



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 05:14 PM GMT

PDB ID : 2A2C
Title : x-ray structure of human N-acetyl galactosamine kinase complexed with Mg-ADP and N-acetyl galactosamine 1-phosphate
Authors : Thoden, J.B.; Holden, H.M.
Deposited on : 2005-06-22
Resolution : 1.65 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>

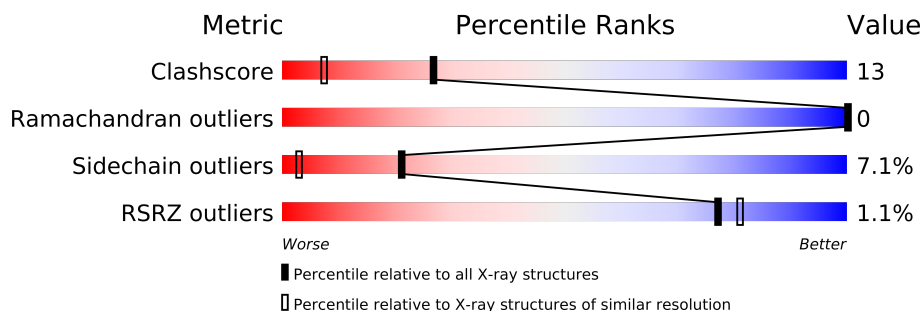
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.65 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1001 (1.66-1.66)
Ramachandran outliers	78287	1581 (1.68-1.64)
Sidechain outliers	78261	1580 (1.68-1.64)
RSRZ outliers	66119	1404 (1.68-1.64)

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	478	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	NA	A	462	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3976 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.

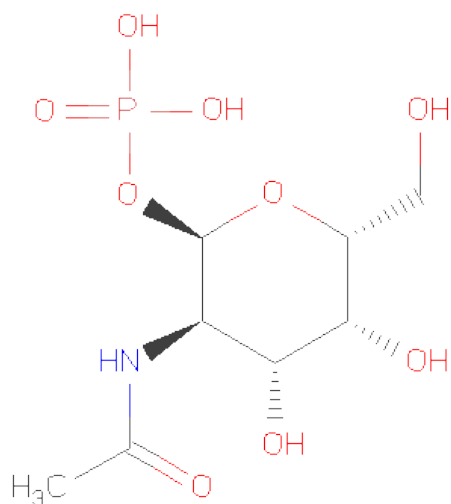
- Molecule 1 is a protein called N-acetylgalactosaminekinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	446	3470	2206	589	645	30	0	9	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	CLONING ARTIFACT	UNP Q01415
A	-18	GLY	-	CLONING ARTIFACT	UNP Q01415
A	-17	SER	-	CLONING ARTIFACT	UNP Q01415
A	-16	SER	-	CLONING ARTIFACT	UNP Q01415
A	-15	HIS	-	EXPRESSION TAG	UNP Q01415
A	-14	HIS	-	EXPRESSION TAG	UNP Q01415
A	-13	HIS	-	EXPRESSION TAG	UNP Q01415
A	-12	HIS	-	EXPRESSION TAG	UNP Q01415
A	-11	HIS	-	EXPRESSION TAG	UNP Q01415
A	-10	HIS	-	EXPRESSION TAG	UNP Q01415
A	-9	SER	-	CLONING ARTIFACT	UNP Q01415
A	-8	SER	-	CLONING ARTIFACT	UNP Q01415
A	-7	GLU	-	CLONING ARTIFACT	UNP Q01415
A	-6	ASN	-	CLONING ARTIFACT	UNP Q01415
A	-5	LEU	-	CLONING ARTIFACT	UNP Q01415
A	-4	TYR	-	CLONING ARTIFACT	UNP Q01415
A	-3	PHE	-	CLONING ARTIFACT	UNP Q01415
A	-2	GLN	-	CLONING ARTIFACT	UNP Q01415
A	-1	GLY	-	CLONING ARTIFACT	UNP Q01415
A	0	HIS	-	CLONING ARTIFACT	UNP Q01415

- Molecule 2 is SUGAR (N-ACETYL-ALPHA-D-GALACTOSAMINE1-PHOSPHATE) (three-letter code: NG1) (formula: C₈H₁₆NO₉P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			19	8	1	9	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

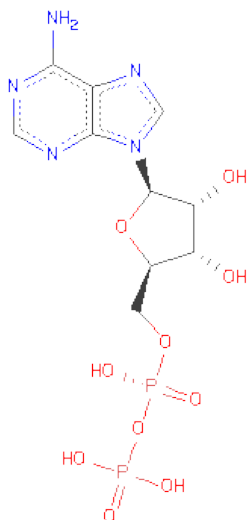
- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Na	0	0
			1	1		

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 7 is water.

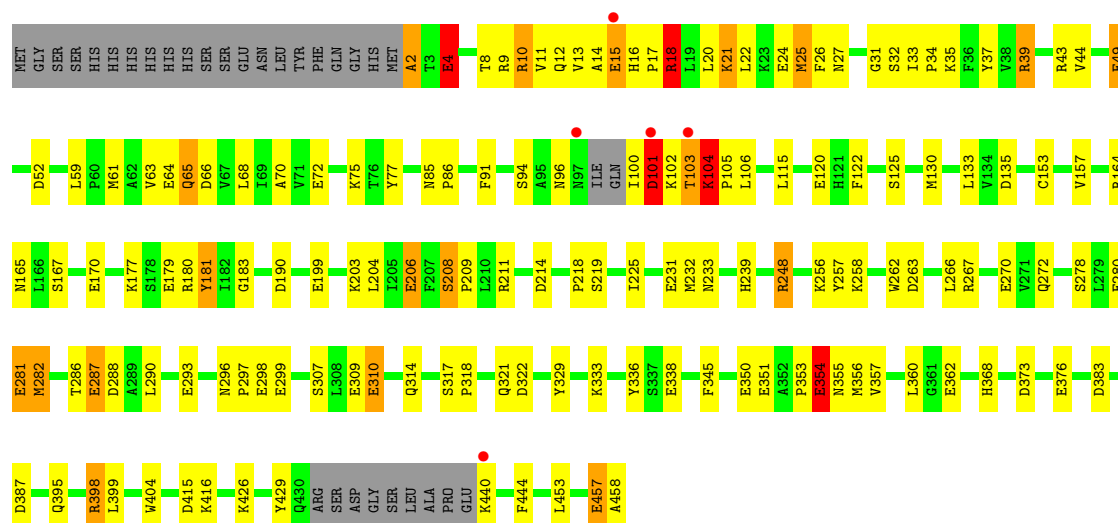
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	457	Total	O	0	0
			457	457		

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: N-acetylgalactosaminekinase

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	123.80Å 123.80Å 60.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 1.65 29.74 – 1.65	Depositor EDS
% Data completeness (in resolution range)	94.3 (50.00-1.65) 94.4 (29.74-1.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.86 (at 1.65Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.167 , 0.201 0.165 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	18.5	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 87.4	EDS
Estimated twinning fraction	0.054 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 59706 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3976	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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: NA, MG, NG1, ADP, CL

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	0.99	25/3572 (0.7%)	1.40	48/4828 (1.0%)

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	49	GLU	CD-OE2	8.03	1.34	1.25
1	A	354	GLU	CD-OE2	7.10	1.33	1.25
1	A	376	GLU	CD-OE2	6.81	1.33	1.25
1	A	338	GLU	CD-OE2	6.62	1.32	1.25
1	A	350	GLU	CD-OE2	6.51	1.32	1.25
1	A	4	GLU	CD-OE2	6.42	1.32	1.25
1	A	299	GLU	CD-OE2	6.39	1.32	1.25
1	A	309	GLU	CD-OE2	6.39	1.32	1.25
1	A	179	GLU	CD-OE2	6.37	1.32	1.25
1	A	206	GLU	CD-OE1	-6.22	1.18	1.25
1	A	120	GLU	CD-OE2	6.08	1.32	1.25
1	A	64	GLU	CD-OE2	6.04	1.32	1.25
1	A	280	GLU	CD-OE2	5.93	1.32	1.25
1	A	457	GLU	CD-OE2	5.83	1.32	1.25
1	A	351	GLU	CD-OE2	5.81	1.32	1.25
1	A	293	GLU	CD-OE2	5.73	1.31	1.25
1	A	310	GLU	CD-OE2	5.67	1.31	1.25
1	A	298	GLU	CD-OE2	5.59	1.31	1.25
1	A	199	GLU	CD-OE2	5.59	1.31	1.25
1	A	24	GLU	CD-OE2	5.45	1.31	1.25
1	A	281	GLU	CD-OE2	5.34	1.31	1.25
1	A	362	GLU	CD-OE2	5.25	1.31	1.25
1	A	15	GLU	CD-OE2	5.24	1.31	1.25
1	A	287	GLU	CD-OE2	5.22	1.31	1.25
1	A	231	GLU	CD-OE2	5.14	1.31	1.25

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	398	ARG	NE-CZ-NH2	-10.22	115.19	120.30
1	A	10	ARG	NE-CZ-NH2	-9.91	115.35	120.30
1	A	398	ARG	NE-CZ-NH1	8.83	124.71	120.30
1	A	52	ASP	CB-CG-OD2	-8.52	110.63	118.30
1	A	248[A]	ARG	NE-CZ-NH1	8.45	124.52	120.30
1	A	248[B]	ARG	NE-CZ-NH1	8.45	124.52	120.30
1	A	101	ASP	CB-CG-OD2	-8.36	110.78	118.30
1	A	288	ASP	CB-CG-OD2	-8.30	110.83	118.30
1	A	383	ASP	CB-CG-OD2	-8.23	110.89	118.30
1	A	248[A]	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	A	248[B]	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	A	373	ASP	CB-CG-OD2	-7.86	111.23	118.30
1	A	181	TYR	CB-CG-CD2	-7.59	116.45	121.00
1	A	373	ASP	CB-CG-OD1	7.39	124.95	118.30
1	A	214	ASP	CB-CG-OD2	-7.24	111.79	118.30
1	A	453	LEU	CB-CA-C	-7.19	96.53	110.20
1	A	18	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	A	180	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	A	322	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	A	8	THR	CA-CB-CG2	-6.90	102.74	112.40
1	A	288	ASP	CB-CG-OD1	6.79	124.41	118.30
1	A	383	ASP	CB-CG-OD1	6.76	124.39	118.30
1	A	257	TYR	CB-CG-CD2	6.55	124.93	121.00
1	A	190	ASP	CB-CG-OD1	6.50	124.15	118.30
1	A	190	ASP	CB-CG-OD2	-6.46	112.49	118.30
1	A	257	TYR	CB-CG-CD1	-6.46	117.13	121.00
1	A	52	ASP	CB-CG-OD1	6.38	124.04	118.30
1	A	135	ASP	CB-CG-OD1	6.36	124.02	118.30
1	A	387	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	A	345	PHE	CB-CG-CD2	-6.19	116.47	120.80
1	A	2	ALA	CB-CA-C	-6.07	101.00	110.10
1	A	429	TYR	CB-CG-CD2	-5.91	117.45	121.00
1	A	263	ASP	CB-CG-OD2	-5.73	113.15	118.30
1	A	135	ASP	CB-CG-OD2	-5.68	113.18	118.30
1	A	429	TYR	CB-CG-CD1	5.67	124.41	121.00
1	A	415	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	387	ASP	CB-CG-OD1	5.57	123.31	118.30
1	A	91	PHE	CB-CG-CD1	-5.56	116.91	120.80
1	A	180	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	164	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	A	39	ARG	NE-CZ-NH2	5.43	123.02	120.30
1	A	68	LEU	CB-CG-CD2	-5.32	101.97	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	LYS	N-CA-CB	-5.25	101.15	110.60
1	A	122	PHE	CB-CG-CD1	5.23	124.46	120.80
1	A	66	ASP	CB-CG-OD1	5.22	123.00	118.30
1	A	164	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	122	PHE	CB-CG-CD2	-5.18	117.18	120.80
1	A	101	ASP	CB-CG-OD1	5.12	122.91	118.30

There are no chirality outliers.

There are no planarity outliers.

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	3470	0	3519	93	0
2	A	19	0	14	0	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
5	A	1	0	0	0	0
6	A	27	0	12	0	0
7	A	457	0	0	13	1
All	All	3976	0	3545	93	1

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 13.

All (93) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:13:VAL:HG12	1:A:20:LEU:HD12	1.15	1.10
1:A:103:THR:HB	1:A:104:LYS:HE2	1.39	1.04
1:A:13:VAL:HG12	1:A:20:LEU:CD1	2.04	0.86
1:A:12:GLN:HG3	1:A:458:ALA:CB	2.07	0.84
1:A:103:THR:CB	1:A:104:LYS:HE2	2.07	0.84
1:A:102:LYS:HE2	1:A:183:GLY:HA2	1.60	0.82
1:A:12:GLN:HG3	1:A:458:ALA:HB3	1.62	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:12:GLN:HB2	1:A:15:GLU:CD	2.07	0.75
1:A:100:ILE:HD13	1:A:181:TYR:HB3	1.69	0.74
1:A:307:SER:OG	1:A:310:GLU:HG3	1.87	0.74
1:A:65:GLN:H	1:A:65:GLN:HE21	1.36	0.74
1:A:21:LYS:HE2	1:A:25[B]:MET:HE2	1.71	0.73
1:A:317:SER:HB2	1:A:318:PRO:HD2	1.72	0.72
1:A:2:ALA:HB1	7:A:914:HOH:O	1.89	0.71
1:A:13:VAL:CG1	1:A:20:LEU:HD12	2.09	0.70
1:A:44:VAL:HG21	1:A:225[A]:ILE:HD11	1.74	0.69
1:A:100:ILE:HD13	1:A:181:TYR:CB	2.23	0.69
1:A:21:LYS:HE2	1:A:25[B]:MET:CE	2.23	0.69
1:A:248[A]:ARG:NH2	7:A:484:HOH:O	2.26	0.68
1:A:256:LYS:HD2	1:A:262:TRP:CD1	2.29	0.68
1:A:102:LYS:HE2	1:A:183:GLY:CA	2.25	0.67
1:A:59[A]:LEU:HD12	1:A:203:LYS:O	1.96	0.66
1:A:21:LYS:HG3	1:A:25[B]:MET:HE3	1.77	0.66
1:A:103:THR:HB	1:A:104:LYS:CE	2.21	0.65
1:A:206:GLU:OE2	1:A:211:ARG:NH1	2.30	0.65
1:A:12:GLN:HB2	1:A:15:GLU:OE1	1.96	0.64
1:A:278:SER:OG	1:A:281:GLU:HG3	1.97	0.64
1:A:13:VAL:HG23	1:A:457:GLU:HG2	1.82	0.60
1:A:65:GLN:H	1:A:65:GLN:NE2	1.99	0.60
1:A:25[A]:MET:HG2	7:A:796:HOH:O	2.03	0.58
1:A:165:ASN:HB2	7:A:811:HOH:O	2.03	0.58
1:A:18:ARG:HB2	7:A:884:HOH:O	2.04	0.58
1:A:272:GLN:HB2	1:A:282:MET:HG2	1.85	0.57
1:A:256:LYS:HD2	1:A:262:TRP:NE1	2.19	0.57
1:A:77:TYR:HB3	7:A:802:HOH:O	2.06	0.54
1:A:167:SER:OG	1:A:170:GLU:HG3	2.09	0.53
1:A:225[B]:ILE:HD12	1:A:444:PHE:CE1	2.44	0.53
1:A:14:ALA:HA	1:A:20:LEU:HD13	1.90	0.51
1:A:11:VAL:O	1:A:458:ALA:N	2.32	0.51
1:A:101:ASP:O	1:A:102:LYS:C	2.50	0.49
1:A:232[B]:MET:HG3	1:A:404:TRP:HB2	1.94	0.49
1:A:368:HIS:HB2	1:A:398:ARG:CB	2.43	0.49
1:A:208:SER:OG	1:A:208:SER:O	2.30	0.48
1:A:27:ASN:HD22	1:A:32:SER:C	2.16	0.48
1:A:34:PRO:HG2	1:A:37:TYR:OH	2.14	0.48
1:A:63:VAL:HG12	7:A:709:HOH:O	2.13	0.47
1:A:218:PRO:HG3	1:A:360:LEU:HD12	1.95	0.47
1:A:287:GLU:OE1	1:A:333:LYS:NZ	2.39	0.47
1:A:329:TYR:CE2	1:A:333:LYS:HE3	2.50	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:115:LEU:HD12	1:A:130:MET:CE	2.45	0.46
1:A:13:VAL:CG2	1:A:457:GLU:HG2	2.45	0.46
1:A:232[B]:MET:HE1	1:A:239:HIS:HD2	1.80	0.46
1:A:296:ASN:HB2	1:A:297:PRO:HD2	1.98	0.46
1:A:354:GLU:HG2	1:A:355:ASN:N	2.31	0.46
1:A:16:HIS:O	1:A:17:PRO:C	2.54	0.46
1:A:12:GLN:OE1	1:A:15:GLU:OE1	2.34	0.46
1:A:353:PRO:HB2	1:A:355:ASN:OD1	2.16	0.46
1:A:310:GLU:O	1:A:314:GLN:N	2.44	0.45
1:A:317:SER:CB	1:A:318:PRO:HD2	2.37	0.45
1:A:356:MET:HE1	7:A:591:HOH:O	2.16	0.45
1:A:310:GLU:O	1:A:314:GLN:HB2	2.17	0.45
1:A:26:PHE:HZ	1:A:72:GLU:HB3	1.80	0.45
1:A:218:PRO:HG3	1:A:360:LEU:CD1	2.47	0.44
1:A:354:GLU:CG	1:A:355:ASN:N	2.80	0.44
1:A:232[B]:MET:CE	1:A:239:HIS:CD2	3.00	0.44
1:A:457:GLU:HG2	7:A:883:HOH:O	2.16	0.44
1:A:282:MET:HG3	1:A:336:TYR:CE1	2.53	0.44
1:A:286:THR:HG23	1:A:290:LEU:HD12	1.99	0.44
1:A:266:LEU:HD23	1:A:266:LEU:HA	1.81	0.43
1:A:106:LEU:HD22	7:A:647:HOH:O	2.19	0.43
1:A:262:TRP:HZ3	7:A:726:HOH:O	2.01	0.43
1:A:22:LEU:HA	1:A:22:LEU:HD12	1.85	0.43
1:A:59[A]:LEU:HD13	1:A:204:LEU:HA	2.00	0.43
1:A:357:VAL:HG12	1:A:395:GLN:HG3	2.01	0.43
1:A:153:CYS:O	1:A:157:VAL:HG23	2.18	0.43
1:A:399:LEU:C	1:A:399:LEU:HD12	2.39	0.42
1:A:232[B]:MET:HE2	1:A:239:HIS:CD2	2.54	0.42
1:A:33:ILE:HB	1:A:34:PRO:HD2	2.01	0.42
1:A:25[A]:MET:HB3	1:A:133:LEU:HD21	2.00	0.42
1:A:248[A]:ARG:HD3	1:A:266:LEU:HD22	2.00	0.42
1:A:248[A]:ARG:HD3	1:A:266:LEU:CD2	2.50	0.42
1:A:177:LYS:NZ	7:A:815:HOH:O	2.51	0.42
1:A:368:HIS:HB2	1:A:398:ARG:HB3	2.01	0.42
1:A:22:LEU:HG	1:A:70:ALA:HB2	2.00	0.42
1:A:49:GLU:HB2	1:A:398:ARG:NH2	2.34	0.41
1:A:85:ASN:HA	1:A:86:PRO:HD2	1.93	0.41
1:A:2:ALA:HB3	1:A:4:GLU:H	1.85	0.41
1:A:282:MET:HG3	1:A:336:TYR:CZ	2.55	0.41
1:A:27:ASN:O	1:A:31:GLY:N	2.42	0.41
1:A:267:ARG:O	1:A:270:GLU:HB2	2.21	0.41
1:A:208:SER:HA	1:A:209:PRO:HA	1.80	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:61:MET:HE3	7:A:709:HOH:O	2.20	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:A:662:HOH:O	7:A:713:HOH:O[2_655]	2.19	0.01

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	449/478 (94%)	434 (97%)	15 (3%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	387/407 (95%)	358 (92%)	29 (8%)	19 2

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	9	ARG
1	A	10	ARG
1	A	18	ARG
1	A	21	LYS

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Mol	Chain	Res	Type
1	A	25[A]	MET
1	A	25[B]	MET
1	A	35	LYS
1	A	39	ARG
1	A	43	ARG
1	A	65	GLN
1	A	75	LYS
1	A	94	SER
1	A	101	ASP
1	A	103	THR
1	A	104	LYS
1	A	105	PRO
1	A	125[A]	SER
1	A	125[B]	SER
1	A	208	SER
1	A	219	SER
1	A	233	ASN
1	A	258	LYS
1	A	282	MET
1	A	321	GLN
1	A	354	GLU
1	A	416	LYS
1	A	426	LYS
1	A	440	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	HIS
1	A	27	ASN
1	A	65	GLN
1	A	109	ASN
1	A	165	ASN
1	A	233	ASN
1	A	239	HIS

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 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	$\# Z > 2$
2	NG1	A	459	3	19,19,19	1.49	3 (15%)	28,28,28	1.61	3 (10%)
6	ADP	A	463	3	29,29,29	1.00	1 (3%)	45,45,45	1.24	4 (8%)

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
2	NG1	A	459	3	-	0/11/31/31	0/1/1/1
6	ADP	A	463	3	-	0/16/32/32	0/1/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	459	NG1	O1-C1	-3.67	1.35	1.42
2	A	459	NG1	C1-C2	3.05	1.58	1.53
6	A	463	ADP	C6-N6	-2.69	1.26	1.35
2	A	459	NG1	P1-OP1	2.12	1.62	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	459	NG1	O5-C1-O1	-5.01	104.82	111.36
6	A	463	ADP	N3-C2-N1	-3.63	125.68	128.71
6	A	463	ADP	C2-N1-C6	3.34	124.80	118.77
2	A	459	NG1	O1-C1-C2	3.27	113.10	107.91
6	A	463	ADP	C5-C6-N6	2.89	127.24	120.72
6	A	463	ADP	C5-C6-N1	-2.74	110.07	119.27
2	A	459	NG1	OP2-P1-OP3	-2.36	102.72	110.44

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	446/478 (93%)	-0.33	5 (1%) 77 81	13, 23, 57, 91	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	103	THR	6.3
1	A	440	LYS	3.6
1	A	101	ASP	3.5
1	A	97	ASN	3.2
1	A	15	GLU	2.7

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
5	NA	A	462	1/1	0.14	5.33	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NG1	A	459	19/19	0.11	0.81	10,13,27,36	0
3	MG	A	460	1/1	0.10	0.79	9,9,9,9	0
6	ADP	A	463	27/27	0.05	-0.78	12,16,19,23	0
4	CL	A	461	1/1	0.03	-1.11	26,26,26,26	0

6.5 Other polymers ⓘ

There are no such residues in this entry.