



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:38 PM UTC

PDB ID : 2HGS / pdb_00002hgs
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

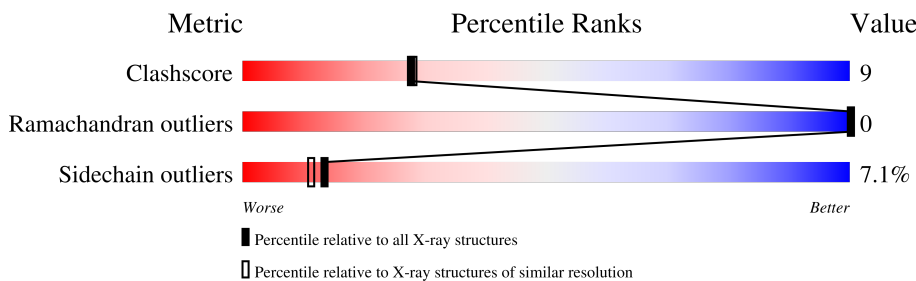
1 Overall quality at a glance

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	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	474	 68% 26% 6% •

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.

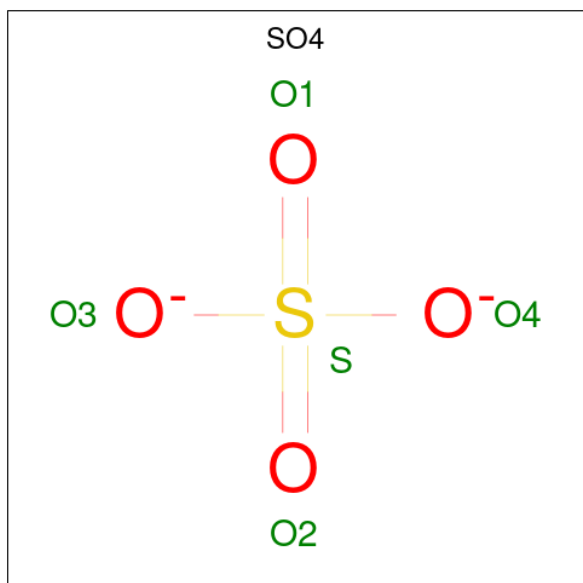
- Molecule 1 is a protein called PROTEIN (GLUTATHIONE SYNTHETASE).

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 (CCD ID: MG) (formula: Mg).

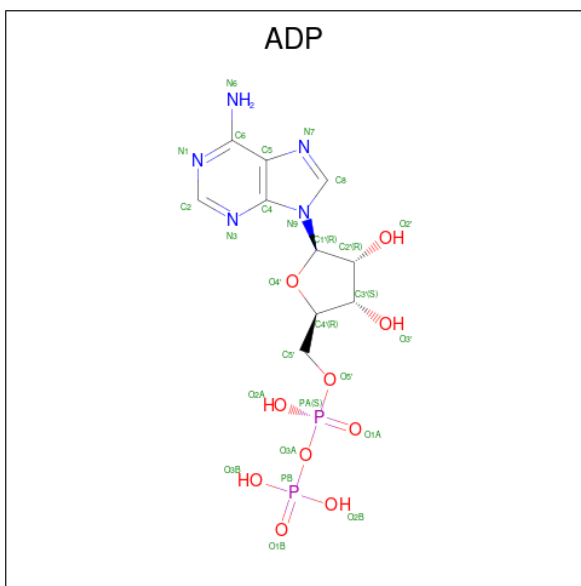
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



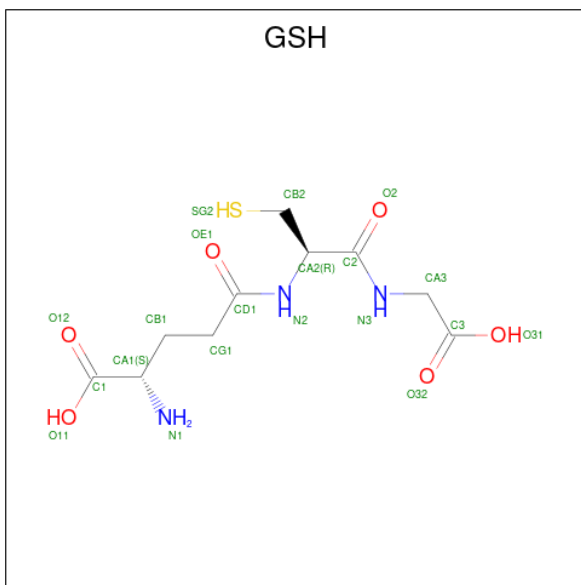
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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 (CCD ID: 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.

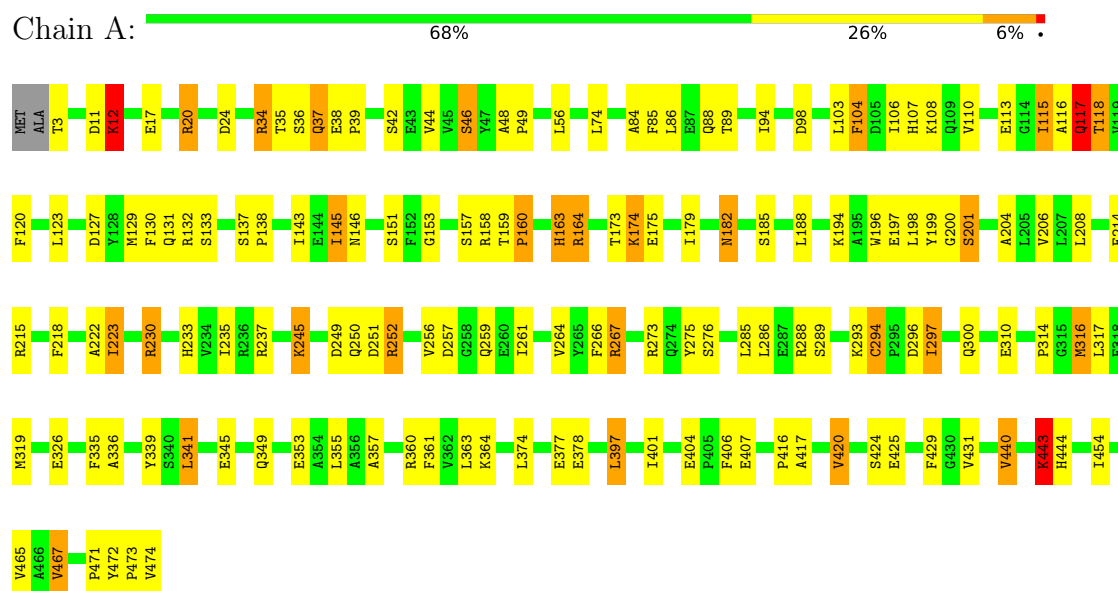
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	230	Total 230	O 230	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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 is therefore 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: MG, SO4, GSH, 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	0.90	0/3738	1.96	96/5057 (1.9%)

There are no bond length outliers.

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	294	CYS	CA-C-O	-11.32	109.00	120.09
1	A	429	PHE	CA-C-N	-10.20	115.14	122.18
1	A	429	PHE	C-N-CA	-10.20	115.14	122.18
1	A	12	LYS	N-CA-C	10.06	122.24	111.28
1	A	420	VAL	CB-CA-C	-7.96	98.24	111.29
1	A	218	PHE	CA-CB-CG	-7.74	106.06	113.80
1	A	151	SER	N-CA-C	7.58	121.62	110.17
1	A	163	HIS	CA-CB-CG	-7.32	106.48	113.80
1	A	420	VAL	CA-CB-CG1	7.27	122.76	110.40
1	A	288	ARG	NE-CZ-NH2	-7.24	112.69	119.20
1	A	257	ASP	CA-CB-CG	7.20	119.80	112.60
1	A	115	ILE	CA-CB-CG1	7.06	122.41	110.40
1	A	233	HIS	CA-CB-CG	-7.00	106.80	113.80
1	A	275	TYR	CB-CA-C	-6.97	98.60	110.16
1	A	34	ARG	NE-CZ-NH1	-6.86	114.64	121.50
1	A	118	THR	N-CA-CB	-6.78	100.70	110.80
1	A	117	GLN	CG-CD-NE2	6.75	126.52	116.40
1	A	267	ARG	CD-NE-CZ	6.74	133.84	124.40
1	A	48	ALA	N-CA-C	-6.68	100.49	110.24
1	A	289	SER	N-CA-C	6.67	118.61	110.41
1	A	129	MET	N-CA-CB	6.64	121.02	111.05
1	A	208	LEU	CA-C-N	-6.57	114.16	122.43
1	A	208	LEU	C-N-CA	-6.57	114.16	122.43
1	A	276	SER	N-CA-C	-6.43	100.39	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	206	VAL	N-CA-C	-6.42	99.17	108.36
1	A	245	LYS	CA-C-N	-6.37	115.50	122.38
1	A	245	LYS	C-N-CA	-6.37	115.50	122.38
1	A	46	SER	N-CA-CB	6.36	121.92	111.31
1	A	164	ARG	NE-CZ-NH1	-6.35	115.15	121.50
1	A	364	LYS	N-CA-C	6.33	120.76	108.85
1	A	98	ASP	CA-CB-CG	-6.23	106.37	112.60
1	A	200	GLY	N-CA-C	6.20	124.62	115.08
1	A	465	VAL	CB-CA-C	-6.18	106.46	111.71
1	A	11	ASP	CA-C-N	6.17	128.55	120.28
1	A	11	ASP	C-N-CA	6.17	128.55	120.28
1	A	117	GLN	CG-CD-OE1	-6.17	108.46	120.80
1	A	104	PHE	CA-CB-CG	-6.09	107.71	113.80
1	A	275	TYR	N-CA-C	6.08	118.33	108.41
1	A	397	LEU	CA-C-O	-6.05	114.27	121.11
1	A	443	LYS	CB-CA-C	-6.04	97.38	111.09
1	A	88	GLN	OE1-CD-NE2	5.99	128.59	122.60
1	A	288	ARG	NE-CZ-NH1	5.96	127.46	121.50
1	A	120	PHE	CA-C-N	-5.96	111.45	121.75
1	A	120	PHE	C-N-CA	-5.96	111.45	121.75
1	A	360	ARG	N-CA-C	5.90	120.60	113.17
1	A	251	ASP	CA-CB-CG	-5.87	106.73	112.60
1	A	256	VAL	CA-C-O	-5.86	114.35	120.27
1	A	237	ARG	CD-NE-CZ	5.83	132.56	124.40
1	A	454	ILE	N-CA-C	5.81	119.19	111.17
1	A	173	THR	CA-C-N	5.80	128.52	120.63
1	A	173	THR	C-N-CA	5.80	128.52	120.63
1	A	444	HIS	CA-CB-CG	5.79	119.59	113.80
1	A	266	PHE	N-CA-C	5.74	118.03	109.25
1	A	196	TRP	CA-C-O	5.68	126.45	120.42
1	A	443	LYS	N-CA-CB	-5.65	102.64	111.56
1	A	314	PRO	CB-CA-C	5.63	118.71	111.56
1	A	267	ARG	N-CA-C	-5.62	106.42	113.72
1	A	341	LEU	N-CA-C	-5.60	105.13	112.41
1	A	74	LEU	CA-C-O	5.58	126.46	120.55
1	A	296	ASP	N-CA-C	-5.55	103.06	110.55
1	A	199	TYR	N-CA-C	-5.52	105.26	111.28
1	A	42	SER	N-CA-C	-5.52	106.43	112.72
1	A	20	ARG	NE-CZ-NH2	-5.50	114.25	119.20
1	A	339	TYR	N-CA-C	5.45	117.78	108.90
1	A	257	ASP	CB-CA-C	-5.42	103.88	111.80
1	A	116	ALA	CA-C-N	5.42	128.40	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	ALA	C-N-CA	5.42	128.40	120.71
1	A	130	PHE	CA-CB-CG	5.41	119.21	113.80
1	A	336	ALA	N-CA-C	-5.41	101.44	109.94
1	A	223	ILE	CB-CA-C	-5.40	104.77	112.22
1	A	222	ALA	O-C-N	5.37	127.81	122.12
1	A	145	ILE	N-CA-CB	5.37	118.81	111.41
1	A	153	GLY	N-CA-C	-5.33	108.05	114.66
1	A	267	ARG	NE-CZ-NH1	5.31	126.81	121.50
1	A	273	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	A	182	ASN	N-CA-CB	-5.28	101.95	110.71
1	A	117	GLN	CB-CG-CD	-5.27	103.64	112.60
1	A	252	ARG	CD-NE-CZ	5.26	131.77	124.40
1	A	86	LEU	CA-C-N	-5.25	113.30	120.44
1	A	86	LEU	C-N-CA	-5.25	113.30	120.44
1	A	164	ARG	CD-NE-CZ	-5.25	117.05	124.40
1	A	261	ILE	O-C-N	-5.24	116.97	122.95
1	A	24	ASP	CA-CB-CG	5.23	117.83	112.60
1	A	276	SER	CA-CB-OG	-5.22	100.67	111.10
1	A	317	LEU	N-CA-CB	5.21	117.56	110.01
1	A	335	PHE	CA-CB-CG	5.19	118.99	113.80
1	A	300	GLN	N-CA-C	-5.18	105.71	111.36
1	A	361	PHE	CA-CB-CG	-5.17	108.63	113.80
1	A	235	ILE	N-CA-CB	5.16	120.37	111.39
1	A	143	ILE	CB-CA-C	-5.14	105.46	111.94
1	A	38	GLU	CA-C-N	5.06	124.78	119.82
1	A	38	GLU	C-N-CA	5.06	124.78	119.82
1	A	223	ILE	N-CA-C	-5.04	105.63	110.72
1	A	84	ALA	O-C-N	5.04	127.90	122.15
1	A	158	ARG	CD-NE-CZ	5.04	131.45	124.40
1	A	357	ALA	N-CA-CB	-5.00	104.29	110.79

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	66	0
2	A	2	0	0	0	0
3	A	10	0	0	1	0
4	A	27	0	12	1	0
5	A	20	0	14	2	0
6	A	230	0	0	3	0
All	All	3964	0	3728	67	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 9.

All (67) 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:264:VAL:HG21	1:A:293:LYS:HZ3	1.61	0.65
1:A:174:LYS:HD2	1:A:174:LYS:H	1.61	0.65
1:A:89:THR:HG23	1:A:310:GLU:HG3	1.80	0.64
1:A:85:PHE:HE1	1:A:316:MET:HE3	1.65	0.61
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: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:286:LEU:C	1:A:293:LYS:HZ2	2.14	0.55
1:A:123:LEU:HD13	1:A:188:LEU:HB3	1.90	0.53
1:A:406:PHE:HZ	1:A:424:SER:HG	1.56	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:H	1:A:12:LYS:HD2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:VAL:HG21	1:A:293:LYS:HZ1	1.75	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:286:LEU:HB3	1:A:293:LYS:NZ	2.28	0.48
1:A:157:SER:HA	1:A:182:ASN:O	2.13	0.48
1:A:353:GLU:OE1	1:A:353:GLU:HA	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
1:A:245:LYS:HD3	6:A:705:HOH:O	2.14	0.48
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:286:LEU:HB3	1:A:293:LYS:HZ3	1.80	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
1:A:117:GLN:H	1:A:117:GLN:HG3	1.38	0.46
3:A:505:SO4:O4	5:A:503:GSH:C2	2.64	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:416:PRO:O	1:A:417:ALA:C	2.60	0.44
1:A:174:LYS:HD2	1:A:174:LYS:N	2.32	0.44
1:A:113:GLU:OE2	1:A:252:ARG:CZ	2.67	0.43
1:A:471:PRO:O	1:A:473:PRO:HD3	2.18	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:249:ASP:OD1	1:A:249:ASP:C	2.62	0.41
1:A:56:LEU:HA	1:A:472:TYR:HB3	2.03	0.41
1:A:472:TYR:HA	1:A:473:PRO:HD3	1.87	0.41
1:A:49:PRO:C	1:A:467:VAL:HB	2.46	0.40
1:A:425:GLU:OE1	4:A:500:ADP:O3'	2.30	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	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%)	364 (93%)	28 (7%)	13	11

All (28) 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	94	ILE
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

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Mol	Chain	Res	Type
1	A	201	SER
1	A	230	ARG
1	A	259	GLN
1	A	285	LEU
1	A	297	ILE
1	A	316	MET
1	A	319	MET
1	A	326	GLU
1	A	355	LEU
1	A	377	GLU
1	A	407	GLU
1	A	420	VAL
1	A	440	VAL
1	A	443	LYS
1	A	467	VAL

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

Mol	Chain	Res	Type
1	A	96	GLN
1	A	107	HIS
1	A	131	GLN
1	A	142	GLN
1	A	372	ASN
1	A	435	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

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
5	GSH	A	503	-	18,19,19	1.61	2 (11%)	21,24,24	3.63	10 (47%)
4	ADP	A	500	2	28,29,29	1.60	7 (25%)	43,45,45	2.30	13 (30%)
3	SO4	A	505	2	4,4,4	0.63	0	6,6,6	0.74	0
3	SO4	A	504	-	4,4,4	0.52	0	6,6,6	0.33	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
5	GSH	A	503	-	-	4/24/24/24	-
4	ADP	A	500	2	-	3/16/32/32	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	503	GSH	CB2-CA2	5.10	1.58	1.53
4	A	500	ADP	C5-N7	-3.85	1.32	1.39
4	A	500	ADP	C8-N7	3.30	1.38	1.31
4	A	500	ADP	PB-O2B	-2.91	1.44	1.54
4	A	500	ADP	C5-C4	-2.45	1.34	1.39
5	A	503	GSH	O12-C1	2.33	1.29	1.22
4	A	500	ADP	C8-N9	-2.21	1.33	1.37
4	A	500	ADP	PA-O2A	-2.09	1.45	1.55
4	A	500	ADP	PA-O3A	-2.01	1.57	1.59

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	503	GSH	CA2-CB2-SG2	-10.72	102.07	114.16
4	A	500	ADP	C6-C5-C4	7.05	126.81	117.18
4	A	500	ADP	C6-C5-N7	-6.53	119.51	132.09
5	A	503	GSH	O11-C1-O12	-5.96	110.57	124.08
5	A	503	GSH	OE1-CD1-N2	5.82	132.81	122.95
4	A	500	ADP	N6-C6-N1	4.74	128.94	118.38
5	A	503	GSH	O2-C2-N3	-4.51	113.44	122.98
5	A	503	GSH	CB1-CA1-N1	3.71	119.80	110.12
4	A	500	ADP	N3-C2-N1	3.48	133.85	128.58
5	A	503	GSH	OE1-CD1-CG1	-3.36	115.93	122.02
4	A	500	ADP	O4'-C1'-N9	3.35	114.53	108.09
5	A	503	GSH	CB1-CA1-C1	3.34	119.30	110.45
4	A	500	ADP	C1'-N9-C8	3.34	134.50	127.09
4	A	500	ADP	O2A-PA-O3A	3.24	116.04	107.27
5	A	503	GSH	O2-C2-CA2	3.05	126.87	120.48
4	A	500	ADP	C5-C6-N1	-2.92	110.09	117.51
5	A	503	GSH	CG1-CD1-N2	-2.80	110.93	115.86
4	A	500	ADP	C4-C5-N7	2.71	113.68	110.58
4	A	500	ADP	O3B-PB-O2B	2.58	117.48	107.80
4	A	500	ADP	C2-N3-C4	-2.52	105.68	111.83
4	A	500	ADP	O2B-PB-O1B	2.25	119.62	110.83
4	A	500	ADP	C4-N9-C1'	-2.25	121.36	126.63
5	A	503	GSH	C2-CA2-N2	-2.10	105.43	111.11

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	503	GSH	C1-CA1-CB1-CG1
5	A	503	GSH	O2-C2-N3-CA3
5	A	503	GSH	N3-C2-CA2-N2
4	A	500	ADP	PA-O3A-PB-O1B
4	A	500	ADP	PA-O3A-PB-O2B
4	A	500	ADP	PA-O3A-PB-O3B
5	A	503	GSH	O11-C1-CA1-N1

There are no ring outliers.

3 monomers are involved in 3 short contacts:

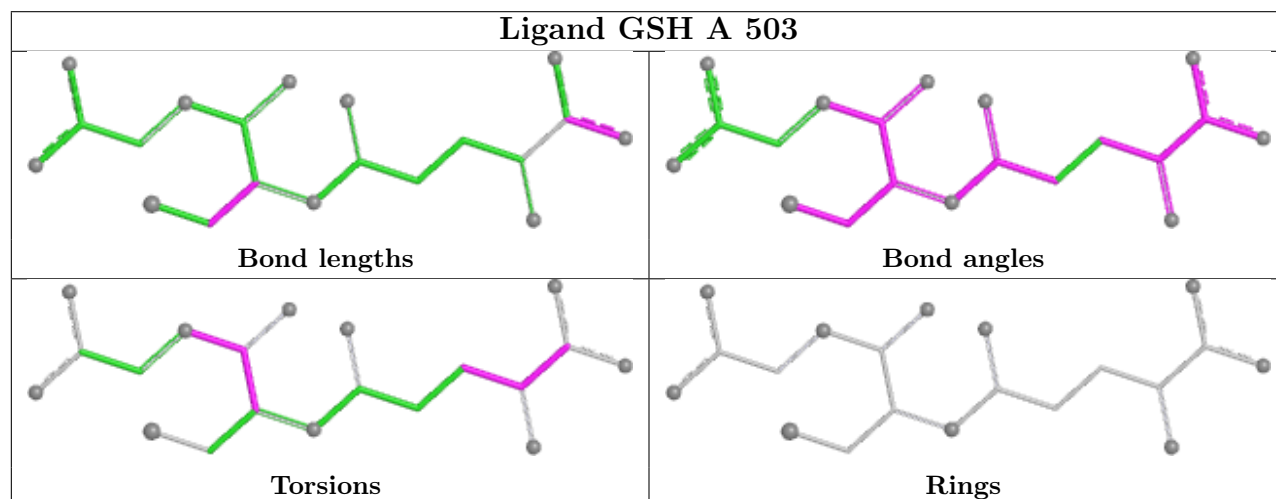
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	503	GSH	2	0
4	A	500	ADP	1	0

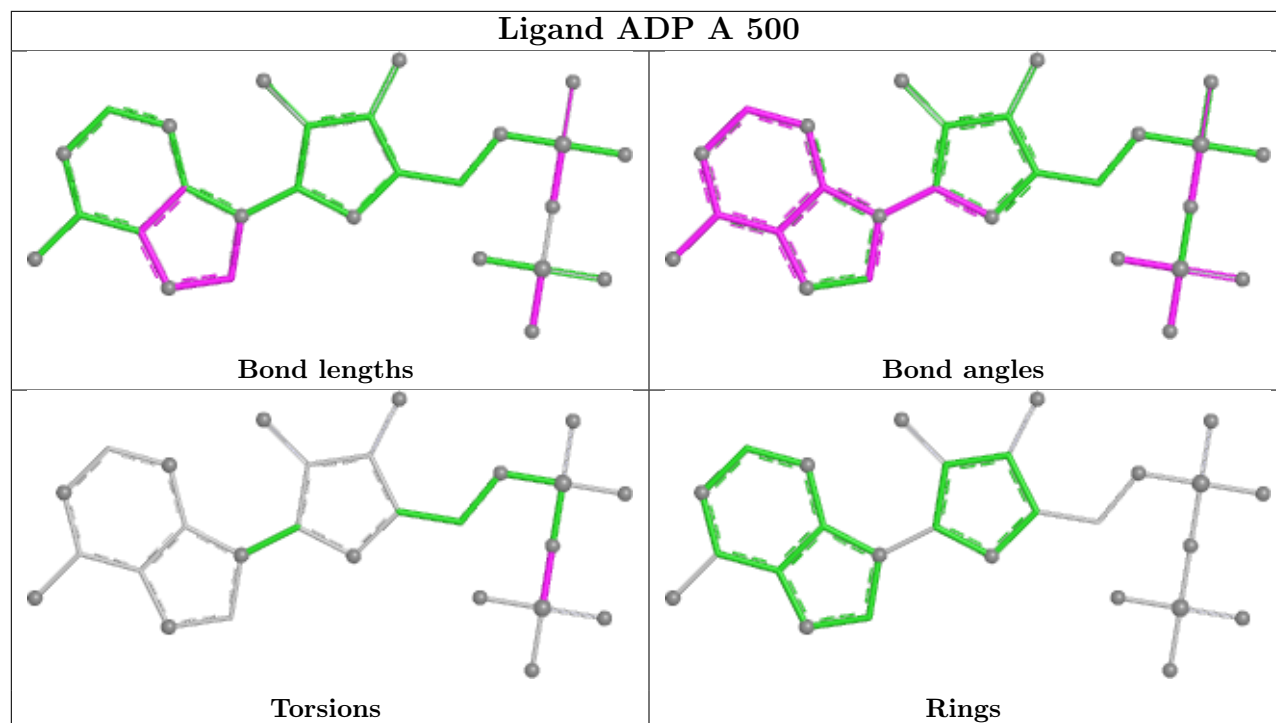
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	505	SO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.