	All	16087	0	14622	56	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 2.

All (56) 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:H:16:PRO:HG3	1:H:187:ARG:HG3	1.64	0.78
1:C:16:PRO:HG3	1:C:187:ARG:HG3	1.68	0.74
1:B:16:PRO:HG3	1:B:187:ARG:HG3	1.68	0.74
1:F:16:PRO:HG3	1:F:187:ARG:HG3	1.72	0.71
1:D:167:LYS:NZ	1:H:163:ALA:O	2.30	0.64
1:B:20:LYS:HG2	1:B:180:ALA:HA	1.86	0.57
1:D:16:PRO:HG3	1:D:187:ARG:HG3	1.87	0.56
1:A:47:ASP:OD1	1:A:51:LYS:NZ	2.41	0.54
1:E:108:LEU:O	1:E:112:ILE:HG12	2.09	0.53
1:B:58:ILE:HG13	2:B:302:GSH:O2	2.08	0.53
1:F:124:GLN:NE2	4:F:493:HOH:O	2.42	0.53
1:A:112:ILE:HA	1:A:115:VAL:HG22	1.91	0.53
1:A:16:PRO:HG3	1:A:187:ARG:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:205:TYR:CE2	1:F:209:LEU:HD11	2.44	0.52
1:C:12:THR:OG1	1:C:13:ALA:N	2.43	0.52
1:B:14:PRO:HD3	1:B:221:PRO:HG2	1.92	0.52
1:A:160:ARG:NH1	1:F:51:LYS:O	2.43	0.51
1:B:9:LYS:HB3	1:B:62:ASN:HB3	1.93	0.51
1:F:165:ASP:HB2	1:F:167:LYS:HD2	1.93	0.50
1:C:92:GLU:HG2	1:C:94:LYS:HG3	1.93	0.50
1:D:210:LYS:NZ	4:D:503:HOH:O	2.44	0.49
2:D:301:GSH:HSG	2:D:302:GSH:HSG	1.60	0.48
1:B:108:LEU:O	1:B:112:ILE:HG12	2.13	0.48
2:B:301:GSH:OE1	2:B:302:GSH:HA32	2.14	0.48
1:A:120:PRO:O	1:A:124:GLN:HG2	2.13	0.48
1:B:120:PRO:O	1:B:124:GLN:HG2	2.14	0.47
1:E:155:GLU:OE2	4:E:479:HOH:O	2.20	0.47
1:B:42:ASN:ND2	4:B:508:HOH:O	2.47	0.47
2:A:301:GSH:HSG	2:A:302:GSH:HSG	1.63	0.46
2:B:301:GSH:HN11	1:G:142:ARG:HH22	1.62	0.45
1:D:9:LYS:HB3	1:D:62:ASN:HB3	1.97	0.45
1:G:120:PRO:O	1:G:124:GLN:HG2	2.18	0.44
1:G:91:LYS:HD3	4:H:520:HOH:O	2.17	0.44
1:F:15:THR:HB	1:F:16:PRO:HD2	2.01	0.43
1:D:53:ASN:ND2	1:D:57:ARG:O	2.52	0.42
1:B:106:LYS:HD3	1:B:106:LYS:HA	1.93	0.42
1:A:108:LEU:HD23	1:A:108:LEU:HA	1.88	0.42
1:H:108:LEU:O	1:H:112:ILE:HG12	2.19	0.42
1:H:12:THR:OG1	1:H:13:ALA:N	2.53	0.42
1:B:12:THR:OG1	1:B:13:ALA:N	2.50	0.41
1:B:58:ILE:HB	1:B:59:PRO:HA	2.02	0.41
1:C:120:PRO:O	1:C:124:GLN:HG2	2.20	0.41
1:G:58:ILE:HB	1:G:59:PRO:HA	2.02	0.41
2:D:301:GSH:HB23	4:D:488:HOH:O	2.19	0.41
1:E:58:ILE:HB	1:E:59:PRO:HA	2.02	0.41
1:B:15:THR:HB	1:B:16:PRO:HD2	2.03	0.41
1:B:144:ILE:HD11	1:B:191:LEU:HD22	2.01	0.41
1:D:120:PRO:O	1:D:124:GLN:HG2	2.21	0.41
1:B:112:ILE:HA	1:B:115:VAL:HG22	2.03	0.41
1:G:209:LEU:HD13	1:G:209:LEU:HA	1.86	0.41
1:C:64:PRO:HA	1:C:72:GLY:HA3	2.03	0.41
1:G:144:ILE:HD13	1:G:144:ILE:HA	1.95	0.41
1:A:144:ILE:HA	1:A:144:ILE:HD13	1.94	0.40
1:D:62:ASN:HA	1:D:73:LEU:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:102:ALA:O	1:H:106:LYS:HG2	2.21	0.40
1:A:156:ASP:O	1:A:160:ARG:HG3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	219/231 (95%)	214 (98%)	4 (2%)	1 (0%)	34	35
1	B	216/231 (94%)	211 (98%)	4 (2%)	1 (0%)	34	35
1	C	224/231 (97%)	218 (97%)	6 (3%)	0	100	100
1	D	217/231 (94%)	215 (99%)	2 (1%)	0	100	100
1	E	224/231 (97%)	220 (98%)	3 (1%)	1 (0%)	39	42
1	F	225/231 (97%)	218 (97%)	7 (3%)	0	100	100
1	G	224/231 (97%)	219 (98%)	5 (2%)	0	100	100
1	H	216/231 (94%)	212 (98%)	3 (1%)	1 (0%)	34	35
All	All	1765/1848 (96%)	1727 (98%)	34 (2%)	4 (0%)	52	59

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	ASN
1	B	77	GLN
1	E	77	GLN
1	H	77	GLN

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	190/199 (96%)	190 (100%)	0	100	100
1	B	188/199 (94%)	187 (100%)	1 (0%)	92	96
1	C	195/199 (98%)	195 (100%)	0	100	100
1	D	189/199 (95%)	189 (100%)	0	100	100
1	E	195/199 (98%)	195 (100%)	0	100	100
1	F	196/199 (98%)	195 (100%)	1 (0%)	92	96
1	G	195/199 (98%)	194 (100%)	1 (0%)	92	96
1	H	188/199 (94%)	186 (99%)	2 (1%)	80	89
All	All	1536/1592 (96%)	1531 (100%)	5 (0%)	94	98

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	62	ASN
1	F	42	ASN
1	G	165	ASP
1	H	42	ASN
1	H	130	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	141	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

17 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	GSH	A	301	-	13,19,19	3.24	4 (30%)	15,24,24	1.86	5 (33%)
2	GSH	A	302	-	13,19,19	3.27	3 (23%)	15,24,24	1.11	1 (6%)
2	GSH	B	301	-	13,19,19	3.37	4 (30%)	15,24,24	1.68	4 (26%)
2	GSH	B	302	-	13,19,19	3.24	3 (23%)	15,24,24	2.35	7 (46%)
2	GSH	C	301	-	13,19,19	3.32	4 (30%)	15,24,24	1.61	5 (33%)
2	GSH	C	302	-	13,19,19	3.24	3 (23%)	15,24,24	1.53	2 (13%)
2	GSH	D	301	-	13,19,19	3.35	4 (30%)	15,24,24	1.29	1 (6%)
2	GSH	D	302	-	13,19,19	3.24	4 (30%)	15,24,24	1.37	3 (20%)
3	CIT	E	301	-	3,12,12	3.17	3 (100%)	3,17,17	2.18	1 (33%)
2	GSH	E	302	-	13,19,19	3.14	4 (30%)	15,24,24	1.64	3 (20%)
2	GSH	E	303	-	13,19,19	2.93	3 (23%)	15,24,24	1.48	3 (20%)
2	GSH	F	301	-	13,19,19	3.38	4 (30%)	15,24,24	1.69	5 (33%)
2	GSH	F	302	-	13,19,19	3.34	3 (23%)	15,24,24	1.59	3 (20%)
2	GSH	G	301	-	13,19,19	3.24	4 (30%)	15,24,24	1.58	5 (33%)
2	GSH	G	302	-	13,19,19	3.19	3 (23%)	15,24,24	1.59	3 (20%)
2	GSH	H	301	-	13,19,19	3.44	4 (30%)	15,24,24	1.62	4 (26%)
2	GSH	H	302	-	13,19,19	3.33	3 (23%)	15,24,24	1.70	2 (13%)

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	301	-	-	0/18/24/24	0/0/0/0
2	GSH	A	302	-	-	0/18/24/24	0/0/0/0
2	GSH	B	301	-	-	0/18/24/24	0/0/0/0
2	GSH	B	302	-	-	0/18/24/24	0/0/0/0
2	GSH	C	301	-	-	0/18/24/24	0/0/0/0
2	GSH	C	302	-	-	0/18/24/24	0/0/0/0
2	GSH	D	301	-	-	0/18/24/24	0/0/0/0
2	GSH	D	302	-	-	0/18/24/24	0/0/0/0
3	CIT	E	301	-	-	0/6/16/16	0/0/0/0
2	GSH	E	302	-	-	0/18/24/24	0/0/0/0
2	GSH	E	303	-	-	0/18/24/24	0/0/0/0
2	GSH	F	301	-	-	0/18/24/24	0/0/0/0
2	GSH	F	302	-	-	0/18/24/24	0/0/0/0
2	GSH	G	301	-	-	0/18/24/24	0/0/0/0
2	GSH	G	302	-	-	0/18/24/24	0/0/0/0
2	GSH	H	301	-	-	0/18/24/24	0/0/0/0
2	GSH	H	302	-	-	0/18/24/24	0/0/0/0

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	GSH	CB2-CA2	-5.69	1.46	1.53
2	F	301	GSH	CB2-CA2	-5.52	1.46	1.53
2	B	301	GSH	CB2-CA2	-5.50	1.46	1.53
2	D	301	GSH	CB2-CA2	-5.47	1.46	1.53
2	F	302	GSH	CB2-CA2	-5.45	1.46	1.53
2	C	301	GSH	CB2-CA2	-5.32	1.46	1.53
2	H	301	GSH	CB2-CA2	-5.31	1.46	1.53
2	C	302	GSH	CB2-CA2	-5.09	1.47	1.53
2	H	302	GSH	CB2-CA2	-5.02	1.47	1.53
2	A	302	GSH	CB2-CA2	-4.95	1.47	1.53
2	G	302	GSH	CB2-CA2	-4.89	1.47	1.53
2	G	301	GSH	CB2-CA2	-4.85	1.47	1.53
2	D	302	GSH	CB2-CA2	-4.73	1.47	1.53
2	E	302	GSH	CB2-CA2	-4.41	1.47	1.53
2	B	302	GSH	CB2-CA2	-4.32	1.48	1.53
2	E	303	GSH	CB2-CA2	-4.05	1.48	1.53
3	E	301	CIT	C4-C3	-3.56	1.49	1.54
3	E	301	CIT	C2-C3	-3.16	1.49	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	301	CIT	O7-C3	-2.74	1.38	1.43
2	B	301	GSH	CB2-SG2	-2.33	1.76	1.81
2	F	301	GSH	CB2-SG2	-2.32	1.76	1.81
2	H	301	GSH	CB2-SG2	-2.22	1.76	1.81
2	E	302	GSH	CB2-SG2	-2.21	1.76	1.81
2	A	301	GSH	CB2-SG2	-2.14	1.76	1.81
2	C	301	GSH	CB2-SG2	-2.14	1.76	1.81
2	G	301	GSH	CB2-SG2	-2.10	1.76	1.81
2	D	302	GSH	CB2-SG2	-2.06	1.76	1.81
2	D	301	GSH	CB2-SG2	-2.02	1.77	1.81
2	A	301	GSH	C2-N3	5.42	1.44	1.33
2	G	301	GSH	C2-N3	5.59	1.45	1.33
2	G	302	GSH	C2-N3	5.60	1.45	1.33
2	B	302	GSH	C2-N3	5.61	1.45	1.33
2	C	302	GSH	C2-N3	5.63	1.45	1.33
2	E	303	GSH	C2-N3	5.64	1.45	1.33
2	D	301	GSH	C2-N3	5.73	1.45	1.33
2	B	301	GSH	C2-N3	5.75	1.45	1.33
2	H	302	GSH	C2-N3	5.76	1.45	1.33
2	E	302	GSH	C2-N3	5.77	1.45	1.33
2	F	301	GSH	C2-N3	5.79	1.45	1.33
2	C	301	GSH	C2-N3	5.81	1.45	1.33
2	D	302	GSH	C2-N3	5.89	1.45	1.33
2	F	302	GSH	C2-N3	6.07	1.46	1.33
2	H	301	GSH	C2-N3	6.10	1.46	1.33
2	A	302	GSH	C2-N3	6.10	1.46	1.33
2	E	303	GSH	CD1-N2	7.54	1.49	1.34
2	E	302	GSH	CD1-N2	8.13	1.50	1.34
2	A	301	GSH	CD1-N2	8.18	1.50	1.34
2	G	302	GSH	CD1-N2	8.24	1.50	1.34
2	A	302	GSH	CD1-N2	8.24	1.50	1.34
2	D	302	GSH	CD1-N2	8.40	1.50	1.34
2	F	302	GSH	CD1-N2	8.44	1.51	1.34
2	C	302	GSH	CD1-N2	8.44	1.51	1.34
2	C	301	GSH	CD1-N2	8.49	1.51	1.34
2	G	301	GSH	CD1-N2	8.50	1.51	1.34
2	B	301	GSH	CD1-N2	8.61	1.51	1.34
2	D	301	GSH	CD1-N2	8.63	1.51	1.34
2	F	301	GSH	CD1-N2	8.65	1.51	1.34
2	B	302	GSH	CD1-N2	8.79	1.51	1.34
2	H	302	GSH	CD1-N2	8.80	1.51	1.34
2	H	301	GSH	CD1-N2	8.95	1.52	1.34

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	302	GSH	O2-C2-N3	-4.35	114.34	123.08
2	C	302	GSH	CA2-CB2-SG2	-3.98	109.26	114.16
2	A	301	GSH	CA2-CB2-SG2	-3.94	109.32	114.16
2	H	302	GSH	CA2-CB2-SG2	-3.69	109.62	114.16
2	E	302	GSH	CA2-CB2-SG2	-3.68	109.63	114.16
2	A	301	GSH	CA3-N3-C2	-3.67	117.29	122.34
3	E	301	CIT	C3-C2-C1	-3.62	109.17	114.96
2	G	302	GSH	CA3-N3-C2	-3.57	117.43	122.34
2	D	301	GSH	CA2-CB2-SG2	-3.47	109.89	114.16
2	E	303	GSH	OE1-CD1-N2	-3.42	117.21	123.01
2	F	302	GSH	CA2-CB2-SG2	-3.33	110.06	114.16
2	G	301	GSH	CB2-CA2-N2	-3.17	106.94	111.40
2	B	301	GSH	OE1-CD1-N2	-3.10	117.75	123.01
2	H	301	GSH	CA2-CB2-SG2	-2.97	110.50	114.16
2	F	301	GSH	OE1-CD1-N2	-2.97	117.97	123.01
2	C	301	GSH	CA3-N3-C2	-2.95	118.29	122.34
2	E	302	GSH	OE1-CD1-N2	-2.80	118.25	123.01
2	F	301	GSH	CA2-CB2-SG2	-2.78	110.75	114.16
2	G	302	GSH	CA2-CB2-SG2	-2.72	110.81	114.16
2	F	301	GSH	CA3-N3-C2	-2.65	118.70	122.34
2	F	302	GSH	OE1-CD1-N2	-2.63	118.54	123.01
2	F	302	GSH	CA3-N3-C2	-2.45	118.97	122.34
2	C	301	GSH	CA2-CB2-SG2	-2.38	111.23	114.16
2	B	301	GSH	CA2-CB2-SG2	-2.36	111.26	114.16
2	B	302	GSH	C3-CA3-N3	-2.27	105.89	111.74
2	A	301	GSH	O2-C2-N3	-2.25	118.58	123.08
2	C	302	GSH	OE1-CD1-N2	-2.24	119.21	123.01
2	A	302	GSH	CA2-CB2-SG2	-2.22	111.43	114.16
2	B	301	GSH	CA3-N3-C2	-2.21	119.31	122.34
2	C	301	GSH	O2-C2-N3	-2.18	118.71	123.08
2	G	302	GSH	OE1-CD1-N2	-2.16	119.34	123.01
2	H	301	GSH	OE1-CD1-N2	-2.15	119.35	123.01
2	D	302	GSH	OE1-CD1-N2	-2.14	119.38	123.01
2	A	301	GSH	CB2-CA2-N2	-2.11	108.43	111.40
2	B	302	GSH	OE1-CD1-N2	-2.10	119.44	123.01
2	C	301	GSH	CB2-CA2-N2	-2.08	108.48	111.40
2	G	301	GSH	O2-C2-N3	-2.06	118.96	123.08
2	B	302	GSH	C2-CA2-N2	-2.03	105.54	111.26
2	G	301	GSH	CA2-CB2-SG2	-2.01	111.69	114.16
2	E	303	GSH	CA2-C2-N3	2.01	120.67	116.72
2	G	301	GSH	CG1-CD1-N2	2.04	119.16	115.83
2	A	301	GSH	CA2-C2-N3	2.10	120.84	116.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	302	GSH	CA2-C2-N3	2.10	120.85	116.72
2	F	301	GSH	CA2-C2-N3	2.14	120.92	116.72
2	D	302	GSH	CG1-CD1-N2	2.15	119.34	115.83
2	G	301	GSH	CA2-C2-N3	2.32	121.27	116.72
2	E	303	GSH	CG1-CD1-N2	2.35	119.66	115.83
2	H	301	GSH	CA2-C2-N3	2.35	121.33	116.72
2	E	302	GSH	CG1-CD1-N2	2.36	119.68	115.83
2	B	302	GSH	CG1-CD1-N2	2.73	120.28	115.83
2	C	301	GSH	CA2-C2-N3	2.78	122.18	116.72
2	F	301	GSH	CG1-CD1-N2	2.83	120.45	115.83
2	H	302	GSH	CG1-CD1-N2	3.04	120.78	115.83
2	H	301	GSH	CG1-CD1-N2	3.08	120.85	115.83
2	B	301	GSH	CG1-CD1-N2	3.22	121.08	115.83
2	B	302	GSH	CA3-N3-C2	3.24	126.80	122.34
2	B	302	GSH	CA2-C2-N3	5.43	127.37	116.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	GSH	1	0
2	A	302	GSH	1	0
2	B	301	GSH	2	0
2	B	302	GSH	2	0
2	D	301	GSH	2	0
2	D	302	GSH	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, 95th 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	221/231 (95%)	-0.42	2 (0%) 85 85	10, 19, 42, 93	0
1	B	218/231 (94%)	-0.06	5 (2%) 64 63	13, 27, 54, 70	0
1	C	226/231 (97%)	-0.19	3 (1%) 79 78	14, 27, 48, 89	0
1	D	219/231 (94%)	-0.44	1 (0%) 91 91	11, 21, 42, 59	0
1	E	226/231 (97%)	-0.44	2 (0%) 85 85	9, 17, 33, 49	0
1	F	227/231 (98%)	-0.42	1 (0%) 93 93	10, 19, 36, 55	0
1	G	226/231 (97%)	-0.48	0 100 100	10, 19, 35, 53	0
1	H	218/231 (94%)	-0.17	6 (2%) 56 55	11, 22, 46, 55	0
All	All	1781/1848 (96%)	-0.33	20 (1%) 82 82	9, 21, 44, 93	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	165	ASP	3.1
1	H	112	ILE	2.7
1	H	115	VAL	2.7
1	A	112	ILE	2.7
1	A	115	VAL	2.7
1	B	115	VAL	2.5
1	C	67	LYS	2.5
1	H	70	ASP	2.5
1	B	112	ILE	2.4
1	H	116	ALA	2.4
1	B	133	LYS	2.4
1	F	115	VAL	2.4
1	B	212	PRO	2.3
1	H	111	LEU	2.3
1	D	133	LYS	2.2
1	C	227	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	219	GLU	2.2
1	C	115	VAL	2.2
1	H	6	LYS	2.1
1	E	115	VAL	2.1

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, 95th 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	CIT	E	301	13/13	0.93	0.12	0.39	37,46,54,56	0
2	GSH	F	302	20/20	0.95	0.15	0.02	9,19,27,31	0
2	GSH	D	301	20/20	0.87	0.13	-0.01	20,30,44,46	0
2	GSH	B	301	20/20	0.92	0.13	-0.07	25,39,59,65	0
2	GSH	C	302	20/20	0.95	0.15	-0.08	16,23,34,39	0
2	GSH	G	301	20/20	0.95	0.14	-0.08	13,25,45,47	0
2	GSH	A	301	20/20	0.91	0.13	-0.13	17,27,40,47	0
2	GSH	F	301	20/20	0.93	0.13	-0.24	21,27,51,52	0
2	GSH	B	302	20/20	0.92	0.12	-0.45	12,24,38,38	0
2	GSH	C	301	20/20	0.94	0.12	-0.45	20,27,55,55	0
2	GSH	G	302	20/20	0.96	0.12	-0.47	11,16,23,24	0
2	GSH	H	301	20/20	0.94	0.12	-0.52	22,31,45,46	0
2	GSH	E	302	20/20	0.97	0.12	-0.52	14,21,35,36	0
2	GSH	A	302	20/20	0.94	0.12	-0.53	12,17,27,29	0
2	GSH	E	303	20/20	0.97	0.12	-0.70	3,12,22,28	0
2	GSH	H	302	20/20	0.96	0.10	-0.76	16,23,33,36	0
2	GSH	D	302	20/20	0.96	0.10	-0.82	11,19,30,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.