



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:30 AM GMT

PDB ID : 2HGS
Title : HUMAN GLUTATHIONE SYNTHETASE
Authors : Polekhina, G.; Board, P.; Rossjohn, J.; Parker, M.W.
Deposited on : 1999-01-04
Resolution : 2.10 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

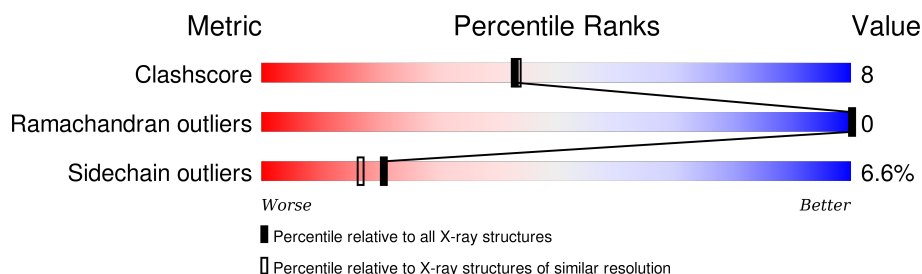
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	474	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3964 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 PROTEIN (GLUTATHIONE SYNTHETASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	472	Total	C	N	O	S	0	0	0
			3675	2318	647	699	11			

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

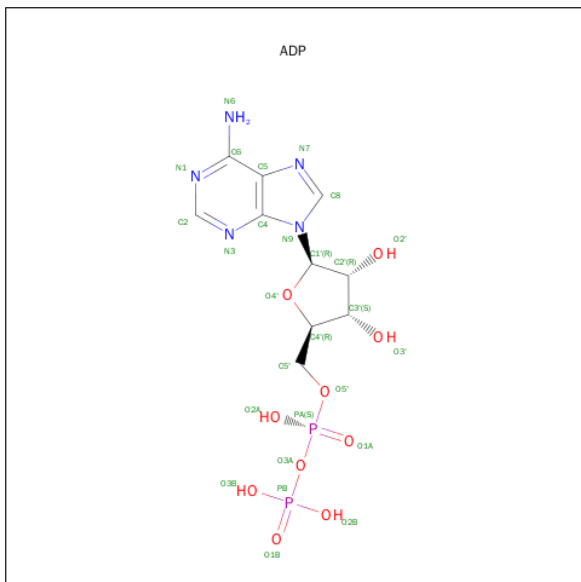
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



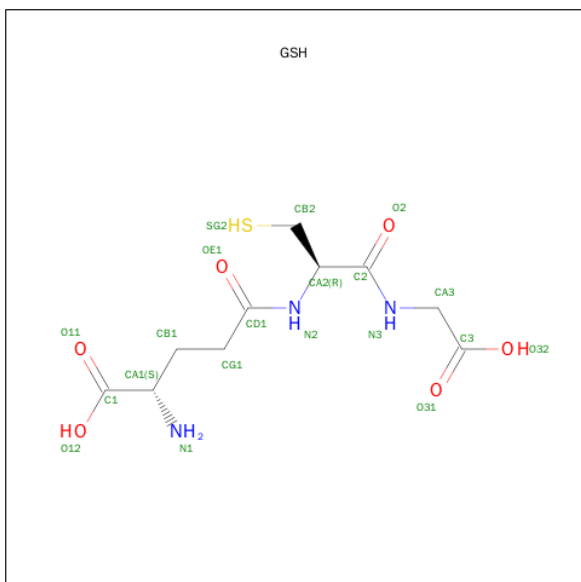
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is GLUTATHIONE (three-letter code: GSH) (formula: $C_{10}H_{17}N_3O_6S$).



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

- Molecule 6 is water.

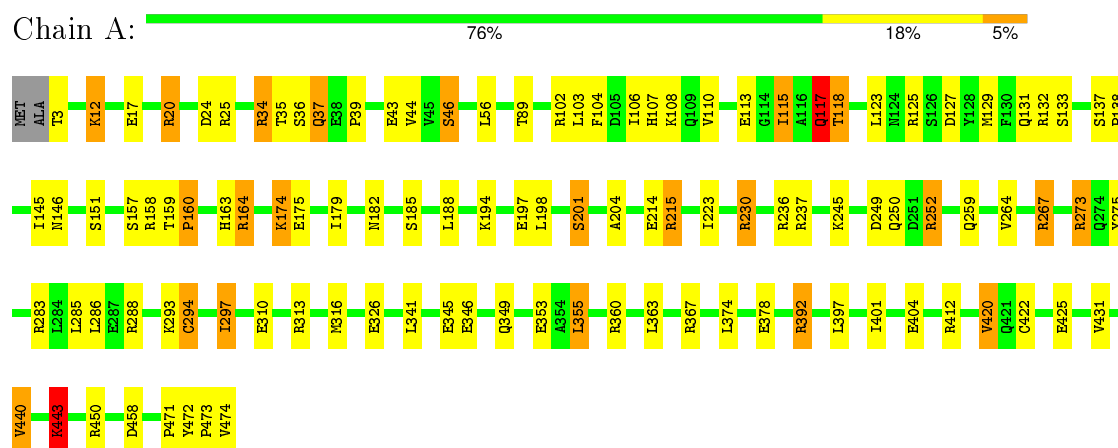
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	230	Total 230	O 230	0	0

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 was not executed.

• Molecule 1: PROTEIN (GLUTATHIONE SYNTHETASE)



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	84.26 Å 84.26 Å 197.62 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10	Depositor
% Data completeness (in resolution range)	95.9 (20.00-2.10)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.218 , 0.281	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3964	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GSH, MG, SO4, ADP

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	0.68	0/3738	1.59	47/5057 (0.9%)

There are no bond length outliers.

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288	ARG	NE-CZ-NH2	-15.23	112.69	120.30
1	A	288	ARG	NE-CZ-NH1	14.32	127.46	120.30
1	A	267	ARG	NE-CZ-NH1	13.03	126.81	120.30
1	A	20	ARG	NE-CZ-NH2	-12.10	114.25	120.30
1	A	34	ARG	NE-CZ-NH1	-11.32	114.64	120.30
1	A	313	ARG	NE-CZ-NH2	-11.11	114.74	120.30
1	A	164	ARG	NE-CZ-NH1	-10.29	115.15	120.30
1	A	450	ARG	NE-CZ-NH1	9.74	125.17	120.30
1	A	20	ARG	NE-CZ-NH1	8.28	124.44	120.30
1	A	420	VAL	CA-CB-CG1	7.91	122.76	110.90
1	A	252	ARG	NE-CZ-NH2	-7.79	116.41	120.30
1	A	215	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	A	46	SER	N-CA-CB	7.62	121.92	110.50
1	A	450	ARG	NE-CZ-NH2	-7.61	116.50	120.30
1	A	273	ARG	NE-CZ-NH2	7.32	123.96	120.30
1	A	267	ARG	CD-NE-CZ	7.31	133.84	123.60
1	A	267	ARG	NE-CZ-NH2	-7.23	116.68	120.30
1	A	313	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	A	420	VAL	CB-CA-C	-6.93	98.24	111.40
1	A	25	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	A	24	ASP	CB-CG-OD1	6.71	124.34	118.30
1	A	117	GLN	CG-CD-OE1	-6.57	108.46	121.60
1	A	443	LYS	CB-CA-C	-6.51	97.38	110.40
1	A	125	ARG	NE-CZ-NH1	-6.46	117.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	360	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	A	237	ARG	CD-NE-CZ	6.40	132.56	123.60
1	A	236	ARG	NE-CZ-NH1	-6.04	117.28	120.30
1	A	115	ILE	CA-CB-CG1	6.00	122.41	111.00
1	A	102	ARG	NE-CZ-NH1	-5.98	117.31	120.30
1	A	275	TYR	CB-CA-C	-5.90	98.60	110.40
1	A	252	ARG	CD-NE-CZ	5.84	131.77	123.60
1	A	129	MET	N-CA-CB	5.79	121.02	110.60
1	A	412	ARG	NE-CZ-NH2	5.78	123.19	120.30
1	A	346	GLU	OE1-CD-OE2	5.77	130.22	123.30
1	A	252	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	A	158	ARG	CD-NE-CZ	5.61	131.45	123.60
1	A	283	ARG	CG-CD-NE	5.33	122.99	111.80
1	A	151	SER	N-CA-CB	-5.32	102.52	110.50
1	A	294	CYS	CA-C-O	-5.29	109.00	120.10
1	A	420	VAL	CA-CB-CG2	5.29	118.83	110.90
1	A	367	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	422	CYS	CB-CA-C	-5.24	99.93	110.40
1	A	215	ARG	CD-NE-CZ	5.22	130.91	123.60
1	A	392	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	355	LEU	CB-CG-CD1	5.12	119.70	111.00
1	A	43	GLU	OE1-CD-OE2	-5.06	117.23	123.30
1	A	118	THR	N-CA-CB	-5.05	100.70	110.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3675	0	3702	60	0
2	A	2	0	0	0	0
3	A	10	0	0	1	0
4	A	27	0	12	0	0
5	A	20	0	14	2	0
6	A	230	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3964	0	3728	61	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 8.

All (61) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:VAL:HG21	1:A:293:LYS:NZ	1.96	0.80
1:A:145:ILE:O	6:A:734:HOH:O	2.04	0.76
1:A:345:GLU:O	1:A:349:GLN:HG3	1.86	0.75
1:A:174:LYS:HG2	1:A:175:GLU:OE1	1.91	0.70
1:A:378:GLU:HG3	6:A:574:HOH:O	1.92	0.69
1:A:174:LYS:HD2	1:A:174:LYS:H	1.61	0.65
1:A:264:VAL:HG21	1:A:293:LYS:HZ1	1.61	0.64
1:A:89:THR:HG23	1:A:310:GLU:HG3	1.80	0.64
1:A:36:SER:O	1:A:39:PRO:HD3	2.01	0.61
1:A:17:GLU:OE1	1:A:20:ARG:NH1	2.33	0.61
1:A:3:THR:HB	1:A:56:LEU:HD11	1.85	0.59
1:A:159:THR:N	1:A:160:PRO:CD	2.67	0.57
1:A:132:ARG:NH2	1:A:404:GLU:HG3	2.20	0.56
1:A:286:LEU:HB3	1:A:293:LYS:HZ3	1.70	0.56
1:A:349:GLN:O	1:A:353:GLU:HG2	2.06	0.56
1:A:56:LEU:HD13	1:A:474:VAL:HG21	1.87	0.56
1:A:123:LEU:HD13	1:A:188:LEU:HB3	1.90	0.53
1:A:264:VAL:HG21	1:A:293:LYS:HZ3	1.74	0.52
1:A:110:VAL:HG12	1:A:115:ILE:HD13	1.92	0.51
1:A:110:VAL:HG12	1:A:115:ILE:CD1	2.40	0.51
1:A:159:THR:N	1:A:160:PRO:HD3	2.26	0.51
1:A:286:LEU:O	1:A:293:LYS:NZ	2.38	0.49
1:A:214:GLU:OE2	5:A:503:GSH:N1	2.45	0.49
1:A:197:GLU:OE2	1:A:230:ARG:NH2	2.46	0.49
1:A:12:LYS:HD2	1:A:12:LYS:H	1.77	0.49
1:A:163:HIS:CB	1:A:179:ILE:HD13	2.43	0.48
1:A:341:LEU:HD21	1:A:397:LEU:HD22	1.94	0.48
1:A:163:HIS:HB3	1:A:179:ILE:HD13	1.96	0.48
1:A:249:ASP:OD1	1:A:250:GLN:N	2.47	0.48
1:A:157:SER:HA	1:A:182:ASN:O	2.13	0.48
1:A:353:GLU:HA	1:A:353:GLU:OE1	2.13	0.48
1:A:185:SER:HB2	1:A:223:ILE:HD13	1.96	0.48
1:A:267:ARG:HA	1:A:267:ARG:HD2	1.70	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:LYS:HD3	6:A:705:HOH:O	2.14	0.48
1:A:286:LEU:HB3	1:A:293:LYS:NZ	2.28	0.47
1:A:286:LEU:C	1:A:293:LYS:HZ2	2.18	0.47
1:A:127:ASP:OD2	1:A:146:ASN:ND2	2.48	0.47
1:A:103:LEU:HB3	1:A:297:ILE:HD11	1.97	0.47
1:A:164:ARG:HH11	1:A:164:ARG:HD2	1.46	0.46
1:A:297:ILE:HD13	1:A:297:ILE:O	2.15	0.46
1:A:174:LYS:H	1:A:174:LYS:CD	2.14	0.46
3:A:505:SO4:O4	5:A:503:GSH:C2	2.64	0.46
1:A:117:GLN:H	1:A:117:GLN:HG3	1.38	0.46
1:A:431:VAL:O	1:A:443:LYS:N	2.43	0.44
1:A:36:SER:HA	1:A:215:ARG:HD2	1.98	0.44
1:A:104:PHE:O	1:A:107:HIS:HB3	2.17	0.44
1:A:131:GLN:HB2	1:A:401:ILE:HG23	1.98	0.44
1:A:174:LYS:N	1:A:174:LYS:HD2	2.32	0.44
1:A:471:PRO:O	1:A:473:PRO:HD3	2.18	0.43
1:A:113:GLU:OE2	1:A:252:ARG:CZ	2.67	0.43
1:A:35:THR:HB	1:A:37:GLN:OE1	2.19	0.43
1:A:34:ARG:HB2	1:A:215:ARG:HA	2.01	0.43
1:A:363:LEU:HD23	1:A:374:LEU:HD12	2.01	0.42
1:A:106:ILE:O	1:A:110:VAL:HG23	2.19	0.42
1:A:201:SER:HB3	1:A:204:ALA:HB2	2.01	0.42
1:A:131:GLN:O	1:A:138:PRO:HA	2.20	0.42
1:A:198:LEU:HD11	1:A:440:VAL:HG11	2.00	0.42
1:A:123:LEU:HG	1:A:294:CYS:SG	2.61	0.41
1:A:127:ASP:HB3	1:A:425:GLU:OE2	2.19	0.41
1:A:472:TYR:HA	1:A:473:PRO:HD3	1.87	0.41
1:A:56:LEU:HA	1:A:472:TYR:HB3	2.03	0.41

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	470/474 (99%)	456 (97%)	14 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	392/393 (100%)	366 (93%)	26 (7%)	21	17

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LYS
1	A	37	GLN
1	A	44	VAL
1	A	46	SER
1	A	108	LYS
1	A	117	GLN
1	A	118	THR
1	A	133	SER
1	A	137	SER
1	A	160	PRO
1	A	174	LYS
1	A	194	LYS
1	A	201	SER
1	A	230	ARG
1	A	259	GLN
1	A	273	ARG
1	A	285	LEU
1	A	297	ILE
1	A	316	MET
1	A	326	GLU
1	A	355	LEU
1	A	392	ARG
1	A	420	VAL

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Mol	Chain	Res	Type
1	A	440	VAL
1	A	443	LYS
1	A	458	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	64	GLN
1	A	107	HIS

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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	ADP	A	500	2	22,29,29	1.45	5 (22%)	27,45,45	2.40	10 (37%)
5	GSH	A	503	-	13,19,19	1.67	2 (15%)	15,24,24	3.72	8 (53%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	A	504	-	4,4,4	0.58	0	6,6,6	0.43	0
3	SO4	A	505	2	4,4,4	0.78	0	6,6,6	0.71	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	ADP	A	500	2	-	0/12/32/32	0/3/3/3
5	GSH	A	503	-	-	0/18/24/24	0/0/0/0
3	SO4	A	504	-	-	0/0/0/0	0/0/0/0
3	SO4	A	505	2	-	0/0/0/0	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	500	ADP	PB-O2B	-2.98	1.44	1.54
4	A	500	ADP	C5-C4	-2.56	1.34	1.40
4	A	500	ADP	O4'-C1'	-2.55	1.38	1.41
4	A	500	ADP	PA-O2A	-2.18	1.45	1.54
4	A	500	ADP	C5-N7	-2.17	1.32	1.39
5	A	503	GSH	C2-N3	2.00	1.37	1.33
5	A	503	GSH	CB2-CA2	4.76	1.58	1.53

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	503	GSH	CA2-CB2-SG2	-9.84	102.07	114.16
5	A	503	GSH	O2-C2-N3	-4.81	113.44	123.08
4	A	500	ADP	C1'-N9-C4	-3.70	121.36	126.94
5	A	503	GSH	OE1-CD1-CG1	-3.51	115.93	121.98
5	A	503	GSH	CG1-CD1-N2	-3.01	110.93	115.83
4	A	500	ADP	C2'-C1'-N9	-2.51	110.46	114.29
5	A	503	GSH	C2-CA2-N2	-2.07	105.43	111.26
4	A	500	ADP	O3A-PA-O5'	2.27	108.96	102.94
4	A	500	ADP	O2A-PA-O3A	2.41	116.04	105.09
4	A	500	ADP	O3B-PB-O2B	2.65	117.48	107.38
4	A	500	ADP	O2B-PB-O1B	2.81	119.62	110.58
5	A	503	GSH	O2-C2-CA2	2.94	126.87	120.36
4	A	500	ADP	O4'-C1'-N9	3.07	114.53	108.10
5	A	503	GSH	CB1-CA1-N1	3.26	119.80	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	500	ADP	N6-C6-N1	4.54	128.94	119.20
4	A	500	ADP	C4-C5-N7	4.56	113.68	109.48
5	A	503	GSH	OE1-CD1-N2	5.78	132.81	123.01
4	A	500	ADP	N3-C2-N1	6.48	133.85	128.89

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
5	A	503	GSH	2	0
3	A	505	SO4	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.