



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 06:16 am BST

PDB ID : 2IO9
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

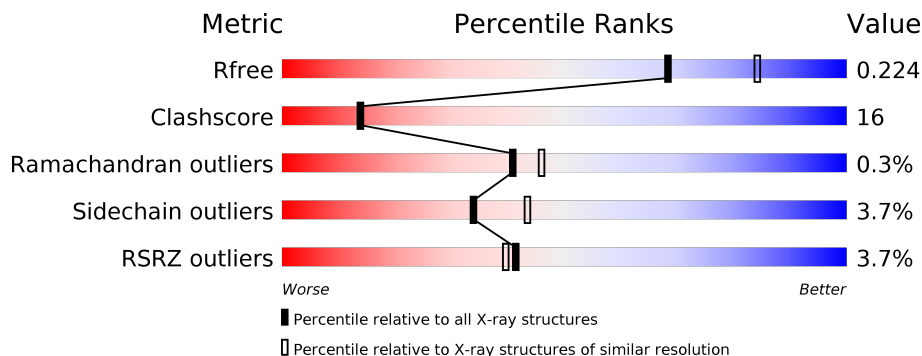
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 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	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 65%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 29%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">3% 65% 29% . .</p>
1	B	619	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 71%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 24%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">4% 71% 24% . .</p>

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.

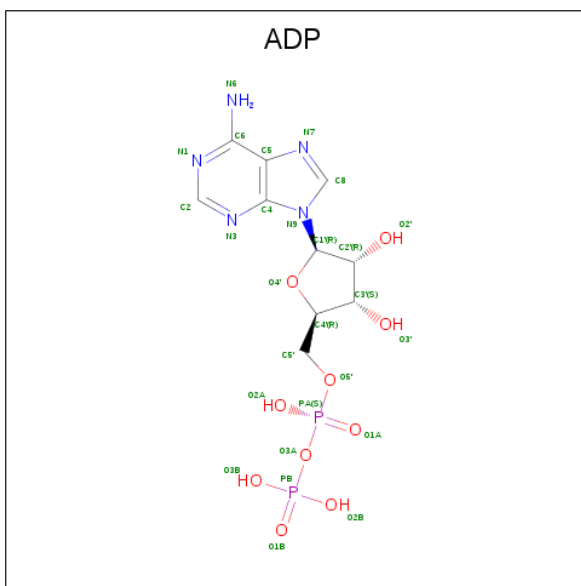
- Molecule 1 is a protein called Bifunctional glutathionylspermidine synthetase/amidase.

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

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

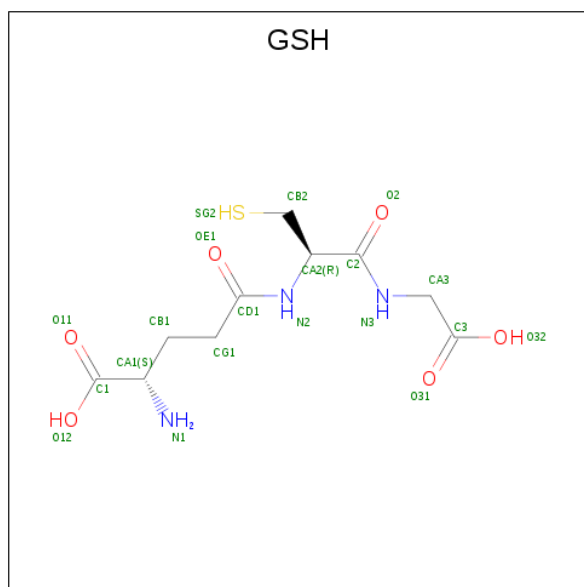
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total 2	Mg 2	0	0
2	A	2	Total 2	Mg 2	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
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 (three-letter code: GSH) (formula: $C_{10}H_{17}N_3O_6S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
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		

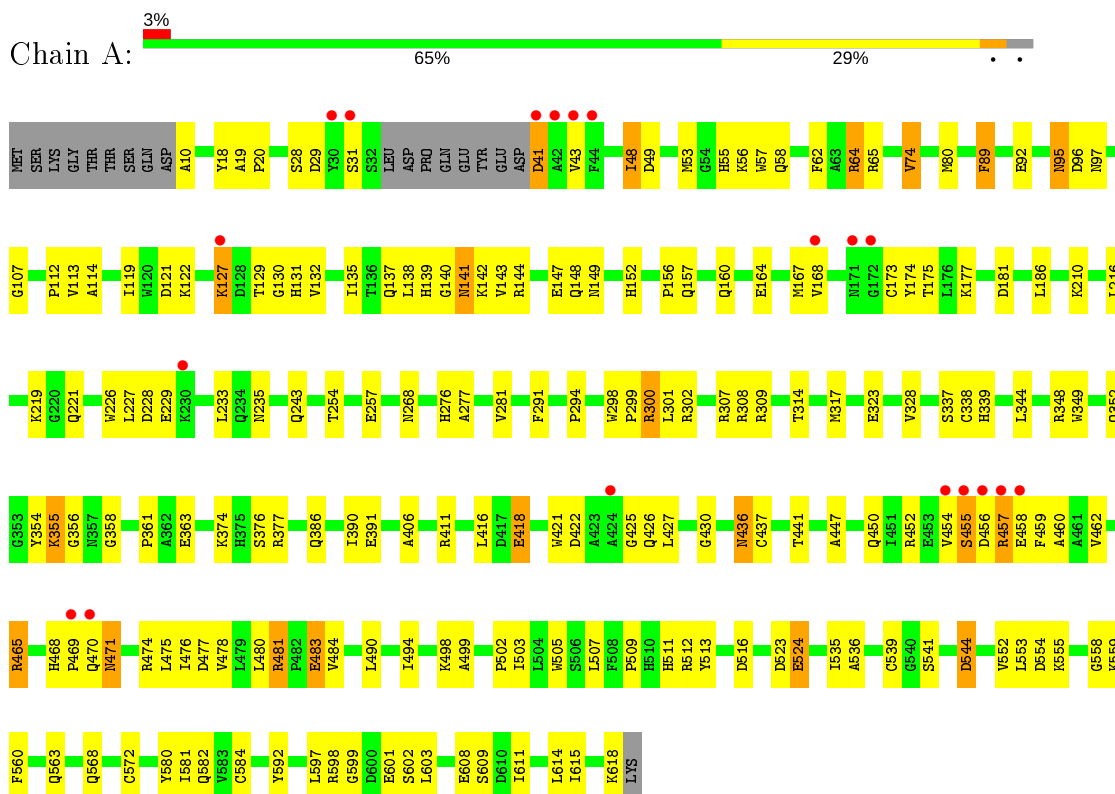
- Molecule 5 is water.

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

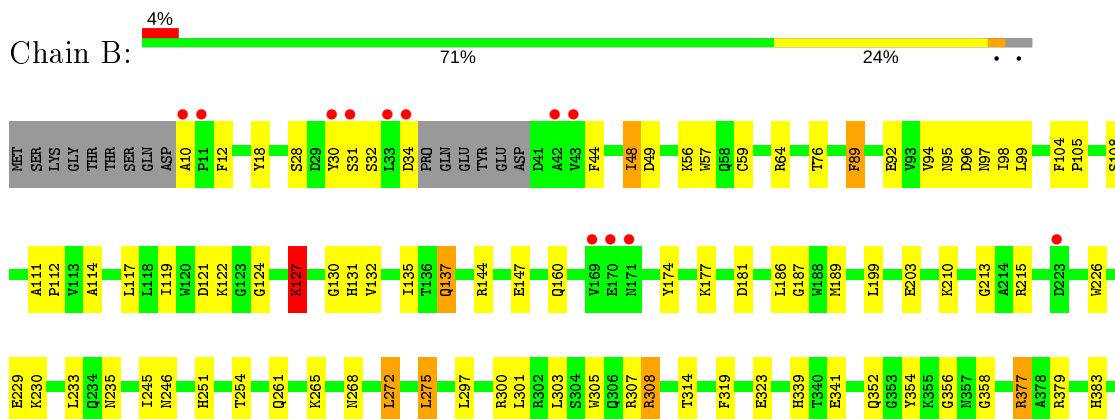
3 Residue-property plots [i](#)

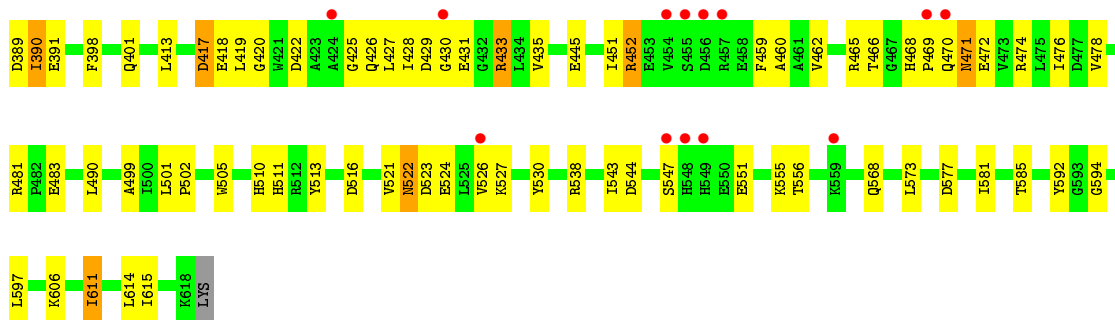
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 29.39 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.20) 91.5 (29.39-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.94 (at 2.20Å)	Xtrriage
Refinement program	CNS, XTALVIEW	Depositor
R, R_{free}	0.170 , 0.232 0.161 , 0.224	Depositor DCC
R_{free} test set	3102 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	27.8	Xtrriage
Anisotropy	0.354	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 68.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: GSH, MG, 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	1/4960 (0.0%)	0.95	10/6736 (0.1%)
1	B	0.86	0/4976	0.93	10/6758 (0.1%)
All	All	0.88	1/9936 (0.0%)	0.94	20/13494 (0.1%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	89	PHE	CD2-CE2	5.05	1.49	1.39

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	308	ARG	NE-CZ-NH2	-8.82	115.89	120.30
1	A	481	ARG	NE-CZ-NH2	-8.13	116.24	120.30
1	A	308	ARG	NE-CZ-NH1	7.25	123.93	120.30
1	A	512	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	A	48	ILE	N-CA-C	-6.51	93.42	111.00
1	B	48	ILE	N-CA-C	-6.19	94.29	111.00
1	B	300	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	B	64	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	B	452	ARG	NE-CZ-NH1	5.91	123.26	120.30
1	A	544	ASP	CB-CG-OD1	5.86	123.58	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	452	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	A	465	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	B	433	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	B	611	ILE	N-CA-C	-5.35	96.56	111.00
1	A	130	GLY	N-CA-C	-5.34	99.76	113.10
1	B	181	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	64	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	B	130	GLY	N-CA-C	-5.29	99.88	113.10
1	A	309	ARG	NE-CZ-NH1	-5.16	117.72	120.30
1	B	272	LEU	CB-CG-CD1	-5.10	102.32	111.00

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	176	0
1	B	4852	0	4718	129	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	305	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 16.

All (305) 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: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
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:157:GLN:CD	1:A:157:GLN:H	1.86	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: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: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:95:ASN:HD22	1:A:95:ASN:C	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:LYS:CD	1:A:323:GLU:HB3	2.17	0.68
1:A:483:GLU:CD	1:A:483:GLU:H	1.97	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:HB3	1:A:457:ARG:HH11	1.62	0.65
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:HG2	1:A:219:LYS:O	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:457:ARG:CB	1:A:457:ARG:HH11	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:B:390:ILE:N	1:B:390:ILE:CD1	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: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:28:SER:HB3	1:A:57:TRP:HB2	1.85	0.58
1:A:300:ARG:HG2	5:A:7159:HOH:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:465:ARG:HG3	1:B:474:ARG:NH2	2.20	0.57
1:B:427:LEU:HD21	1:B:478:VAL:HG13	1.87	0.57
1:B:44:PHE:O	1:B:56:LYS:HG3	2.05	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:A:411:ARG:HH21	1:A:418:GLU:CD	2.07	0.56
1:B:390:ILE:HD13	1:B:390:ILE:N	2.21	0.56
1:A:536:ALA:H	1:A:563:GLN:HE22	1.54	0.56
1:A:436:ASN:HD22	1:A:436:ASN:C	2.10	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:460:ALA:HB2	1:B:114:ALA:HB1	1.87	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:568:GLN:HE21	3:B:3002:ADP:HN61	1.54	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:543:ILE:O	1:B:555:LYS:HA	2.09	0.53
1:B:275:LEU:HD23	1:B:275:LEU:N	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:112:PRO:HB2	1:B:135:ILE:HD13	1.91	0.52
1:B:89:PHE:C	1:B:89:PHE:CD1	2.82	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:522:ASN:C	1:B:522:ASN:ND2	2.64	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:268:ASN:ND2	1:B:592:TYR:H	2.05	0.49
1:A:458:GLU:CG	5:A:7530:HOH:O	2.52	0.49
1:A:95:ASN:ND2	1:A:97:ASN:H	2.11	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: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:119:ILE:HD13	1:B:132:VAL:HG23	1.95	0.49
1:A:221:GLN:N	1:A:221:GLN:OE1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:B:92:GLU:HB3	1:B:97:ASN:HB3	1.94	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:107:GLY:HA2	1:A:174:TYR:O	2.15	0.47
1:A:96:ASP:O	1:A:276:HIS:HD2	1.97	0.47
1:A:294:PRO:HD3	1:A:452:ARG:NH1	2.30	0.47
1:A:457:ARG:CG	1:A:457:ARG:HH11	2.27	0.47
1:B:431:GLU:O	1:B:431:GLU:HG3	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:A:95:ASN:C	1:A:95:ASN:ND2	2.66	0.47
1:B:121:ASP:HB2	1:B:186:LEU:HD21	1.97	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:LEU:CD2	1:A:490:LEU:HG	2.45	0.45
1:A:361:PRO:HG3	1:A:614:LEU:HD23	1.99	0.45
1:A:418:GLU:HG3	1:A:418:GLU:O	2.15	0.45
1:A:121:ASP:OD2	1:A:122:LYS:N	2.49	0.45
1:A:302:ARG:NH1	5:A:7133:HOH:O	2.42	0.45
1:A:216:LEU:HD11	1:A:349:TRP:CZ2	2.52	0.45
1:B:522:ASN:HD22	1:B:522:ASN:C	2.19	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: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:291:PHE:N	1:A:291:PHE:CD1	2.85	0.44
1:A:354:TYR:CZ	1:A:356:GLY:HA3	2.52	0.44
1:A:122:LYS:HB2	1:A:127:LYS:O	2.17	0.44
1:A:29:ASP:OD1	1:A:31:SER:OG	2.34	0.44
1:B:89:PHE:HD1	1:B:89:PHE:C	2.21	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: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:608:GLU:H	1:A:608:GLU:CD	2.20	0.43
1:A:544:ASP:OD1	1:A:555:LYS:HG2	2.19	0.43
1:A:18:TYR:HB2	1:B:466:THR:HG21	1.99	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:121:ASP:HB2	1:B:186:LEU:CD2	2.49	0.43
1:B:56:LYS:HA	1:B:57:TRP:HA	1.67	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:539:CYS:SG	5:A:7301:HOH:O	2.50	0.43
1:A:268:ASN:ND2	1:A:592:TYR:H	2.10	0.43
1:B:358:GLY:HA3	1:B:615:ILE:CG2	2.49	0.43
1:B:471:ASN:HA	1:B:471:ASN:HD22	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: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:436:ASN:ND2	1:A:436:ASN:C	2.71	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: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:105:PRO:HD3	1:B:199:LEU:HG	2.02	0.42
1:B:429:ASP:C	1:B:429:ASP:OD1	2.57	0.42
1:B:97:ASN:O	1:B:98:ILE:HD13	2.19	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:A:281:VAL:HG22	1:A:503:ILE:HD13	2.01	0.42
1:A:181:ASP:C	1:A:181:ASP:OD1	2.58	0.42
1:B:433:ARG:NH2	5:B:7050:HOH:O	2.49	0.42
1:A:300:ARG:HB3	1:A:300:ARG:HH11	1.85	0.42
1:A:598:ARG:HD2	1:A:611:ILE:HD12	2.02	0.42
1:A:608:GLU:O	1:A:609:SER:C	2.58	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:374:LYS:HG3	1:A:406:ALA:HB1	2.01	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:B:105:PRO:O	1:B:108:SER:HB2	2.20	0.41
1:B:390:ILE:H	1:B:390:ILE:CD1	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
1:A:317:MET:O	1:A:584:CYS:HA	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:ILE:CG2	1:A:597:LEU:HD22	2.50	0.41
1:A:55:HIS:HB3	1:A:58:GLN:HG3	2.02	0.41
1:B:501:LEU:HD23	1:B:501:LEU:HA	1.90	0.41
1:B:251:HIS:CE1	1:B:577:ASP:OD2	2.63	0.41
1:A:112:PRO:O	1:A:138:LEU:HD22	2.20	0.41
1:A:95:ASN:H	1:A:95:ASN:ND2	2.18	0.41
1:B:121:ASP:HB2	1:B:186:LEU:HG	2.03	0.41
1:A:301:LEU:HD13	1:A:494:ILE:HD11	2.02	0.41
1:B:547:SER:OG	1:B:551:GLU:HG2	2.21	0.41
1:A:219:LYS:O	1:A:219:LYS:CG	2.68	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: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:A:507:LEU:C	1:A:509:PRO:HD3	2.41	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	597/619 (96%)	568 (95%)	27 (4%)	2 (0%)	41 46
1	B	599/619 (97%)	577 (96%)	21 (4%)	1 (0%)	47 55
All	All	1196/1238 (97%)	1145 (96%)	48 (4%)	3 (0%)	41 46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	LYS

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Mol	Chain	Res	Type
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%)	492 (96%)	21 (4%)	30	39
1	B	515/530 (97%)	498 (97%)	17 (3%)	38	49
All	All	1028/1060 (97%)	990 (96%)	38 (4%)	34	43

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ASP
1	A	43	VAL
1	A	74	VAL
1	A	95	ASN
1	A	141	ASN
1	A	149	ASN
1	A	156	PRO
1	A	164	GLU
1	A	173	CYS
1	A	300	ARG
1	A	355	LYS
1	A	418	GLU
1	A	436	ASN
1	A	457	ARG
1	A	459	PHE
1	A	470	GLN
1	A	471	ASN
1	A	483	GLU
1	A	523	ASP
1	A	524	GLU
1	A	602	SER

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Mol	Chain	Res	Type
1	B	32	SER
1	B	76	THR
1	B	89	PHE
1	B	96	ASP
1	B	127	LYS
1	B	137	GLN
1	B	261	GLN
1	B	272	LEU
1	B	275	LEU
1	B	308	ARG
1	B	377	ARG
1	B	379	ARG
1	B	390	ILE
1	B	417	ASP
1	B	459	PHE
1	B	471	ASN
1	B	522	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) 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	159	GLN
1	A	201	GLN
1	A	235	ASN
1	A	239	GLN
1	A	268	ASN
1	A	276	HIS
1	A	339	HIS
1	A	352	GLN
1	A	395	HIS
1	A	405	GLN
1	A	436	ASN
1	A	470	GLN
1	A	471	ASN
1	A	563	GLN

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Mol	Chain	Res	Type
1	A	568	GLN
1	A	582	GLN
1	B	70	ASN
1	B	102	GLN
1	B	131	HIS
1	B	247	GLN
1	B	251	HIS
1	B	268	ASN
1	B	286	ASN
1	B	339	HIS
1	B	357	ASN
1	B	367	ASN
1	B	375	HIS
1	B	471	ASN
1	B	522	ASN
1	B	563	GLN
1	B	568	GLN

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 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
4	GSH	B	5002	1	14,18,19	1.01	1 (7%)	16,22,24	1.63	3 (18%)
3	ADP	A	3001	2	24,29,29	1.13	2 (8%)	29,45,45	1.57	5 (17%)
3	ADP	B	3002	2	24,29,29	1.21	2 (8%)	29,45,45	1.53	4 (13%)
4	GSH	A	5001	1	14,18,19	1.10	1 (7%)	16,22,24	1.61	2 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GSH	B	5002	1	-	2/18/23/24	-
3	ADP	A	3001	2	-	3/12/32/32	0/3/3/3
3	ADP	B	3002	2	-	3/12/32/32	0/3/3/3
4	GSH	A	5001	1	-	4/18/23/24	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3001	ADP	C2-N1	3.83	1.41	1.33
3	B	3002	ADP	C2-N1	3.04	1.39	1.33
3	B	3002	ADP	C8-N7	-2.53	1.30	1.34
3	A	3001	ADP	C2-N3	2.35	1.35	1.32
4	B	5002	GSH	CA2-N2	2.22	1.50	1.45
4	A	5001	GSH	CB2-SG2	-2.22	1.76	1.81

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3001	ADP	C5-C6-N6	4.35	126.97	120.35
4	B	5002	GSH	CA2-CB2-SG2	-3.92	109.79	114.19
4	A	5001	GSH	CA2-CB2-SG2	-3.77	109.95	114.19
3	B	3002	ADP	C5-C6-N6	3.62	125.85	120.35
3	B	3002	ADP	N3-C2-N1	-3.50	123.21	128.68
3	A	3001	ADP	C5-C6-N1	-3.25	112.99	120.35
3	A	3001	ADP	N3-C2-N1	-3.11	123.81	128.68
3	B	3002	ADP	C5-C6-N1	-3.04	113.47	120.35
3	A	3001	ADP	C2-N1-C6	2.70	123.38	118.75
3	B	3002	ADP	C2-N1-C6	2.67	123.33	118.75
4	B	5002	GSH	CG1-CD1-N2	2.41	120.00	115.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	5001	GSH	CG1-CD1-N2	2.23	119.70	115.83
4	B	5002	GSH	O31-C3-CA3	-2.22	119.01	125.42
3	A	3001	ADP	O4'-C1'-C2'	-2.05	103.93	106.93

There are no chirality outliers.

All (12) torsion outliers are listed below:

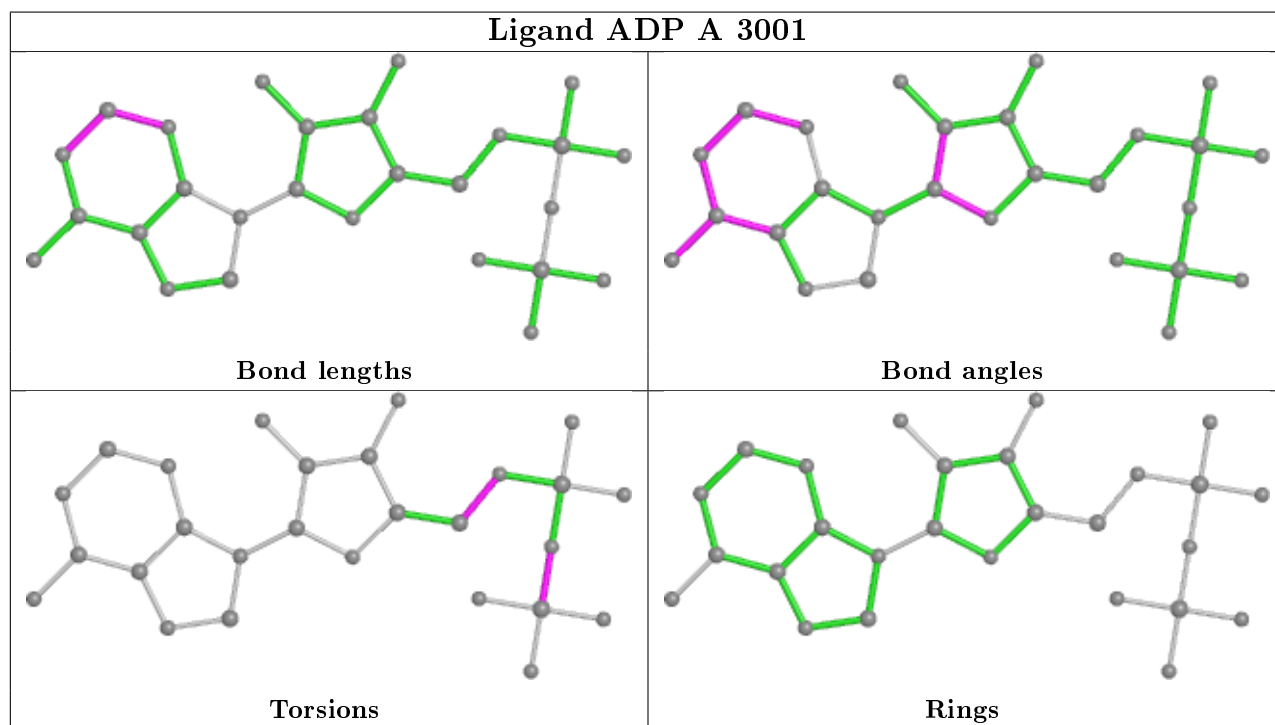
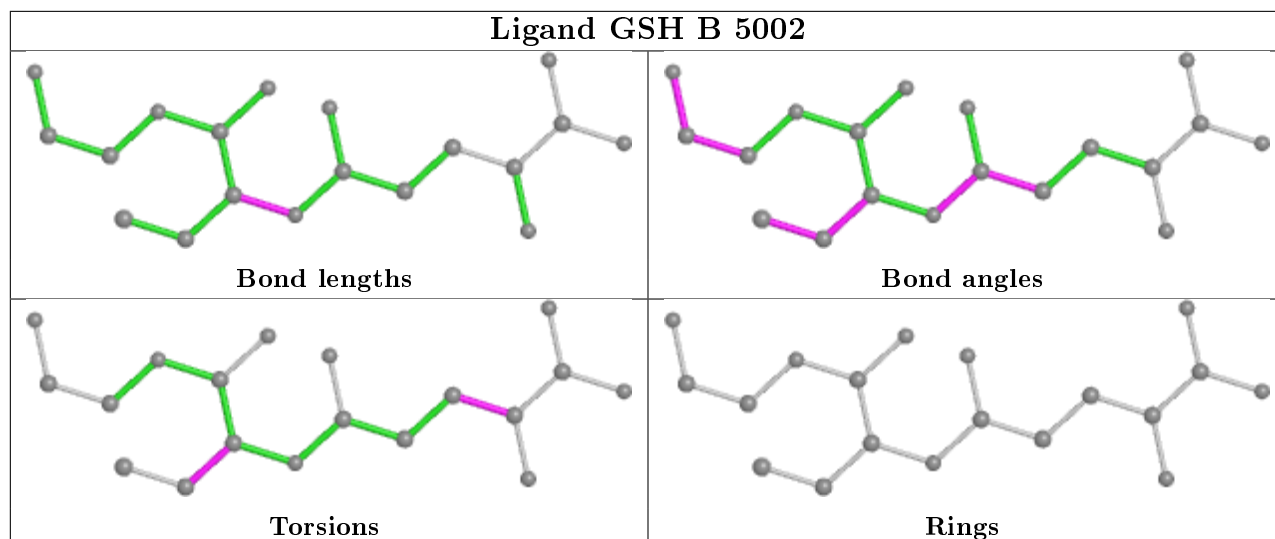
Mol	Chain	Res	Type	Atoms
3	B	3002	ADP	PA-O3A-PB-O3B
3	A	3001	ADP	PA-O3A-PB-O3B
4	B	5002	GSH	C1-CA1-CB1-CG1
4	A	5001	GSH	C1-CA1-CB1-CG1
4	B	5002	GSH	C2-CA2-CB2-SG2
4	A	5001	GSH	C2-CA2-CB2-SG2
4	A	5001	GSH	O2-C2-CA2-N2
3	B	3002	ADP	PA-O3A-PB-O2B
3	A	3001	ADP	PA-O3A-PB-O2B
3	B	3002	ADP	C4'-C5'-O5'-PA
3	A	3001	ADP	C4'-C5'-O5'-PA
4	A	5001	GSH	N3-C2-CA2-N2

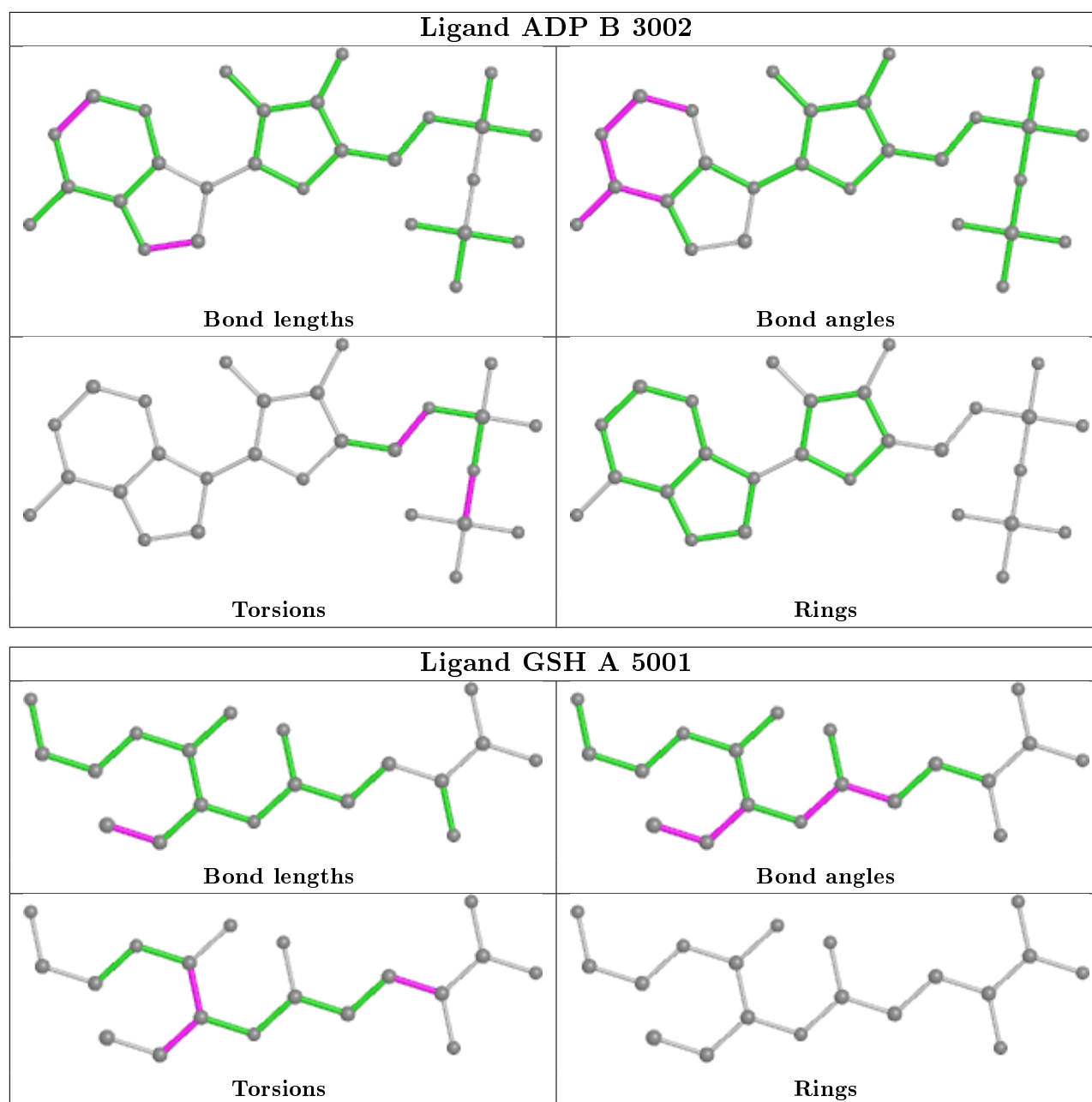
There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	5002	GSH	2	0
3	A	3001	ADP	2	0
3	B	3002	ADP	2	0
4	A	5001	GSH	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

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	601/619 (97%)	-0.18	19 (3%) 47 45	14, 28, 52, 80	0
1	B	603/619 (97%)	-0.07	25 (4%) 37 35	15, 29, 53, 81	0
All	All	1204/1238 (97%)	-0.12	44 (3%) 41 39	14, 29, 53, 81	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	10	ALA	6.1
1	B	43	VAL	6.0
1	B	456	ASP	5.3
1	B	455	SER	4.9
1	A	455	SER	4.6
1	B	170	GLU	4.4
1	A	172	GLY	4.3
1	B	33	LEU	4.1
1	A	454	VAL	4.1
1	B	454	VAL	3.9
1	A	456	ASP	3.7
1	B	171	ASN	3.6
1	A	30	TYR	3.4
1	B	42	ALA	3.4
1	B	549	HIS	3.2
1	A	168	VAL	3.0
1	A	43	VAL	3.0
1	A	458	GLU	2.8
1	A	127	LYS	2.7
1	B	470	GLN	2.7
1	B	31	SER	2.6
1	B	223	ASP	2.6
1	A	42	ALA	2.6
1	A	171	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	230	LYS	2.6
1	B	30	TYR	2.5
1	B	469	PRO	2.5
1	B	548	HIS	2.5
1	A	457	ARG	2.5
1	B	424	ALA	2.4
1	B	526	VAL	2.4
1	A	44	PHE	2.4
1	A	469	PRO	2.3
1	A	31	SER	2.3
1	B	430	GLY	2.2
1	B	34	ASP	2.2
1	B	559	LYS	2.1
1	B	457	ARG	2.1
1	B	169	VAL	2.1
1	B	547	SER	2.1
1	A	470	GLN	2.1
1	A	424	ALA	2.0
1	B	11	PRO	2.0
1	A	41	ASP	2.0

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. 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.

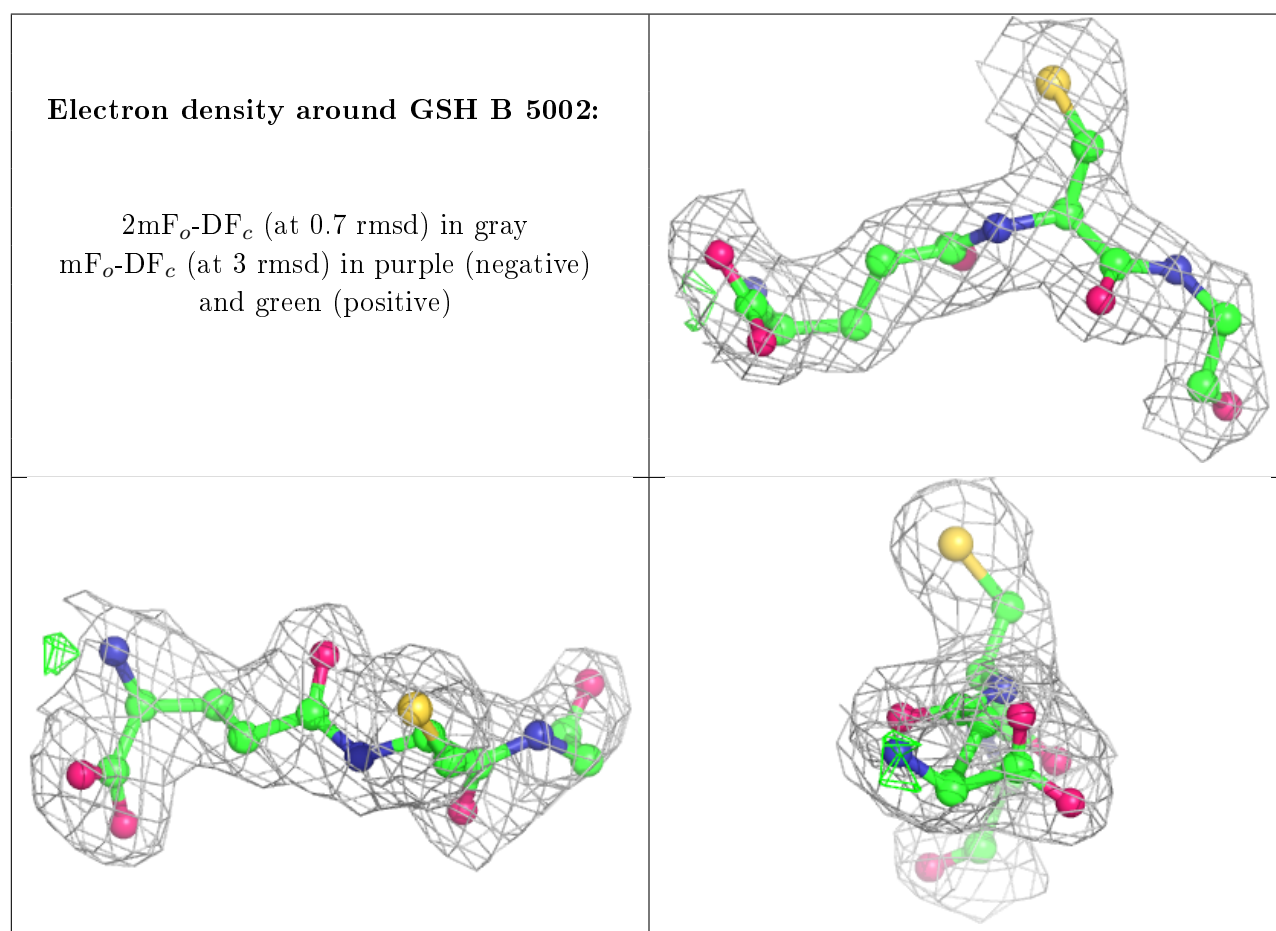
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GSH	B	5002	19/20	0.93	0.16	28,31,43,46	0
2	MG	A	7001	1/1	0.94	0.06	19,19,19,19	0
4	GSH	A	5001	19/20	0.94	0.15	24,27,40,43	0

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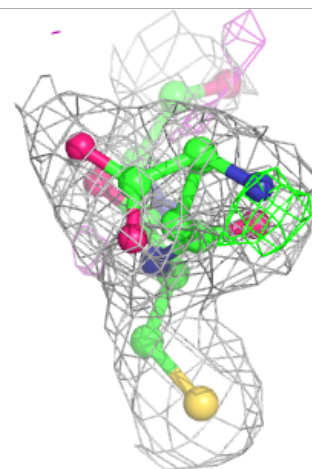
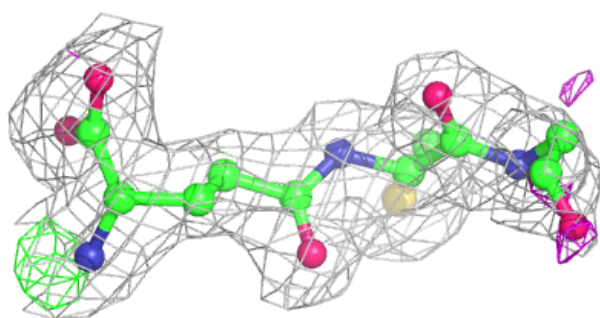
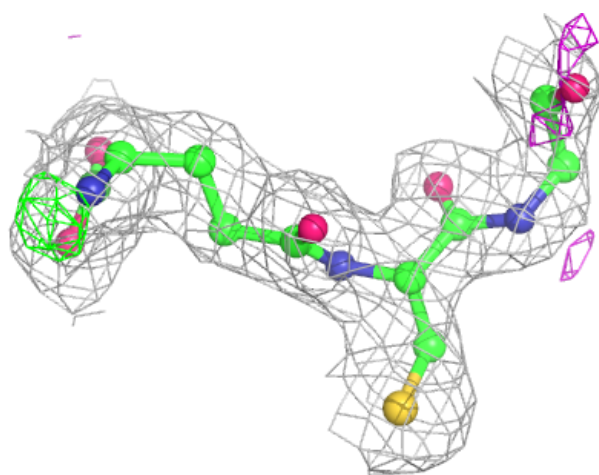
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	B	7003	1/1	0.96	0.05	21,21,21,21	0
3	ADP	B	3002	27/27	0.98	0.10	17,22,25,26	0
2	MG	B	7004	1/1	0.99	0.04	21,21,21,21	0
2	MG	A	7002	1/1	0.99	0.04	17,17,17,17	0
3	ADP	A	3001	27/27	0.99	0.09	14,19,24,25	0

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.



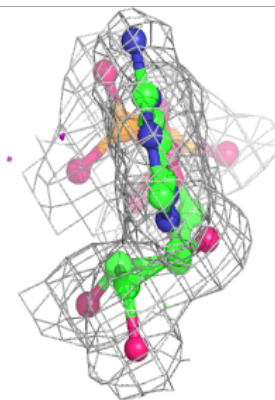
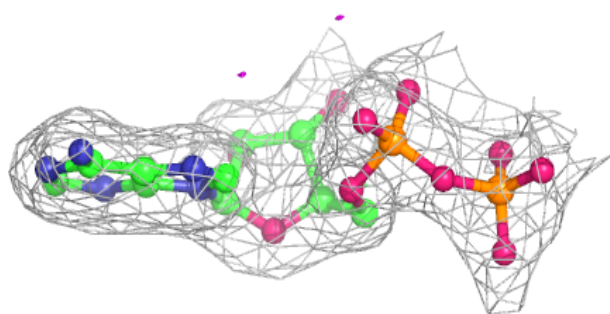
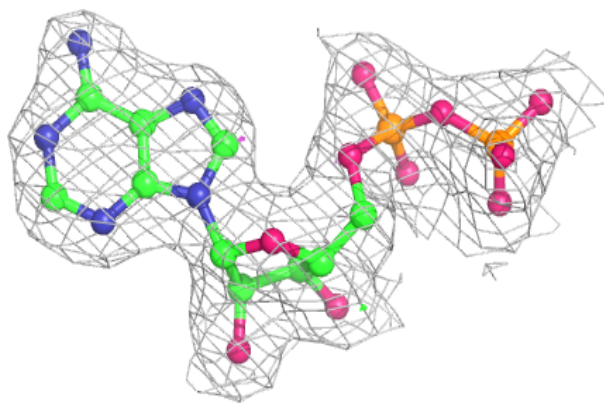
Electron density around GSH A 5001:

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

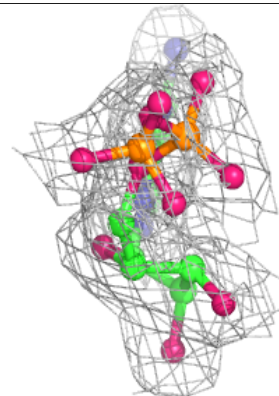
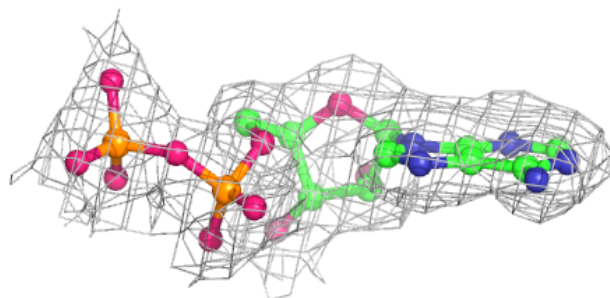
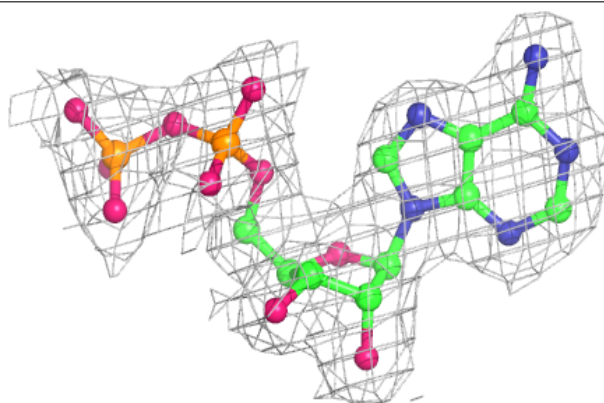


Electron density around ADP B 3002:

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

**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)



6.5 Other polymers

There are no such residues in this entry.