



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:49 AM UTC

PDB ID : 2IO9 / pdb_00002io9
Title : E. coli Bifunctional glutathionylspermidine synthetase/amidase Incomplex with Mg²⁺, GSH and ADP
Authors : Pai, C.H.; Chiang, B.Y.; Ko, T.P.; Chou, C.C.; Chong, C.M.; Yen, F.J.; Coward, J.K.; Wang, A.H.-J.; Lin, C.H.
Deposited on : 2006-10-10
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

<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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

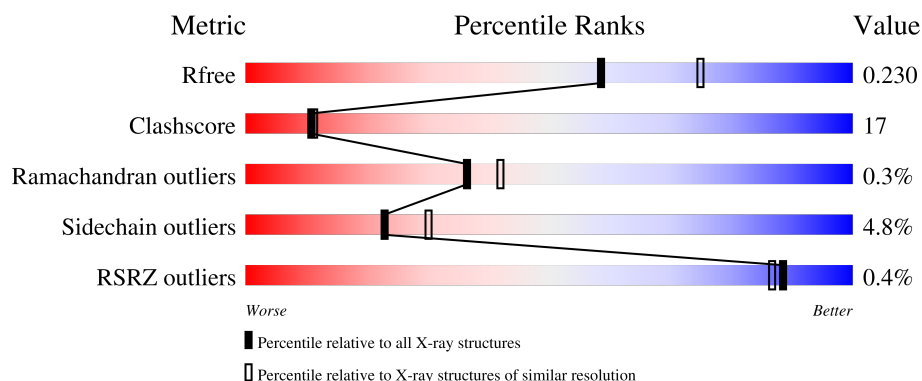
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 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 $\leq 5\%$. 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	619	 61% 30% 6% .
1	B	619	 % 66% 27% . .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11020 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.

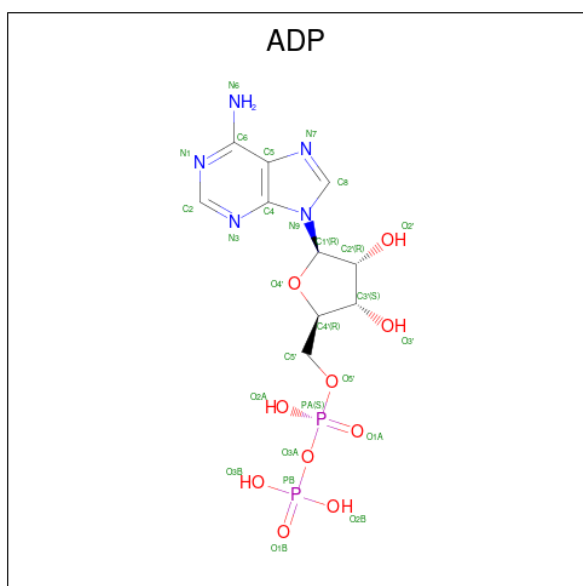
- Molecule 1 is a protein called Bifunctional glutathionylspermidine synthetase/amidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	601	Total	C	N	O	S	0	0	0
			4836	3094	828	895	19			
1	B	603	Total	C	N	O	S	0	0	0
			4852	3104	830	899	19			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

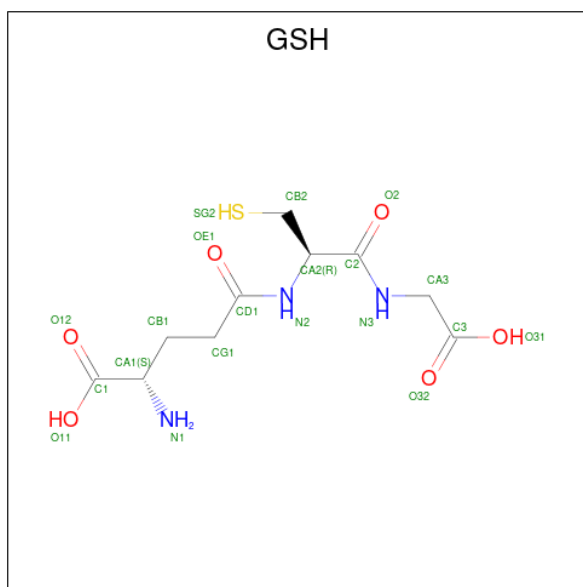
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		
2	B	2	Total	Mg	0	0
			2	2		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 4 is GLUTATHIONE (CCD ID: GSH) (formula: C₁₀H₁₇N₃O₆S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			19	10	3	5	1		
4	B	1	Total	C	N	O	S	0	0
			19	10	3	5	1		

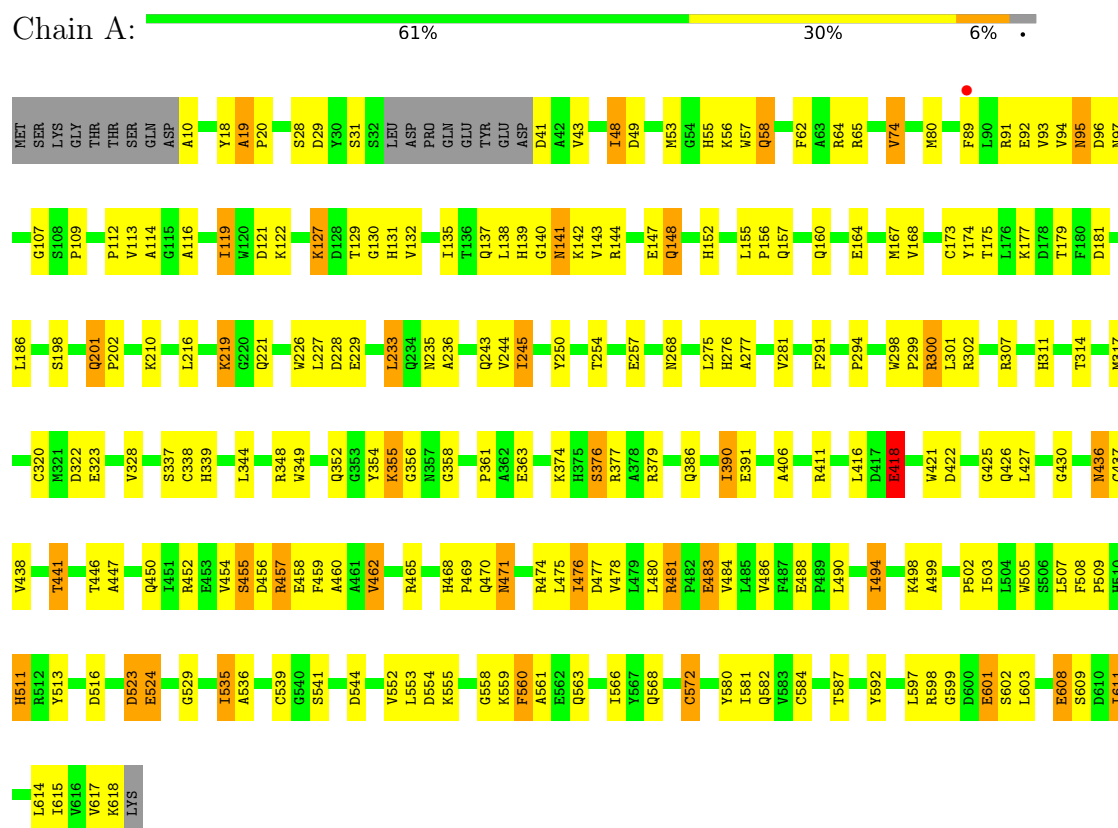
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	625	Total	O	0	0
			625	625		
5	B	611	Total	O	0	0
			611	611		

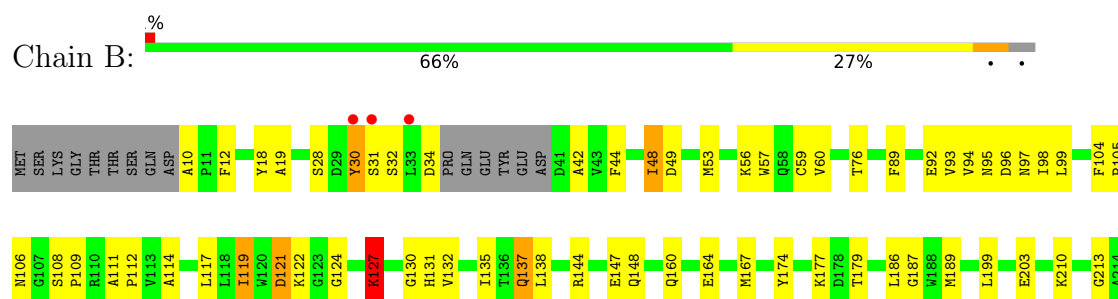
3 Residue-property plots [i](#)

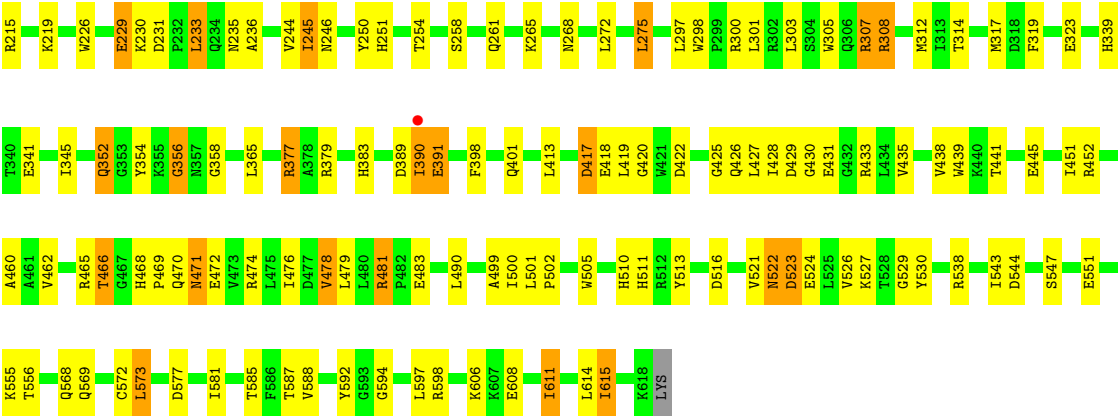
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Bifunctional glutathionylspermidine synthetase/amidase



- Molecule 1: Bifunctional glutathionylspermidine synthetase/amidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	59.91Å 75.48Å 84.01Å 70.44° 74.17° 78.06°	Depositor
Resolution (Å)	30.00 – 2.20 30.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.20) 91.4 (30.00-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.94 (at 2.20Å)	Xtriage
Refinement program	CNS, XTALVIEW	Depositor
R, R_{free}	0.170 , 0.232 0.168 , 0.230	Depositor DCC
R_{free} test set	3102 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	27.8	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 69.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11020	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: MG, ADP, 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	1.07	3/4960 (0.1%)	1.24	45/6736 (0.7%)
1	B	1.01	8/4976 (0.2%)	1.24	40/6758 (0.6%)
All	All	1.04	11/9936 (0.1%)	1.24	85/13494 (0.6%)

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	B	0	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	617	VAL	CA-CB	7.43	1.64	1.54
1	B	60	VAL	CA-CB	6.11	1.62	1.54
1	B	500	ILE	CA-CB	6.11	1.61	1.54
1	B	615	ILE	CA-CB	5.83	1.62	1.54
1	B	312	MET	SD-CE	5.63	1.93	1.79
1	B	317	MET	SD-CE	5.35	1.93	1.79
1	B	345	ILE	CA-CB	5.33	1.60	1.54
1	B	236	ALA	CA-CB	5.32	1.61	1.53
1	B	19	ALA	CA-CB	-5.24	1.45	1.53
1	A	245	ILE	CA-CB	-5.16	1.47	1.54
1	A	476	ILE	CA-CB	-5.06	1.47	1.54

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	93	VAL	N-CA-C	9.64	120.48	110.36
1	A	93	VAL	N-CA-C	8.88	119.69	110.36
1	A	441	THR	N-CA-C	-8.63	102.89	113.50
1	B	441	THR	N-CA-C	-8.29	103.18	113.38
1	B	611	ILE	N-CA-C	-8.25	96.56	108.36
1	A	48	ILE	N-CA-C	-8.23	93.42	107.24
1	A	529	GLY	N-CA-C	-7.89	102.74	112.68
1	B	48	ILE	N-CA-C	-7.71	94.29	107.24
1	B	478	VAL	CB-CA-C	-7.60	105.25	111.71
1	B	529	GLY	N-CA-C	-7.47	103.27	112.68
1	A	611	ILE	N-CA-C	-7.45	97.71	108.36
1	A	148	GLN	CA-C-N	-7.40	110.67	122.95
1	A	148	GLN	C-N-CA	-7.40	110.67	122.95
1	A	601	GLU	N-CA-C	-6.96	104.05	112.54
1	A	130	GLY	N-CA-C	-6.85	99.76	112.37
1	A	109	PRO	N-CA-C	-6.80	105.36	113.86
1	B	130	GLY	N-CA-C	-6.79	99.88	112.37
1	A	376	SER	N-CA-C	-6.77	101.01	110.35
1	B	42	ALA	N-CA-C	-6.69	104.93	113.23
1	B	573	LEU	CA-C-N	-6.68	113.77	120.31
1	B	573	LEU	C-N-CA	-6.68	113.77	120.31
1	B	572	CYS	N-CA-C	6.65	119.87	110.23
1	B	588	VAL	N-CA-C	-6.61	97.93	107.78
1	A	236	ALA	N-CA-C	-6.49	104.28	111.36
1	B	481	ARG	N-CA-C	-6.43	99.90	109.42
1	A	462	VAL	N-CA-C	-6.35	102.04	108.96
1	B	236	ALA	N-CA-C	-6.30	104.41	111.28
1	B	219	LYS	N-CA-C	-6.17	104.39	112.41
1	B	119	ILE	N-CA-C	6.06	117.32	108.53
1	A	250	TYR	N-CA-C	-6.05	105.90	113.28
1	A	446	THR	N-CA-C	-6.01	104.72	111.28
1	B	587	THR	N-CA-C	-6.01	99.60	109.40
1	B	121	ASP	N-CA-C	-5.96	103.08	110.41
1	B	258	SER	N-CA-C	-5.94	104.80	111.28
1	A	155	LEU	CA-C-N	5.86	126.20	119.93
1	A	155	LEU	C-N-CA	5.86	126.20	119.93
1	A	587	THR	N-CA-C	-5.85	100.17	109.59
1	A	311	HIS	N-CA-C	5.80	120.05	112.92
1	B	245	ILE	CB-CA-C	-5.77	105.92	111.05
1	A	511	HIS	N-CA-C	-5.75	102.53	110.35
1	B	356	GLY	N-CA-C	5.72	121.41	112.31
1	A	19	ALA	N-CA-C	-5.72	102.70	110.36
1	B	298	TRP	CA-C-N	-5.71	113.14	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	298	TRP	C-N-CA	-5.71	113.14	119.19
1	B	179	THR	N-CA-C	-5.65	106.35	113.18
1	B	307	ARG	N-CA-C	5.65	120.32	113.38
1	A	481	ARG	N-CA-C	-5.64	101.07	109.42
1	B	109	PRO	N-CA-C	-5.60	106.40	114.18
1	A	508	PHE	CA-C-N	5.54	126.77	119.84
1	A	508	PHE	C-N-CA	5.54	126.77	119.84
1	A	572	CYS	N-CA-C	5.53	118.46	110.28
1	A	119	ILE	N-CA-C	5.51	116.52	108.53
1	B	365	LEU	N-CA-C	5.48	117.69	111.11
1	A	488	GLU	CA-C-N	5.45	125.40	119.78
1	A	488	GLU	C-N-CA	5.45	125.40	119.78
1	A	535	ILE	N-CA-C	5.44	117.85	111.05
1	B	250	TYR	N-CA-C	-5.42	106.62	113.18
1	A	494	ILE	CA-C-N	-5.41	114.10	119.56
1	A	494	ILE	C-N-CA	-5.41	114.10	119.56
1	A	418	GLU	N-CA-C	5.40	119.13	112.54
1	B	439	TRP	N-CA-C	-5.37	100.42	109.07
1	B	231	ASP	CA-C-N	5.36	125.44	119.32
1	B	231	ASP	C-N-CA	5.36	125.44	119.32
1	B	244	VAL	N-CA-C	5.35	115.99	108.17
1	B	479	LEU	N-CA-C	5.35	117.11	111.28
1	A	179	THR	N-CA-C	-5.34	106.76	113.28
1	B	598	ARG	N-CA-C	-5.33	100.72	109.40
1	A	116	ALA	N-CA-C	5.32	118.00	110.50
1	B	96	ASP	CA-C-N	5.32	130.65	120.97
1	B	96	ASP	C-N-CA	5.32	130.65	120.97
1	B	30	TYR	N-CA-C	-5.30	102.20	110.42
1	A	486	VAL	N-CA-C	5.30	116.61	108.71
1	A	219	LYS	N-CA-C	-5.26	104.46	111.87
1	A	560	PHE	N-CA-C	5.26	119.00	112.59
1	B	106	ASN	N-CA-C	-5.26	102.61	110.23
1	A	320	CYS	N-CA-C	-5.24	100.64	109.07
1	B	164	GLU	N-CA-C	-5.18	101.43	109.72
1	A	201	GLN	CA-C-N	-5.14	114.64	119.89
1	A	201	GLN	C-N-CA	-5.14	114.64	119.89
1	A	94	VAL	N-CA-C	5.13	119.28	111.89
1	B	523	ASP	N-CA-C	5.12	116.55	111.07
1	A	438	VAL	N-CA-C	5.11	116.08	108.46
1	A	561	ALA	N-CA-C	5.06	118.22	111.75
1	A	523	ASP	N-CA-C	5.04	117.43	111.33
1	A	198	SER	N-CA-C	5.00	116.98	110.43

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	319	PHE	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	4836	0	4704	186	0
1	B	4852	0	4718	133	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	27	0	12	2	0
3	B	27	0	12	2	0
4	A	19	0	14	2	0
4	B	19	0	14	2	0
5	A	625	0	0	26	0
5	B	611	0	0	20	0
All	All	11020	0	9474	319	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 17.

All (319) 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:210:LYS:HD3	1:A:323:GLU:HB3	1.35	1.05
1:B:422:ASP:HB3	5:B:7400:HOH:O	1.61	1.00
1:B:522:ASN:O	1:B:526:VAL:HG23	1.69	0.93
1:B:95:ASN:OD1	1:B:97:ASN:HB2	1.72	0.90
1:A:465:ARG:HD2	5:A:7329:HOH:O	1.72	0.88
4:A:5001:GSH:N1	5:A:7626:HOH:O	1.99	0.88
1:B:31:SER:HB3	1:B:34:ASP:OD2	1.76	0.85
1:A:157:GLN:CD	1:A:157:GLN:H	1.86	0.84
1:A:168:VAL:HG23	1:A:175:THR:HB	1.60	0.82
1:A:210:LYS:NZ	1:A:323:GLU:HG2	1.94	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:5002:GSH:N1	5:B:7614:HOH:O	2.11	0.81
1:A:228:ASP:HB2	1:A:348:ARG:HH12	1.44	0.81
1:B:323:GLU:HG2	5:B:7430:HOH:O	1.80	0.81
1:B:268:ASN:HD21	1:B:592:TYR:H	1.28	0.80
1:B:445:GLU:OE2	1:B:452:ARG:NH2	2.12	0.79
1:A:138:LEU:CD1	1:A:143:VAL:HG12	2.13	0.79
1:B:425:GLY:O	1:B:481:ARG:NH2	2.16	0.79
1:A:41:ASP:N	5:A:7559:HOH:O	2.16	0.77
1:B:390:ILE:HD13	1:B:391:GLU:H	1.48	0.77
1:B:215:ARG:HD3	5:B:7266:HOH:O	1.84	0.77
1:A:95:ASN:C	1:A:95:ASN:HD22	1.93	0.76
1:B:203:GLU:HA	5:B:7119:HOH:O	1.86	0.75
1:A:210:LYS:HZ2	1:A:323:GLU:H	1.35	0.74
1:A:559:LYS:HG2	5:A:7401:HOH:O	1.87	0.74
1:B:177:LYS:HB2	5:B:7363:HOH:O	1.87	0.74
1:A:458:GLU:HG2	5:A:7530:HOH:O	1.88	0.73
1:B:390:ILE:HD13	1:B:391:GLU:N	2.03	0.73
1:B:510:HIS:HD2	5:B:7449:HOH:O	1.71	0.73
1:A:483:GLU:CD	1:A:483:GLU:H	1.97	0.73
1:B:265:LYS:HE2	5:B:7371:HOH:O	1.89	0.72
1:B:251:HIS:HE1	1:B:577:ASP:OD2	1.73	0.72
1:A:141:ASN:HD22	1:A:141:ASN:H	1.36	0.72
1:B:230:LYS:HE2	5:B:7273:HOH:O	1.88	0.72
1:A:411:ARG:NH2	1:A:418:GLU:OE1	2.22	0.72
1:A:447:ALA:HB1	1:A:476:ILE:HG22	1.70	0.71
1:A:425:GLY:O	1:A:481:ARG:NH2	2.24	0.71
1:B:233:LEU:HD12	1:B:401:GLN:OE1	1.90	0.71
1:A:137:GLN:NE2	1:A:144:ARG:HD2	2.05	0.71
1:B:245:ILE:HG13	1:B:246:ASN:N	2.06	0.70
1:A:268:ASN:HD21	1:A:592:TYR:H	1.37	0.70
1:A:137:GLN:HE21	1:A:144:ARG:HD2	1.57	0.69
1:B:413:LEU:HD13	1:B:419:LEU:HD21	1.73	0.69
1:A:138:LEU:HD12	1:A:143:VAL:HG12	1.73	0.68
1:A:210:LYS:CD	1:A:323:GLU:HB3	2.17	0.68
1:A:210:LYS:HZ3	1:A:323:GLU:HG2	1.58	0.67
1:B:389:ASP:HB3	1:B:391:GLU:HG3	1.75	0.67
1:A:137:GLN:HE22	1:A:144:ARG:HH11	1.43	0.66
1:A:168:VAL:CG2	1:A:175:THR:HB	2.26	0.66
1:A:450:GLN:OE1	1:A:476:ILE:HG12	1.95	0.66
1:A:113:VAL:HG22	1:A:114:ALA:N	2.11	0.65
1:A:457:ARG:HH11	1:A:457:ARG:HB3	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:GLN:HG3	1:B:144:ARG:HB2	1.77	0.65
1:B:301:LEU:HD23	1:B:490:LEU:HG	1.79	0.65
1:A:307:ARG:HD3	1:B:49:ASP:OD2	1.97	0.65
1:A:452:ARG:O	1:A:455:SER:HB2	1.97	0.64
1:A:568:GLN:HE21	3:A:3001:ADP:HN61	1.45	0.64
1:A:137:GLN:NE2	1:A:144:ARG:HH11	1.95	0.64
1:A:137:GLN:HG3	1:A:144:ARG:HB2	1.78	0.64
1:B:111:ALA:HB2	1:B:174:TYR:CZ	2.32	0.64
1:A:142:LYS:HE3	5:A:7207:HOH:O	1.98	0.63
1:B:210:LYS:HG2	5:B:7430:HOH:O	1.98	0.63
1:A:219:LYS:O	1:A:219:LYS:HG2	1.99	0.62
1:A:138:LEU:HD13	1:A:143:VAL:HG12	1.79	0.62
1:A:301:LEU:HD23	1:A:490:LEU:HG	1.81	0.62
1:A:411:ARG:HH21	1:A:418:GLU:CD	2.07	0.62
1:A:457:ARG:HH11	1:A:457:ARG:CB	2.12	0.62
1:B:245:ILE:HG13	1:B:246:ASN:H	1.65	0.62
1:B:390:ILE:HD13	1:B:391:GLU:HG2	1.81	0.61
1:A:168:VAL:HG11	1:A:177:LYS:HE3	1.81	0.61
1:B:522:ASN:HD22	1:B:523:ASP:N	1.99	0.61
1:A:210:LYS:HZ2	1:A:323:GLU:HG2	1.62	0.61
4:A:5001:GSH:N1	5:A:7625:HOH:O	2.31	0.60
1:A:436:ASN:HD22	1:A:436:ASN:C	2.10	0.60
1:B:390:ILE:CD1	1:B:390:ILE:N	2.63	0.60
1:A:210:LYS:HD3	1:A:323:GLU:CB	2.23	0.59
1:A:233:LEU:HD23	1:A:344:LEU:HD22	1.85	0.59
1:A:277:ALA:O	1:A:281:VAL:HG23	2.03	0.59
1:A:376:SER:O	5:A:7087:HOH:O	2.16	0.59
1:A:337:SER:O	1:A:338:CYS:HB2	2.03	0.58
1:B:215:ARG:CD	5:B:7266:HOH:O	2.49	0.58
1:A:421:TRP:H	1:A:471:ASN:HD21	1.51	0.58
1:A:28:SER:HB3	1:A:57:TRP:HB2	1.85	0.58
1:A:138:LEU:HD11	1:A:167:MET:SD	2.43	0.58
1:A:481:ARG:HB3	1:A:484:VAL:HG23	1.85	0.58
1:A:300:ARG:HG2	5:A:7159:HOH:O	2.03	0.58
1:B:303:LEU:HD22	1:B:307:ARG:HH21	1.68	0.58
1:A:559:LYS:HE2	1:A:560:PHE:CZ	2.38	0.57
1:B:117:LEU:HB2	1:B:189:MET:HB2	1.87	0.57
1:A:355:LYS:HG2	5:A:7387:HOH:O	2.03	0.57
1:A:89:PHE:HB2	5:A:7103:HOH:O	2.05	0.57
1:A:89:PHE:CD1	5:A:7335:HOH:O	2.52	0.57
1:B:44:PHE:O	1:B:56:LYS:HG3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:LEU:HD21	1:B:478:VAL:HG13	1.87	0.57
1:B:465:ARG:HG3	1:B:474:ARG:NH2	2.20	0.57
1:A:597:LEU:HD11	1:A:614:LEU:HD13	1.85	0.56
1:B:226:TRP:HB2	1:B:352:GLN:HG2	1.85	0.56
1:A:10:ALA:N	5:A:7323:HOH:O	2.38	0.56
1:A:148:GLN:O	5:A:7560:HOH:O	2.17	0.56
1:B:417:ASP:HB2	5:B:7179:HOH:O	2.03	0.56
1:B:390:ILE:HD13	1:B:390:ILE:N	2.21	0.56
1:B:522:ASN:C	1:B:522:ASN:ND2	2.64	0.56
1:B:89:PHE:CD1	1:B:89:PHE:C	2.82	0.56
1:A:536:ALA:H	1:A:563:GLN:HE22	1.54	0.56
1:A:460:ALA:HB2	1:B:114:ALA:HB1	1.87	0.56
1:A:541:SER:HB3	1:A:558:GLY:HA3	1.87	0.56
1:A:572:CYS:HB3	1:A:603:LEU:HD22	1.88	0.56
1:A:254:THR:HA	1:A:615:ILE:O	2.06	0.56
1:A:137:GLN:HE21	1:A:139:HIS:HE1	1.52	0.55
1:A:114:ALA:HB1	1:B:460:ALA:HB2	1.87	0.55
1:A:454:VAL:O	1:A:456:ASP:N	2.32	0.55
1:A:18:TYR:O	1:A:160:GLN:HA	2.06	0.55
1:A:226:TRP:HB2	1:A:352:GLN:HG2	1.87	0.55
1:A:536:ALA:H	1:A:563:GLN:NE2	2.05	0.55
1:B:354:TYR:CZ	1:B:356:GLY:HA3	2.42	0.55
1:B:544:ASP:OD1	1:B:555:LYS:HE2	2.06	0.55
1:B:568:GLN:HE21	3:B:3002:ADP:HN61	1.54	0.55
1:B:383:HIS:CE1	1:B:435:VAL:HG22	2.42	0.55
1:B:213:GLY:HA3	1:B:577:ASP:OD2	2.07	0.55
1:B:468:HIS:CG	1:B:469:PRO:HD2	2.42	0.55
1:A:377:ARG:N	5:A:7184:HOH:O	2.19	0.54
1:B:314:THR:OG1	1:B:339:HIS:HE1	1.89	0.54
1:A:89:PHE:HD1	5:A:7335:HOH:O	1.86	0.54
1:B:138:LEU:HD11	1:B:167:MET:HE1	1.89	0.54
1:B:462:VAL:HB	5:B:7184:HOH:O	2.07	0.54
1:A:131:HIS:HE1	1:A:147:GLU:OE2	1.91	0.54
1:B:511:HIS:HE1	1:B:513:TYR:CD2	2.25	0.54
1:B:307:ARG:HG3	1:B:308:ARG:HG2	1.90	0.54
1:B:341:GLU:HG2	1:B:611:ILE:HG13	1.88	0.54
1:A:121:ASP:HB2	1:A:186:LEU:HG	1.90	0.54
1:B:131:HIS:HE1	1:B:147:GLU:OE1	1.91	0.54
1:B:303:LEU:HD13	1:B:307:ARG:NH2	2.24	0.53
1:A:229:GLU:HG2	1:A:235:ASN:HD22	1.73	0.53
1:B:505:TRP:CD2	1:B:516:ASP:HA	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:543:ILE:O	1:B:555:LYS:HA	2.09	0.53
1:B:275:LEU:N	1:B:275:LEU:HD23	2.24	0.52
1:A:112:PRO:HB2	1:A:135:ILE:HD13	1.91	0.52
1:A:358:GLY:HA3	1:A:615:ILE:CG2	2.39	0.52
1:B:465:ARG:HG3	1:B:474:ARG:HH21	1.75	0.52
1:B:53:MET:HE2	1:B:53:MET:HA	1.91	0.52
1:B:112:PRO:HB2	1:B:135:ILE:HD13	1.91	0.52
1:B:28:SER:HB2	1:B:57:TRP:O	2.09	0.52
1:A:28:SER:H	1:A:152:HIS:CD2	2.27	0.51
1:A:53:MET:SD	1:A:65:ARG:HA	2.49	0.51
1:B:59:CYS:SG	5:B:7235:HOH:O	2.43	0.51
1:A:257:GLU:OE2	1:A:618:LYS:HB3	2.10	0.51
1:A:498:LYS:HB2	1:A:535:ILE:HA	1.92	0.51
1:A:474:ARG:CZ	1:A:476:ILE:HD11	2.42	0.50
1:A:436:ASN:HD22	1:A:437:CYS:N	2.09	0.50
1:B:215:ARG:NE	5:B:7266:HOH:O	2.43	0.50
1:A:462:VAL:HB	5:A:7513:HOH:O	2.10	0.50
1:A:505:TRP:CD2	1:A:516:ASP:HA	2.47	0.50
1:B:481:ARG:NH1	1:B:483:GLU:OE1	2.45	0.50
1:B:521:VAL:HG11	1:B:530:TYR:CE2	2.46	0.50
1:A:141:ASN:HD22	1:A:141:ASN:N	2.06	0.50
1:A:62:PHE:HB2	1:A:148:GLN:HB2	1.94	0.50
1:B:522:ASN:HD22	1:B:522:ASN:C	2.19	0.49
1:B:268:ASN:ND2	1:B:592:TYR:H	2.05	0.49
1:A:95:ASN:ND2	1:A:97:ASN:H	2.11	0.49
1:A:458:GLU:CG	5:A:7530:HOH:O	2.52	0.49
1:B:89:PHE:HB2	1:B:99:LEU:O	2.12	0.49
1:B:10:ALA:N	5:B:7232:HOH:O	2.46	0.49
1:A:608:GLU:H	1:A:608:GLU:CD	2.20	0.49
1:A:314:THR:OG1	1:A:339:HIS:HE1	1.95	0.49
1:A:92:GLU:HB3	1:A:95:ASN:HD21	1.78	0.49
1:A:95:ASN:HD22	1:A:96:ASP:N	2.10	0.49
1:B:89:PHE:C	1:B:89:PHE:HD1	2.21	0.49
1:B:119:ILE:HD13	1:B:132:VAL:HG23	1.95	0.49
1:A:221:GLN:OE1	1:A:221:GLN:N	2.44	0.49
1:A:113:VAL:CG2	1:A:114:ALA:N	2.76	0.48
1:A:553:LEU:O	1:A:554:ASP:HB2	2.11	0.48
1:B:418:GLU:HG3	1:B:430:GLY:N	2.28	0.48
1:A:427:LEU:HD21	1:A:478:VAL:HG13	1.95	0.48
1:A:80:MET:SD	1:A:129:THR:HA	2.54	0.48
1:B:522:ASN:ND2	1:B:524:GLU:H	2.10	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:GLY:O	1:B:127:LYS:HE2	2.13	0.48
1:B:522:ASN:ND2	1:B:524:GLU:N	2.61	0.48
1:A:436:ASN:C	1:A:436:ASN:ND2	2.71	0.48
1:A:468:HIS:CG	1:A:469:PRO:HD2	2.48	0.48
1:A:210:LYS:NZ	1:A:323:GLU:CG	2.71	0.48
1:B:92:GLU:HB3	1:B:97:ASN:HB3	1.94	0.48
1:B:233:LEU:HD11	1:B:398:PHE:HA	1.96	0.48
1:B:427:LEU:HD22	1:B:481:ARG:HD2	1.95	0.48
1:A:618:LYS:HE2	5:A:7420:HOH:O	2.14	0.47
1:B:573:LEU:HD22	1:B:581:ILE:O	2.14	0.47
1:A:96:ASP:O	1:A:276:HIS:HD2	1.97	0.47
1:A:107:GLY:HA2	1:A:174:TYR:O	2.15	0.47
1:A:294:PRO:HD3	1:A:452:ARG:NH1	2.30	0.47
1:A:457:ARG:HH11	1:A:457:ARG:CG	2.27	0.47
1:B:431:GLU:HG3	1:B:431:GLU:O	2.15	0.47
1:B:468:HIS:CE1	1:B:470:GLN:HB2	2.49	0.47
1:A:210:LYS:HZ2	1:A:323:GLU:N	2.08	0.47
1:A:511:HIS:HE1	1:A:513:TYR:CD2	2.32	0.47
1:B:229:GLU:HG2	1:B:235:ASN:OD1	2.14	0.47
1:B:104:PHE:O	1:B:187:GLY:HA3	2.14	0.47
1:B:121:ASP:HB2	1:B:186:LEU:HD21	1.97	0.47
1:A:181:ASP:OD1	1:A:181:ASP:C	2.58	0.47
1:A:608:GLU:O	1:A:609:SER:C	2.58	0.47
1:B:465:ARG:NH2	1:B:472:GLU:O	2.32	0.47
1:B:56:LYS:HB3	1:B:57:TRP:CD1	2.50	0.46
1:A:56:LYS:HA	1:A:57:TRP:HA	1.74	0.46
1:A:390:ILE:HD12	1:A:391:GLU:N	2.30	0.46
1:A:416:LEU:HD11	1:A:475:LEU:N	2.30	0.46
1:B:12:PHE:CE1	1:B:30:TYR:CE1	3.03	0.46
1:A:422:ASP:OD2	1:A:426:GLN:HB2	2.16	0.46
1:B:429:ASP:OD1	1:B:429:ASP:C	2.57	0.46
1:A:601:GLU:HG2	5:A:7318:HOH:O	2.16	0.46
1:B:418:GLU:HG3	1:B:430:GLY:H	1.80	0.46
1:A:580:TYR:O	1:A:599:GLY:HA2	2.14	0.46
1:B:254:THR:HA	1:B:615:ILE:O	2.15	0.46
1:B:555:LYS:HE3	1:B:555:LYS:HB2	1.68	0.46
1:A:390:ILE:HD12	1:A:391:GLU:HG3	1.97	0.46
1:A:618:LYS:HG2	5:A:7374:HOH:O	2.15	0.46
1:A:582:GLN:NE2	3:A:3001:ADP:O3'	2.39	0.46
1:A:138:LEU:HD13	1:A:143:VAL:CG1	2.46	0.45
1:A:301:LEU:CD2	1:A:490:LEU:HG	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:MET:HE2	1:A:53:MET:HA	1.98	0.45
1:A:361:PRO:HG3	1:A:614:LEU:HD23	1.99	0.45
1:A:418:GLU:O	1:A:418:GLU:HG3	2.15	0.45
1:A:121:ASP:OD2	1:A:122:LYS:N	2.49	0.45
1:A:216:LEU:HD11	1:A:349:TRP:CZ2	2.52	0.45
1:A:302:ARG:NH1	5:A:7133:HOH:O	2.42	0.45
1:A:20:PRO:HD3	1:A:160:GLN:O	2.16	0.45
1:A:328:VAL:O	1:A:328:VAL:HG13	2.17	0.45
1:A:480:LEU:HD23	1:A:480:LEU:HA	1.83	0.45
1:A:507:LEU:C	1:A:509:PRO:HD3	2.41	0.45
1:A:572:CYS:HB3	1:A:603:LEU:CD2	2.46	0.45
1:B:119:ILE:CD1	1:B:132:VAL:HG23	2.46	0.45
4:B:5002:GSH:N1	5:B:7613:HOH:O	2.36	0.45
1:A:566:ILE:C	1:A:566:ILE:HD12	2.42	0.45
1:A:291:PHE:CD1	1:A:291:PHE:N	2.85	0.44
1:A:354:TYR:CZ	1:A:356:GLY:HA3	2.52	0.44
1:A:29:ASP:OD1	1:A:31:SER:OG	2.34	0.44
1:A:122:LYS:HB2	1:A:127:LYS:O	2.17	0.44
1:B:521:VAL:CG1	1:B:530:TYR:CE2	3.00	0.44
1:B:48:ILE:O	1:B:49:ASP:HB2	2.17	0.44
1:A:114:ALA:HA	1:A:135:ILE:HG22	2.00	0.44
1:A:257:GLU:CD	1:A:618:LYS:HB3	2.43	0.44
1:B:94:VAL:HG13	5:B:7088:HOH:O	2.16	0.44
1:A:552:VAL:HG11	1:A:555:LYS:HE3	2.00	0.44
1:B:499:ALA:O	1:B:502:PRO:HD2	2.18	0.44
1:B:18:TYR:O	1:B:160:GLN:HA	2.18	0.43
1:A:18:TYR:HB2	1:B:466:THR:HG21	1.99	0.43
1:A:544:ASP:OD1	1:A:555:LYS:HG2	2.19	0.43
1:B:122:LYS:HB2	1:B:127:LYS:O	2.18	0.43
1:B:297:LEU:HD11	1:B:451:ILE:HD12	2.00	0.43
1:A:416:LEU:CD1	1:A:475:LEU:N	2.81	0.43
1:B:522:ASN:HD22	1:B:524:GLU:N	2.17	0.43
1:B:56:LYS:HA	1:B:57:TRP:HA	1.67	0.43
1:B:121:ASP:HB2	1:B:186:LEU:CD2	2.49	0.43
1:A:418:GLU:HG3	1:A:430:GLY:N	2.34	0.43
1:B:585:THR:HA	1:B:594:GLY:O	2.18	0.43
1:A:268:ASN:ND2	1:A:592:TYR:H	2.10	0.43
1:A:539:CYS:SG	5:A:7301:HOH:O	2.50	0.43
1:B:358:GLY:HA3	1:B:615:ILE:CG2	2.49	0.43
1:B:471:ASN:HD22	1:B:471:ASN:HA	1.40	0.43
1:B:505:TRP:CH2	1:B:510:HIS:HA	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ASN:C	1:A:95:ASN:ND2	2.66	0.43
1:A:119:ILE:HD13	1:A:132:VAL:HG23	2.01	0.43
1:A:138:LEU:HD11	1:A:167:MET:CE	2.49	0.43
1:A:476:ILE:HG13	1:A:477:ASP:N	2.33	0.43
1:A:524:GLU:HB2	5:A:7279:HOH:O	2.18	0.43
1:B:468:HIS:HE1	1:B:470:GLN:HB2	1.83	0.43
1:A:137:GLN:CG	1:A:144:ARG:HB2	2.45	0.43
1:A:140:GLY:HA2	5:A:7622:HOH:O	2.19	0.42
1:A:157:GLN:CD	1:A:157:GLN:N	2.65	0.42
1:A:227:LEU:HB2	1:A:243:GLN:OE1	2.18	0.42
1:A:48:ILE:O	1:A:49:ASP:HB2	2.19	0.42
1:B:538:ARG:HA	3:B:3002:ADP:O2B	2.19	0.42
1:A:229:GLU:OE1	1:A:235:ASN:ND2	2.51	0.42
1:A:298:TRP:HB2	1:A:299:PRO:HD3	2.01	0.42
1:B:420:GLY:O	1:B:428:ILE:HG12	2.20	0.42
1:B:556:THR:HG21	1:B:606:LYS:HE3	2.00	0.42
1:A:499:ALA:O	1:A:502:PRO:HD2	2.18	0.42
1:A:137:GLN:NE2	1:A:144:ARG:CD	2.79	0.42
1:B:97:ASN:O	1:B:98:ILE:HD13	2.19	0.42
1:B:105:PRO:HD3	1:B:199:LEU:HG	2.02	0.42
1:A:281:VAL:HG22	1:A:503:ILE:HD13	2.01	0.42
1:A:363:GLU:HG3	5:A:7413:HOH:O	2.20	0.42
1:A:386:GLN:HA	1:A:441:THR:OG1	2.20	0.42
1:B:433:ARG:NH2	5:B:7050:HOH:O	2.49	0.42
1:A:300:ARG:HH11	1:A:300:ARG:HB3	1.85	0.42
1:A:598:ARG:HD2	1:A:611:ILE:HD12	2.02	0.42
1:B:597:LEU:HD11	1:B:614:LEU:HD13	2.02	0.42
1:A:64:ARG:CG	1:A:74:VAL:CG2	2.98	0.42
1:B:524:GLU:O	1:B:527:LYS:HG3	2.20	0.42
1:A:322:ASP:OD2	1:A:322:ASP:C	2.63	0.41
1:A:374:LYS:HG3	1:A:406:ALA:HB1	2.01	0.41
1:B:608:GLU:CD	1:B:608:GLU:H	2.28	0.41
1:A:421:TRP:HA	1:A:426:GLN:O	2.20	0.41
1:B:413:LEU:CD1	1:B:419:LEU:HD21	2.45	0.41
1:A:243:GLN:C	1:A:244:VAL:HG23	2.45	0.41
1:A:454:VAL:C	1:A:456:ASP:H	2.23	0.41
1:A:483:GLU:CD	1:A:483:GLU:N	2.69	0.41
1:B:105:PRO:O	1:B:108:SER:HB2	2.20	0.41
1:B:390:ILE:CD1	1:B:390:ILE:H	2.32	0.41
1:A:64:ARG:HG3	1:A:74:VAL:CG2	2.50	0.41
1:A:95:ASN:HD22	1:A:97:ASN:H	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:568:GLN:O	1:B:569:GLN:C	2.63	0.41
1:A:201:GLN:O	1:A:202:PRO:C	2.61	0.41
1:A:317:MET:O	1:A:584:CYS:HA	2.21	0.41
1:A:422:ASP:OD1	1:A:422:ASP:C	2.63	0.41
1:B:275:LEU:HB3	1:B:305:TRP:HH2	1.84	0.41
1:A:19:ALA:HB1	1:A:20:PRO:HD2	2.02	0.41
1:A:55:HIS:HB3	1:A:58:GLN:HG3	2.02	0.41
1:A:581:ILE:CG2	1:A:597:LEU:HD22	2.50	0.41
1:B:251:HIS:CE1	1:B:577:ASP:OD2	2.63	0.41
1:B:501:LEU:HA	1:B:501:LEU:HD23	1.90	0.41
1:A:95:ASN:ND2	1:A:95:ASN:H	2.18	0.41
1:A:112:PRO:O	1:A:138:LEU:HD22	2.20	0.41
1:B:121:ASP:HB2	1:B:186:LEU:HG	2.03	0.41
1:A:219:LYS:O	1:A:219:LYS:CG	2.68	0.41
1:A:301:LEU:HD13	1:A:494:ILE:HD11	2.02	0.41
1:A:447:ALA:HB1	1:A:476:ILE:CG2	2.45	0.41
1:B:426:GLN:NE2	5:B:7557:HOH:O	2.34	0.41
1:B:547:SER:OG	1:B:551:GLU:HG2	2.21	0.41
1:B:377:ARG:NH2	1:B:377:ARG:HG3	2.35	0.41
1:B:522:ASN:HD22	1:B:524:GLU:H	1.66	0.41
1:A:337:SER:O	1:A:338:CYS:CB	2.69	0.40
1:B:451:ILE:HG13	1:B:476:ILE:CD1	2.52	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	576/619 (93%)	550 (96%)	24 (4%)	2 (0%)	36	42
1	B	599/619 (97%)	577 (96%)	21 (4%)	1 (0%)	43	51
All	All	1175/1238 (95%)	1127 (96%)	45 (4%)	3 (0%)	36	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	LYS
1	A	455	SER
1	B	127	LYS

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	513/530 (97%)	486 (95%)	27 (5%)	20	26
1	B	515/530 (97%)	493 (96%)	22 (4%)	26	35
All	All	1028/1060 (97%)	979 (95%)	49 (5%)	23	30

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	VAL
1	A	58	GLN
1	A	74	VAL
1	A	91	ARG
1	A	95	ASN
1	A	141	ASN
1	A	156	PRO
1	A	164	GLU
1	A	173	CYS
1	A	233	LEU
1	A	245	ILE
1	A	275	LEU
1	A	300	ARG
1	A	355	LYS
1	A	379	ARG
1	A	390	ILE
1	A	418	GLU
1	A	436	ASN
1	A	457	ARG
1	A	459	PHE

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Mol	Chain	Res	Type
1	A	470	GLN
1	A	471	ASN
1	A	483	GLU
1	A	523	ASP
1	A	524	GLU
1	A	602	SER
1	A	608	GLU
1	B	32	SER
1	B	76	THR
1	B	127	LYS
1	B	137	GLN
1	B	148	GLN
1	B	229	GLU
1	B	233	LEU
1	B	261	GLN
1	B	272	LEU
1	B	275	LEU
1	B	300	ARG
1	B	308	ARG
1	B	352	GLN
1	B	377	ARG
1	B	379	ARG
1	B	390	ILE
1	B	391	GLU
1	B	417	ASP
1	B	438	VAL
1	B	466	THR
1	B	471	ASN
1	B	522	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	95	ASN
1	A	131	HIS
1	A	137	GLN
1	A	139	HIS
1	A	141	ASN
1	A	149	ASN
1	A	201	GLN
1	A	235	ASN

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Mol	Chain	Res	Type
1	A	241	ASN
1	A	268	ASN
1	A	276	HIS
1	A	339	HIS
1	A	352	GLN
1	A	395	HIS
1	A	397	GLN
1	A	405	GLN
1	A	436	ASN
1	A	470	GLN
1	A	471	ASN
1	A	563	GLN
1	A	565	ASN
1	A	568	GLN
1	A	591	ASN
1	B	70	ASN
1	B	102	GLN
1	B	131	HIS
1	B	171	ASN
1	B	191	GLN
1	B	201	GLN
1	B	247	GLN
1	B	251	HIS
1	B	268	ASN
1	B	286	ASN
1	B	339	HIS
1	B	352	GLN
1	B	357	ASN
1	B	367	ASN
1	B	375	HIS
1	B	426	GLN
1	B	471	ASN
1	B	510	HIS
1	B	522	ASN
1	B	563	GLN
1	B	565	ASN
1	B	568	GLN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 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$
3	ADP	A	3001	2	28,29,29	1.24	2 (7%)	43,45,45	1.15	2 (4%)
4	GSH	A	5001	1	17,18,19	1.75	5 (29%)	19,22,24	1.61	4 (21%)
4	GSH	B	5002	1	17,18,19	1.70	4 (23%)	19,22,24	1.56	3 (15%)
3	ADP	B	3002	2	28,29,29	1.42	4 (14%)	43,45,45	1.13	2 (4%)

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
3	ADP	A	3001	2	-	3/16/32/32	0/3/3/3
4	GSH	A	5001	1	-	3/23/23/24	-
4	GSH	B	5002	1	-	3/23/23/24	-
3	ADP	B	3002	2	-	4/16/32/32	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	5002	GSH	O31-C3	-4.23	1.20	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3001	ADP	C2-N1	3.99	1.41	1.33
4	A	5001	GSH	O31-C3	-3.76	1.22	1.42
4	A	5001	GSH	O12-C1	3.37	1.32	1.22
4	B	5002	GSH	O12-C1	3.32	1.31	1.22
3	B	3002	ADP	PA-O3A	-3.25	1.56	1.59
3	A	3001	ADP	C5-C6	3.20	1.49	1.41
3	B	3002	ADP	C2-N1	3.17	1.39	1.33
3	B	3002	ADP	C5-N7	-2.82	1.33	1.39
4	B	5002	GSH	O11-C1	-2.60	1.22	1.30
4	A	5001	GSH	CB1-CA1	2.60	1.58	1.53
4	A	5001	GSH	O11-C1	-2.35	1.23	1.30
4	B	5002	GSH	CA2-N2	2.24	1.50	1.45
4	A	5001	GSH	CB2-SG2	-2.23	1.76	1.81
3	B	3002	ADP	C6-N6	-2.07	1.28	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	5002	GSH	CA2-CB2-SG2	-3.88	109.79	114.16
4	A	5001	GSH	CA2-CB2-SG2	-3.73	109.95	114.16
3	B	3002	ADP	N3-C2-N1	-3.55	123.21	128.58
3	A	3001	ADP	N3-C2-N1	-3.15	123.81	128.58
3	A	3001	ADP	C2-N1-C6	2.83	123.38	118.73
3	B	3002	ADP	C2-N1-C6	2.80	123.33	118.73
4	B	5002	GSH	CG1-CD1-N2	2.35	120.00	115.86
4	A	5001	GSH	O31-C3-CA3	2.24	119.75	111.50
4	A	5001	GSH	CG1-CD1-N2	2.18	119.70	115.86
4	A	5001	GSH	C3-CA3-N3	-2.14	106.56	111.60
4	B	5002	GSH	O31-C3-CA3	2.04	119.01	111.50

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	3001	ADP	PA-O3A-PB-O3B
3	B	3002	ADP	PA-O3A-PB-O3B
4	B	5002	GSH	O31-C3-CA3-N3
4	A	5001	GSH	O31-C3-CA3-N3
4	B	5002	GSH	C1-CA1-CB1-CG1
4	A	5001	GSH	C2-CA2-CB2-SG2
4	B	5002	GSH	C2-CA2-CB2-SG2
3	A	3001	ADP	PA-O3A-PB-O2B

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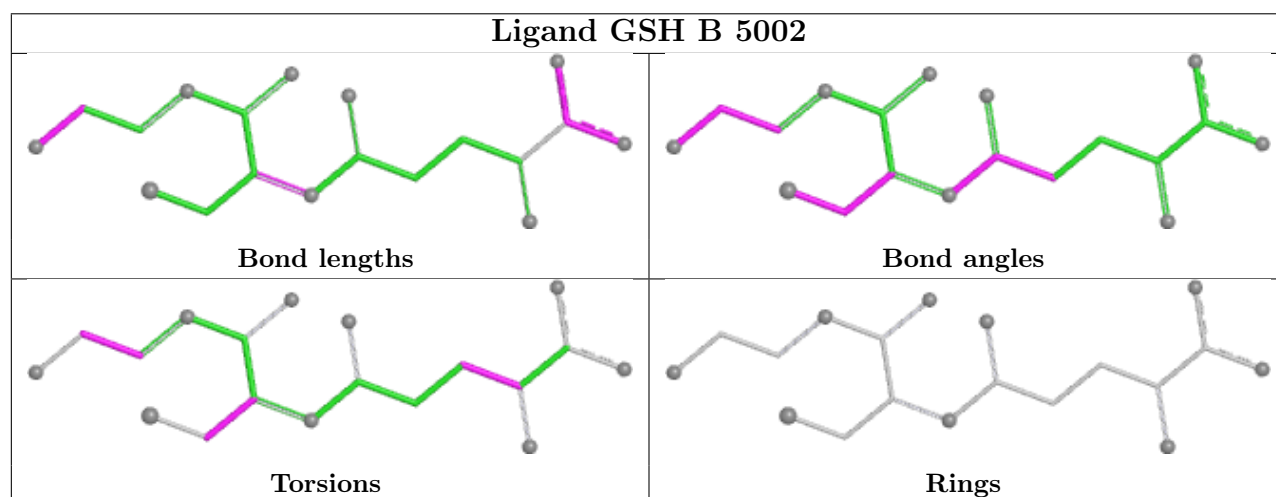
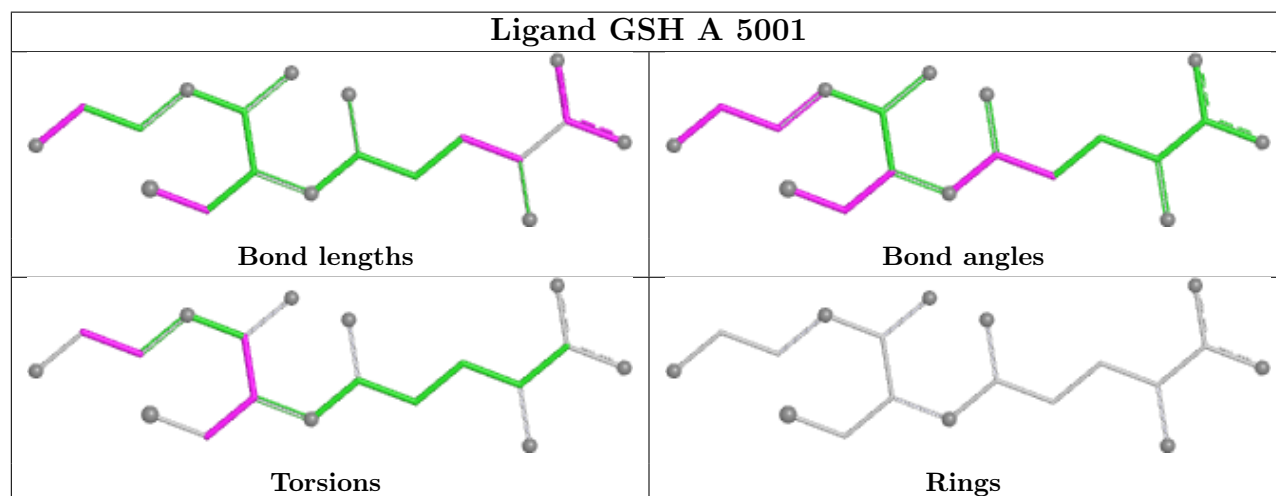
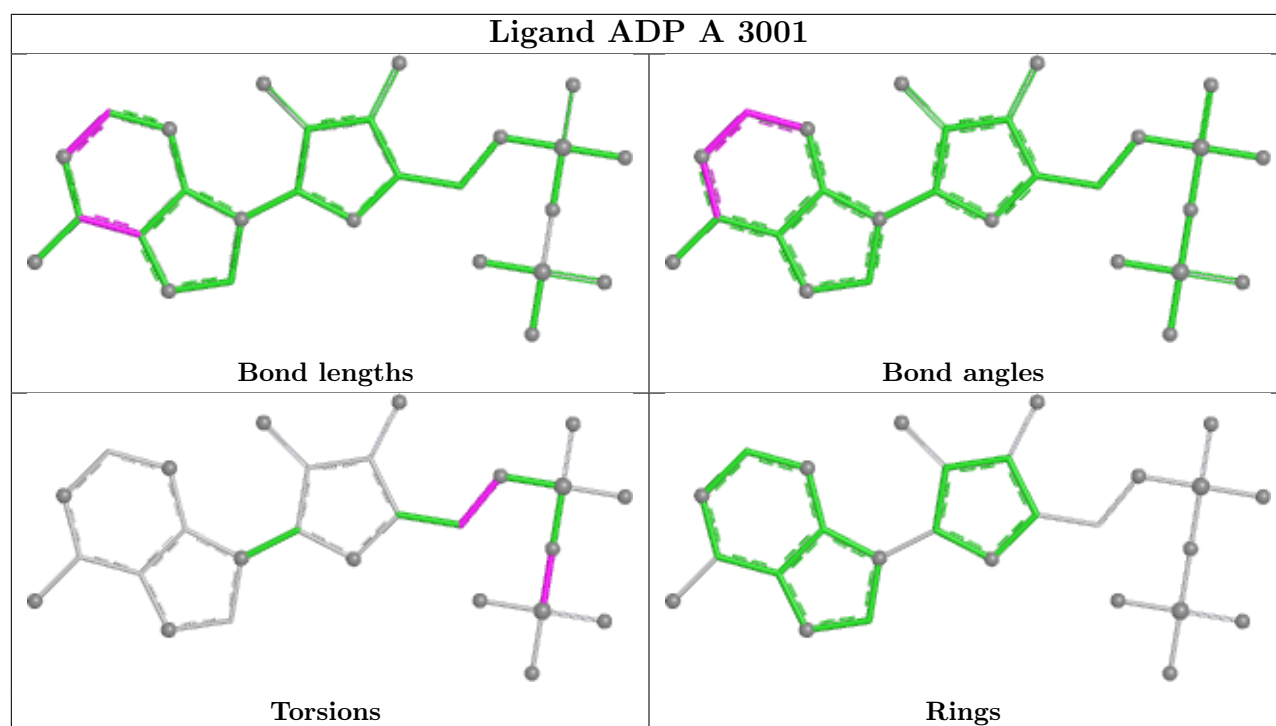
Mol	Chain	Res	Type	Atoms
3	B	3002	ADP	PA-O3A-PB-O2B
4	A	5001	GSH	O2-C2-CA2-N2
3	B	3002	ADP	C4'-C5'-O5'-PA
3	A	3001	ADP	C4'-C5'-O5'-PA
3	B	3002	ADP	PB-O3A-PA-O2A

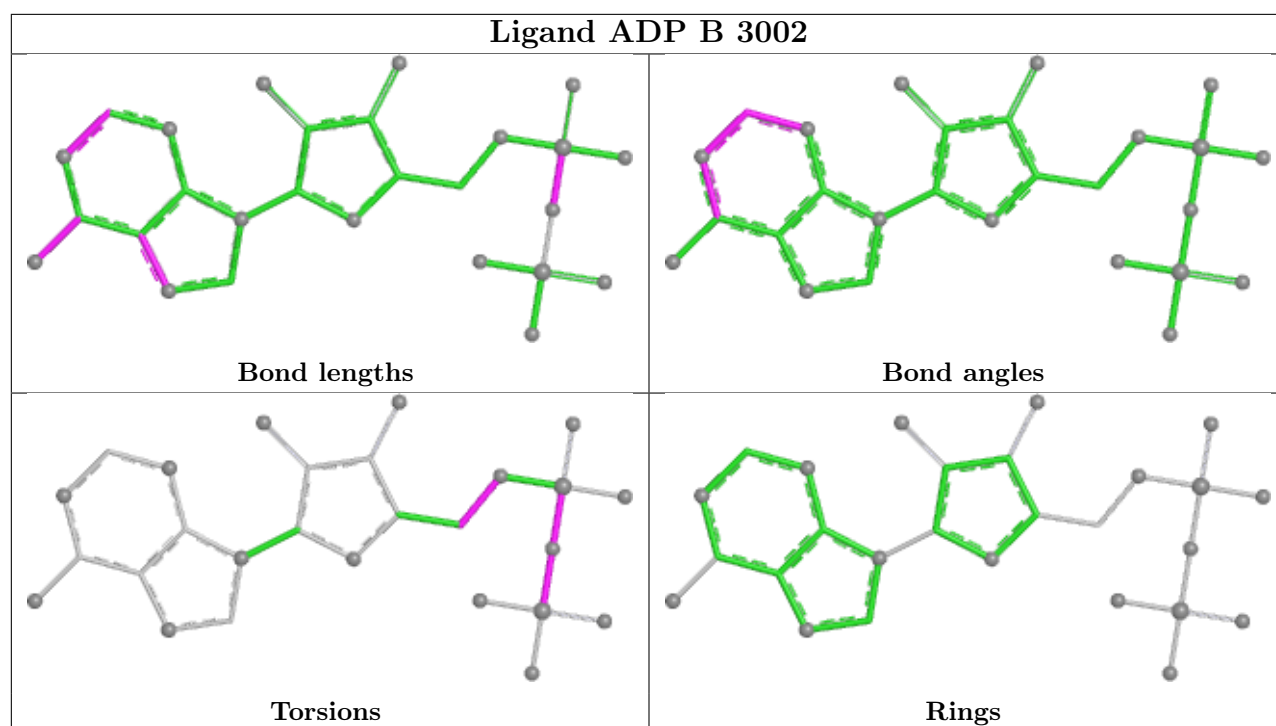
There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3001	ADP	2	0
4	A	5001	GSH	2	0
4	B	5002	GSH	2	0
3	B	3002	ADP	2	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	601/619 (97%)	-0.49	1 (0%)	91 90	14, 28, 52, 80	0
1	B	603/619 (97%)	-0.43	4 (0%)	84 82	15, 29, 53, 81	0
All	All	1204/1238 (97%)	-0.46	5 (0%)	88 87	14, 29, 53, 81	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	33	LEU	3.5
1	B	30	TYR	2.8
1	A	89	PHE	2.5
1	B	390	ILE	2.3
1	B	31	SER	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

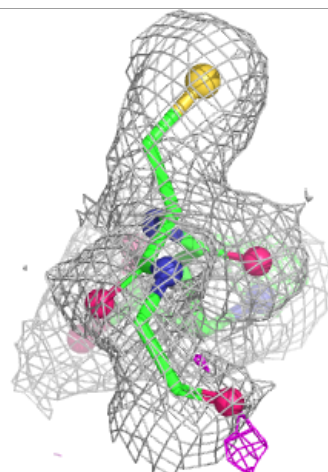
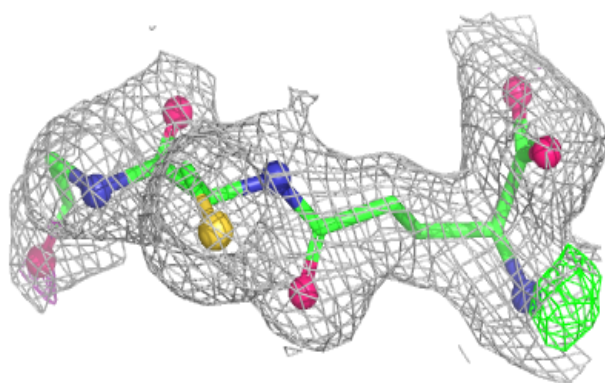
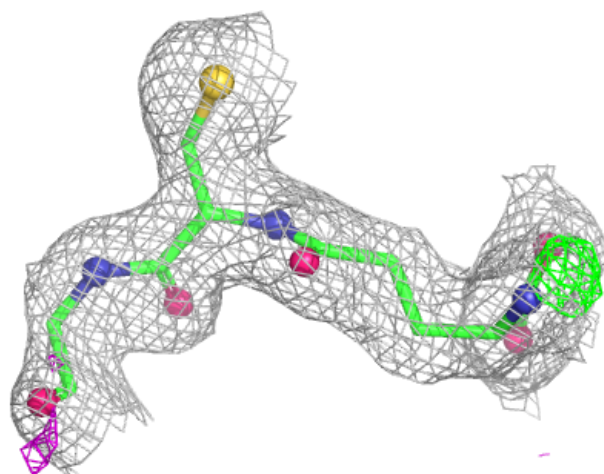
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GSH	A	5001	19/20	0.95	0.07	24,27,40,43	0
4	GSH	B	5002	19/20	0.95	0.08	28,31,43,46	0
2	MG	B	7003	1/1	0.98	0.02	21,21,21,21	0
3	ADP	A	3001	27/27	0.99	0.04	14,19,24,25	0
3	ADP	B	3002	27/27	0.99	0.04	17,22,25,26	0
2	MG	A	7001	1/1	0.99	0.03	19,19,19,19	0
2	MG	B	7004	1/1	0.99	0.02	21,21,21,21	0
2	MG	A	7002	1/1	1.00	0.01	17,17,17,17	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

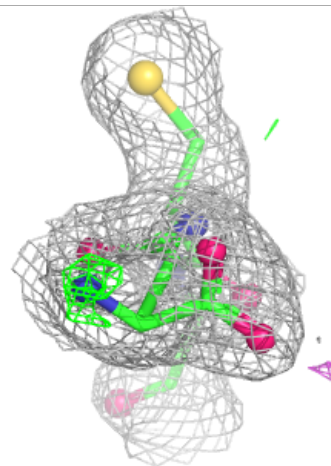
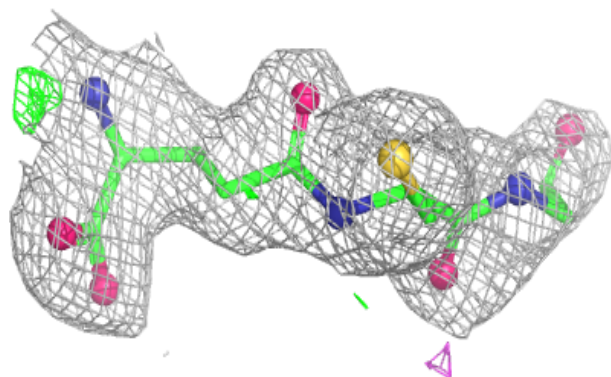
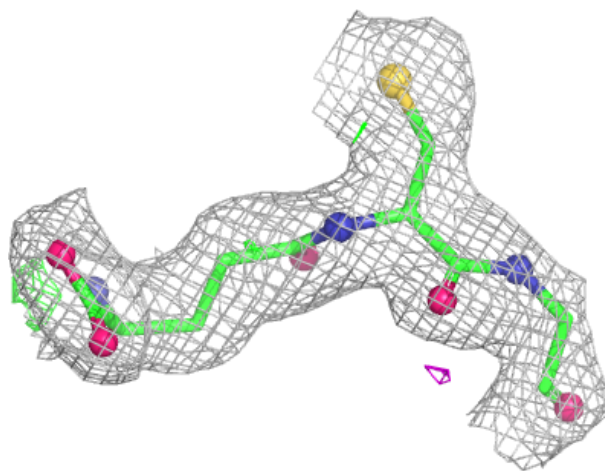
Electron density around GSH A 5001:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



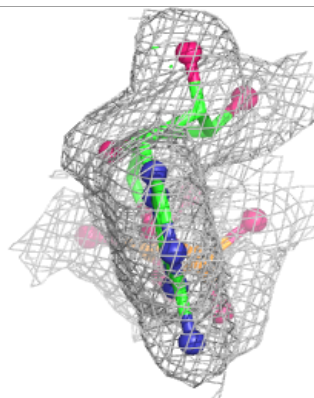
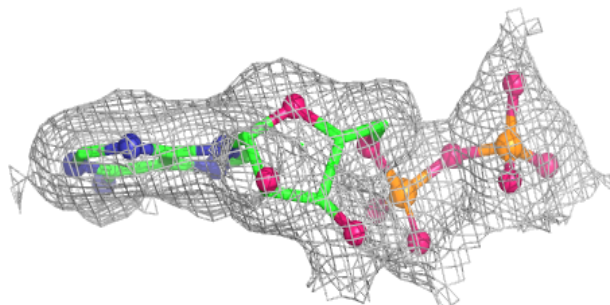
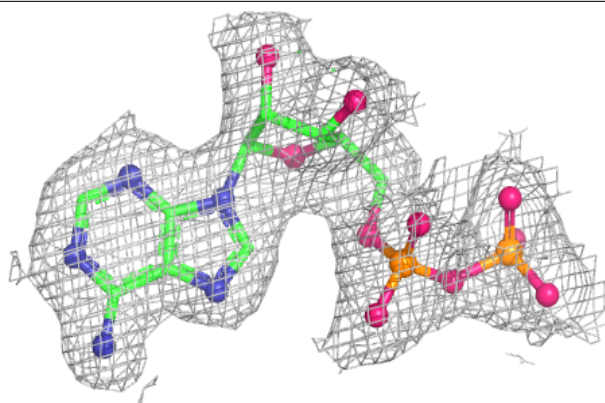
Electron density around GSH B 5002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

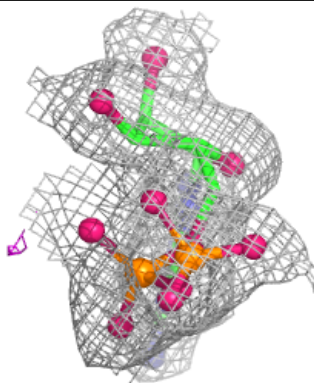
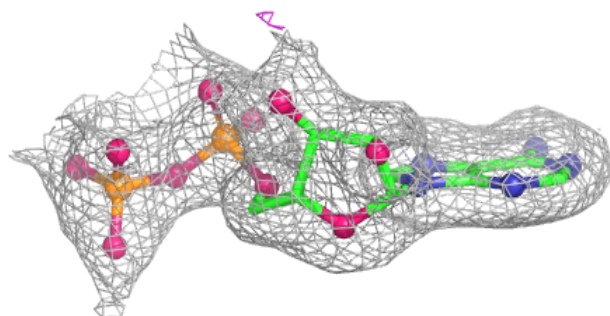
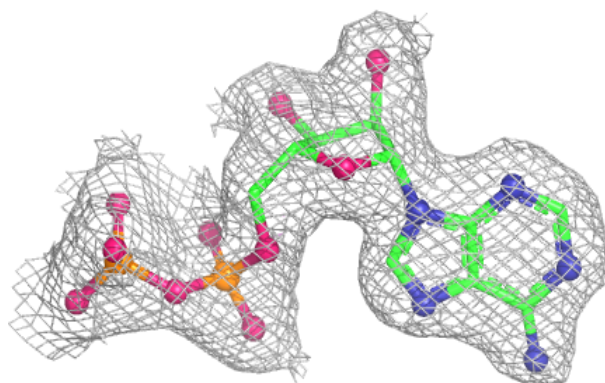


Electron density around ADP A 3001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ADP B 3002:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.