



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:23 PM GMT

PDB ID : 2IO9
Title : E. coli Bifunctional glutathionylspermidinesynthetase/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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

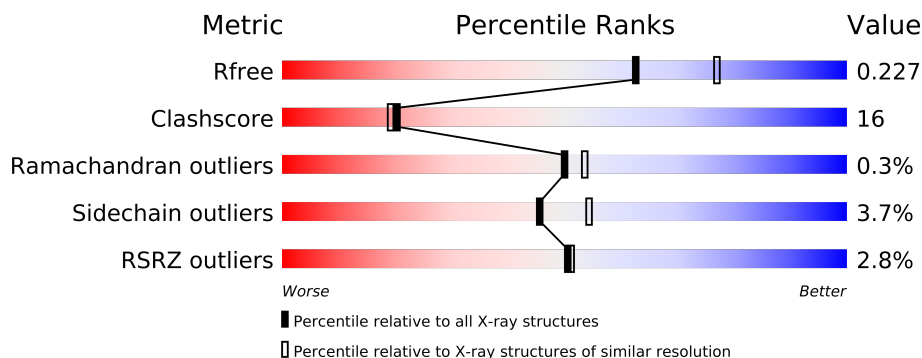
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	619	
1	B	619	

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 11020 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

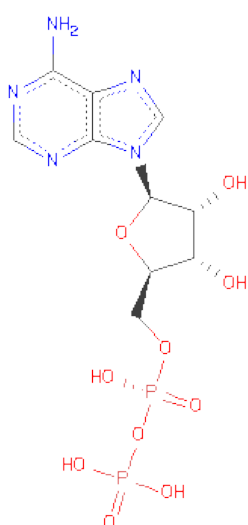
- Molecule 1 is a protein called Bifunctional glutathionylspermidinesynthetase/amidase.

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 (three-letter code: MG) (formula: Mg).

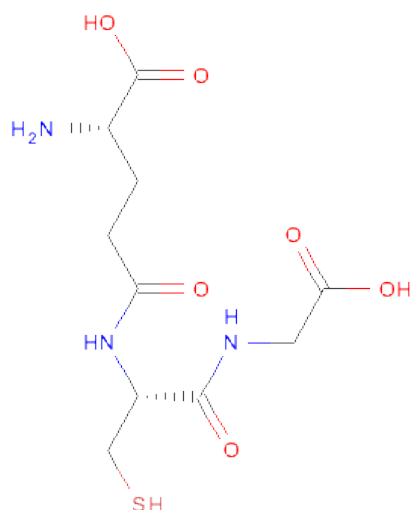
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mg	0	0
			2	2		
2	A	2	Total	Mg	0	0
			2	2		

- 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
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
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.

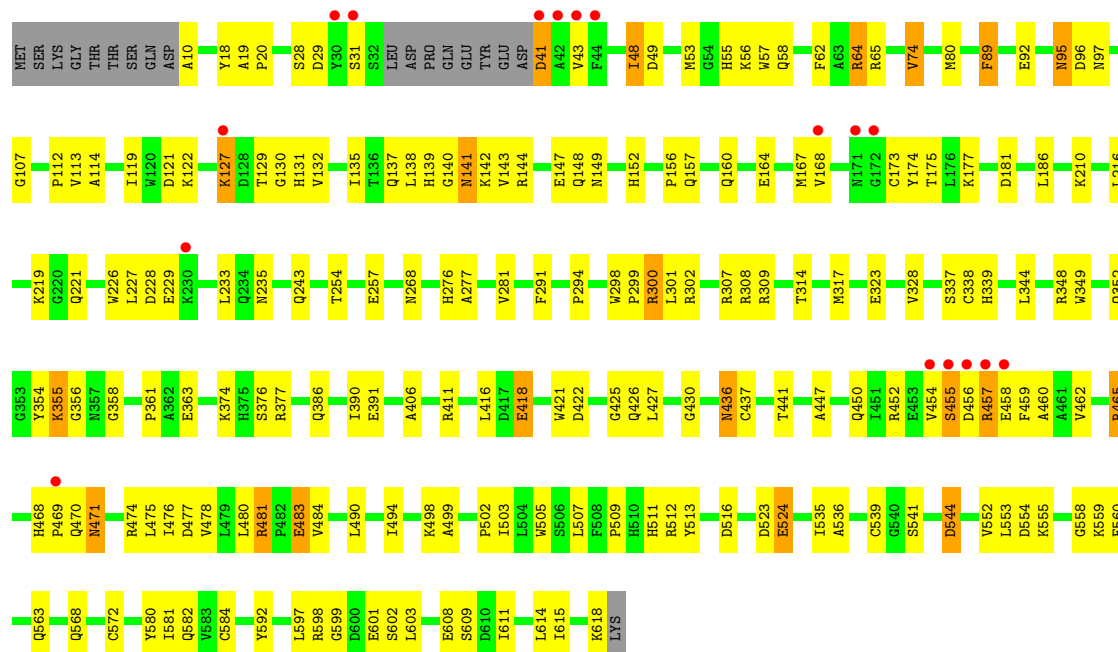
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	625	Total	O	0	0
			625	625		
5	B	611	Total	O	0	0
			611	611		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

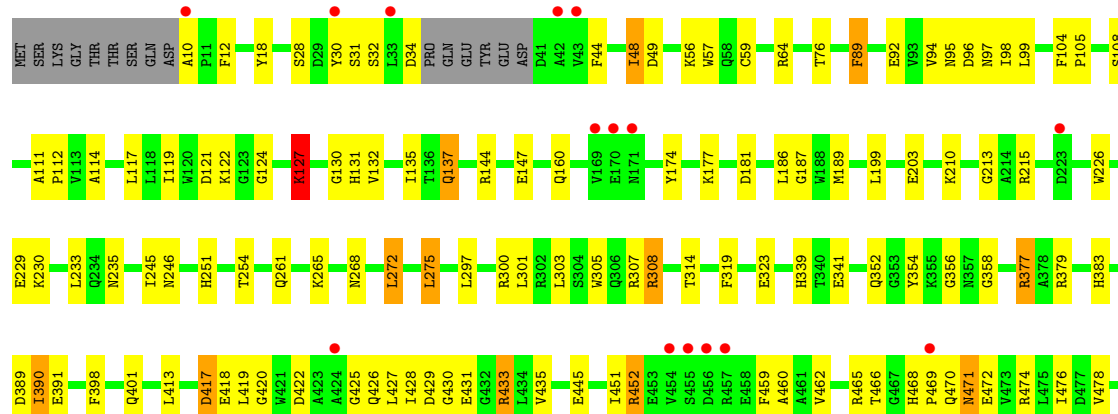
- Molecule 1: Bifunctional glutathionylspermidinesynthetase/amidase

Chain A: 



- Molecule 1: Bifunctional glutathionylspermidinesynthetase/amidase

Chain B: 





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)	Xtriage
Refinement program	XTALVIEW	Depositor
R, R_{free}	0.170 , 0.232 0.165 , 0.227	Depositor DCC
R_{free} test set	3102 reflections (5.32%)	DCC
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 , 49.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 61422 reflections	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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GSH, MG, 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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (305) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:B:323:GLU:HG2	5:B:7430:HOH:O	1.80	0.81
1:A:228:ASP:HB2	1:A:348:ARG:HH12	1.44	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:B:390:ILE:HD13	1:B:391:GLU:H	1.48	0.77
1:A:41:ASP:N	5:A:7559:HOH:O	2.16	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:B:233:LEU:HD12	1:B:401:GLN:OE1	1.90	0.71
1:A:425:GLY:O	1:A:481:ARG:NH2	2.24	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	Distance(Å)	Clash(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:B:245:ILE:HG13	1:B:246:ASN:H	1.65	0.62
1:A:457:ARG:CB	1:A:457:ARG:HH11	2.12	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:B:303:LEU:HD22	1:B:307:ARG:HH21	1.68	0.58
1:A:300:ARG:HG2	5:A:7159:HOH:O	2.03	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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:B:44:PHE:O	1:B:56:LYS:HG3	2.05	0.57
1:B:226:TRP:HB2	1:B:352:GLN:HG2	1.85	0.56
1:A:597:LEU:HD11	1:A:614:LEU:HD13	1.85	0.56
1:A:411:ARG:HH21	1:A:418:GLU:CD	2.07	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:10:ALA:N	5:A:7323:HOH:O	2.38	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: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:436:ASN:HD22	1:A:436:ASN:C	2.10	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:536:ALA:H	1:A:563:GLN:NE2	2.05	0.55
1:A:226:TRP:HB2	1:A:352:GLN:HG2	1.87	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: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:B:131:HIS:HE1	1:B:147:GLU:OE1	1.91	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:121:ASP:HB2	1:A:186:LEU:HG	1.90	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:B:215:ARG:NE	5:B:7266:HOH:O	2.43	0.50
1:A:436:ASN:HD22	1:A:437:CYS:N	2.09	0.50
1:B:481:ARG:NH1	1:B:483:GLU:OE1	2.45	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: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
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:B:522:ASN:ND2	1:B:524:GLU:H	2.10	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:80:MET:SD	1:A:129:THR:HA	2.54	0.48
1:B:522:ASN:ND2	1:B:524:GLU:N	2.61	0.48
1:B:124:GLY:O	1:B:127:LYS:HE2	2.13	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:427:LEU:HD22	1:B:481:ARG:HD2	1.95	0.48
1:B:233:LEU:HD11	1:B:398:PHE:HA	1.96	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:457:ARG:CG	1:A:457:ARG:HH11	2.27	0.47
1:A:294:PRO:HD3	1:A:452:ARG:NH1	2.30	0.47
1:A:107:GLY:HA2	1:A:174:TYR:O	2.15	0.47
1:B:468:HIS:CE1	1:B:470:GLN:HB2	2.49	0.47
1:B:431:GLU:O	1:B:431:GLU:HG3	2.15	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:ND2	1:A:95:ASN:C	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:B:418:GLU:HG3	1:B:430:GLY:H	1.80	0.46
1:A:601:GLU:HG2	5:A:7318:HOH:O	2.16	0.46
1:B:555:LYS:HE3	1:B:555:LYS:HB2	1.68	0.46
1:B:254:THR:HA	1:B:615:ILE:O	2.15	0.46
1:A:580:TYR:O	1:A:599:GLY:HA2	2.14	0.46
1:A:618:LYS:HG2	5:A:7374:HOH:O	2.15	0.46
1:A:390:ILE:HD12	1:A:391:GLU:HG3	1.97	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:522:ASN:HD22	1:B:522:ASN:C	2.19	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
4:B:5002:GSH:N1	5:B:7613:HOH:O	2.36	0.45
1:A:572:CYS:HB3	1:A:603:LEU:CD2	2.46	0.45
1:A:20:PRO:HD3	1:A:160:GLN:O	2.16	0.45
1:B:119:ILE:CD1	1:B:132:VAL:HG23	2.46	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: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:B:89:PHE:HD1	1:B:89:PHE:C	2.21	0.44
1:A:29:ASP:OD1	1:A:31:SER:OG	2.34	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: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:B:522:ASN:HD22	1:B:524:GLU:N	2.17	0.43
1:A:416:LEU:CD1	1:A:475:LEU:N	2.81	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:B:505:TRP:CH2	1:B:510:HIS:HA	2.53	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:A:539:CYS:SG	5:A:7301:HOH:O	2.50	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:436:ASN:ND2	1:A:436:ASN:C	2.71	0.43
1:B:468:HIS:HE1	1:B:470:GLN:HB2	1.83	0.43
1:A:119:ILE:HD13	1:A:132:VAL:HG23	2.01	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:524:GLU:HB2	5:A:7279:HOH:O	2.18	0.43
1:A:137:GLN:CG	1:A:144:ARG:HB2	2.45	0.43
1:A:227:LEU:HB2	1:A:243:GLN:OE1	2.18	0.42
1:A:140:GLY:HA2	5:A:7622:HOH:O	2.19	0.42
1:B:538:ARG:HA	3:B:3002:ADP:O2B	2.19	0.42
1:A:48:ILE:O	1:A:49:ASP:HB2	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:556:THR:HG21	1:B:606:LYS:HE3	2.00	0.42
1:B:420:GLY:O	1:B:428:ILE:HG12	2.20	0.42
1:A:499:ALA:O	1:A:502:PRO:HD2	2.18	0.42
1:B:97:ASN:O	1:B:98:ILE:HD13	2.19	0.42
1:A:137:GLN:NE2	1:A:144:ARG:CD	2.79	0.42
1:B:429:ASP:C	1:B:429:ASP:OD1	2.57	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:386:GLN:HA	1:A:441:THR:OG1	2.20	0.42
1:A:363:GLU:HG3	5:A:7413:HOH:O	2.20	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: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:598:ARG:HD2	1:A:611:ILE:HD12	2.02	0.42
1:B:524:GLU:O	1:B:527:LYS:HG3	2.20	0.42
1:A:64:ARG:CG	1:A:74:VAL:CG2	2.98	0.42
1:A:374:LYS:HG3	1:A:406:ALA:HB1	2.01	0.41
1:B:413:LEU:CD1	1:B:419:LEU:HD21	2.45	0.41
1:A:421:TRP:HA	1:A:426:GLN:O	2.20	0.41
1:B:390:ILE:H	1:B:390:ILE:CD1	2.32	0.41
1:B:105:PRO:O	1:B:108:SER:HB2	2.20	0.41
1:A:95:ASN:HD22	1:A:97:ASN:H	1.69	0.41
1:A:64:ARG:HG3	1:A:74:VAL:CG2	2.50	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:B:251:HIS:CE1	1:B:577:ASP:OD2	2.63	0.41
1:A:581:ILE:CG2	1:A:597:LEU:HD22	2.50	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:B:501:LEU:HD23	1:B:501:LEU:HA	1.90	0.41
1:A:112:PRO:O	1:A:138:LEU:HD22	2.20	0.41
1:A:95:ASN:ND2	1:A:95:ASN:H	2.18	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:121:ASP:HB2	1:B:186:LEU:HG	2.03	0.41
1:A:447:ALA:HB1	1:A:476:ILE:CG2	2.45	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:B:547:SER:OG	1:B:551:GLU:HG2	2.21	0.41
1:B:426:GLN:NE2	5:B:7557:HOH:O	2.34	0.41
1:B:522:ASN:HD22	1:B:524:GLU:H	1.66	0.41
1:B:377:ARG:NH2	1:B:377:ARG:HG3	2.35	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
1:A:507:LEU:C	1:A:509:PRO:HD3	2.41	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	597/619 (96%)	568 (95%)	27 (4%)	2 (0%)	50	53
1	B	599/619 (97%)	577 (96%)	21 (4%)	1 (0%)	56	62
All	All	1196/1238 (97%)	1145 (96%)	48 (4%)	3 (0%)	50	53

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 ⓘ

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%)	41	49
1	B	515/530 (97%)	498 (97%)	17 (3%)	50	60
All	All	1028/1060 (97%)	990 (96%)	38 (4%)	45	54

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
1	B	471	ASN
1	B	522	ASN
1	B	563	GLN
1	B	568	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	29,29,29	1.12	2 (6%)	45,45,45	1.46	5 (11%)
4	GSH	A	5001	1	18,18,19	4.24	3 (16%)	20,22,24	1.25	2 (10%)
3	ADP	B	3002	2	29,29,29	1.28	4 (13%)	45,45,45	1.53	5 (11%)
4	GSH	B	5002	1	18,18,19	3.43	4 (22%)	20,22,24	1.13	1 (5%)

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	-	0/16/32/32	0/1/3/3
4	GSH	A	5001	1	-	0/22/23/24	0/0/0/0
3	ADP	B	3002	2	-	0/16/32/32	0/1/3/3
4	GSH	B	5002	1	-	0/22/23/24	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	5001	GSH	O31-C3	16.76	1.22	1.11
4	B	5002	GSH	O31-C3	13.31	1.20	1.11
4	A	5001	GSH	CA3-C3	4.60	1.54	1.48
4	B	5002	GSH	CA3-C3	3.89	1.53	1.48
3	A	3001	ADP	C2-N1	3.62	1.41	1.33
4	A	5001	GSH	CA3-N3	2.93	1.48	1.46
4	B	5002	GSH	CA3-N3	2.93	1.48	1.46
3	B	3002	ADP	C2-N1	2.87	1.39	1.33
3	A	3001	ADP	PB-O3A	2.68	1.64	1.60
3	B	3002	ADP	C4-N9	-2.63	1.33	1.37
3	B	3002	ADP	C8-N7	-2.24	1.30	1.34
3	B	3002	ADP	PA-O3A	-2.15	1.56	1.59
4	B	5002	GSH	CA2-N2	2.09	1.50	1.45

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3002	ADP	N3-C2-N1	-6.58	123.21	128.71
3	A	3001	ADP	N3-C2-N1	-5.86	123.81	128.71
3	A	3001	ADP	O4'-C1'-N9	-3.08	105.58	108.44
3	B	3002	ADP	O4'-C1'-N9	-3.02	105.63	108.44
3	B	3002	ADP	C4'-O4'-C1'	2.77	112.76	109.75
3	A	3001	ADP	C5-C6-N6	2.76	126.97	120.72
4	A	5001	GSH	CA3-N3-C2	-2.61	119.06	121.62
3	A	3001	ADP	C2-N1-C6	2.55	123.38	118.77
3	B	3002	ADP	C2-N1-C6	2.52	123.33	118.77
3	A	3001	ADP	C4'-O4'-C1'	2.50	112.46	109.75
3	B	3002	ADP	C5-C6-N6	2.27	125.85	120.72
4	B	5002	GSH	CG1-CD1-N2	2.20	120.00	115.83
4	A	5001	GSH	CG1-CD1-N2	2.04	119.70	115.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	601/619 (97%)	-0.31	17 (2%)	50	51	14, 28, 52, 80	0
1	B	603/619 (97%)	-0.21	17 (2%)	50	51	15, 29, 53, 81	0
All	All	1204/1238 (97%)	-0.26	34 (2%)	50	51	14, 29, 53, 81	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	10	ALA	5.2
1	B	43	VAL	4.9
1	B	456	ASP	4.7
1	B	455	SER	4.5
1	A	172	GLY	4.3
1	A	456	ASP	3.7
1	A	458	GLU	3.5
1	B	42	ALA	3.4
1	A	455	SER	3.3
1	B	171	ASN	3.1
1	B	549	HIS	3.0
1	B	33	LEU	3.0
1	B	170	GLU	2.8
1	A	42	ALA	2.7
1	B	223	ASP	2.6
1	B	30	TYR	2.6
1	A	454	VAL	2.6
1	A	469	PRO	2.5
1	A	30	TYR	2.5
1	A	43	VAL	2.5
1	B	457	ARG	2.4
1	B	469	PRO	2.4
1	A	171	ASN	2.2
1	B	454	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	169	VAL	2.2
1	A	127	LYS	2.1
1	A	44	PHE	2.1
1	A	230	LYS	2.1
1	B	424	ALA	2.1
1	A	168	VAL	2.0
1	A	31	SER	2.0
1	B	548	HIS	2.0
1	A	41	ASP	2.0
1	A	457	ARG	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	GSH	B	5002	19/20	0.14	0.82	28,31,43,46	0
4	GSH	A	5001	19/20	0.14	0.66	24,27,40,43	0
3	ADP	A	3001	27/27	0.09	0.22	14,19,24,25	0
3	ADP	B	3002	27/27	0.10	-0.37	17,22,25,26	0
2	MG	A	7001	1/1	0.07	-1.37	19,19,19,19	0
2	MG	A	7002	1/1	0.06	-1.70	17,17,17,17	0
2	MG	B	7003	1/1	0.07	-2.05	21,21,21,21	0
2	MG	B	7004	1/1	0.07	-3.21	21,21,21,21	0

6.5 Other polymers ⓘ

There are no such residues in this entry.