



Full wwPDB X-ray Structure Validation Report i

Feb 28, 2014 – 06:51 AM GMT

PDB ID : 2C54
Title : GDP-MANNOSE-3', 5' -EPIMERASE (ARABIDOPSIS THALIANA),
K178R, WITH GDP-BETA-L-GULOSE AND GDP-4-KETO-BETA-L-G
ULOSEBOUND IN ACTIVE SITE.
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Deposited on : 2005-10-25
Resolution : 1.50 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>

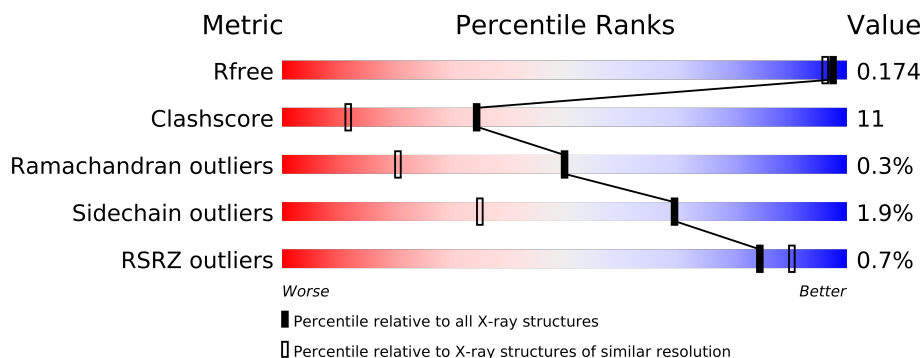
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.50 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	1513 (1.50-1.50)
Clashscore	79885	1768 (1.50-1.50)
Ramachandran outliers	78287	1720 (1.50-1.50)
Sidechain outliers	78261	1718 (1.50-1.50)
RSRZ outliers	66119	1514 (1.50-1.50)

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	379	
1	B	379	

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	FMT	A	1384	-	X
5	FMT	A	1386	-	X
5	FMT	A	1387	-	X
5	FMT	A	1388	-	X
5	FMT	A	1389	-	X
5	FMT	B	1380	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
5	FMT	B	1381	-	X
5	FMT	B	1383	-	X
5	FMT	B	1384	-	X
5	FMT	B	1385	-	X
6	EPE	A	1390	-	X

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 7269 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.

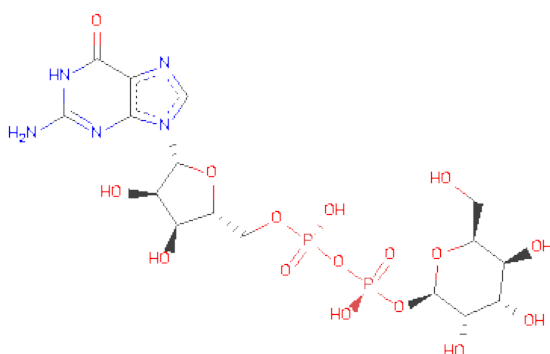
- Molecule 1 is a protein called GDP-MANNOSE-3', 5'-EPIMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	19	0
			3000	1906	513	556	25			
1	B	360	Total	C	N	O	S	0	15	0
			2976	1890	509	553	24			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	178	ARG	LYS	ENGINEERED MUTATION	UNP Q93VR3
B	178	ARG	LYS	ENGINEERED MUTATION	UNP Q93VR3

- Molecule 2 is GUANOSINE 5'-DIPHOSPHATE-BETA-L-GULOSE (three-letter code: GKE) (formula: C₁₆H₂₅N₅O₁₆P₂).



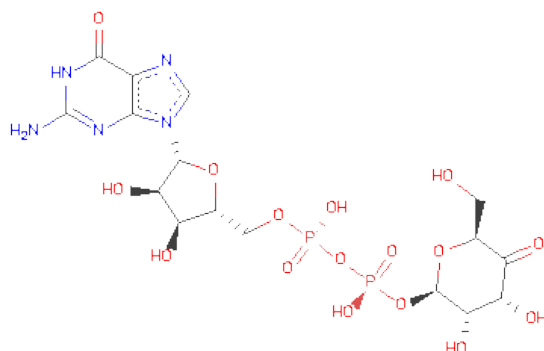
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	1
			39	16	5	16	2		

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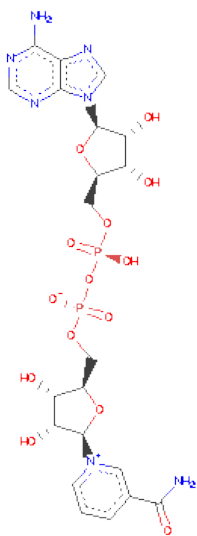
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	1
			39	16	5	16	2		

- Molecule 3 is GUANOSINE 5'-DIPHOSPHATE-4-KETO-BETA-L-GULOSE (three-letter code: GKD) (formula: $C_{16}H_{23}N_5O_{16}P_2$).



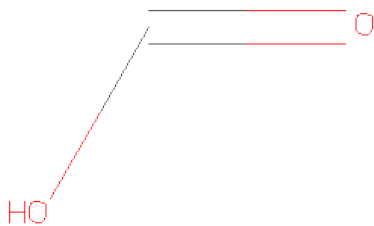
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	1
			39	16	5	16	2		
3	B	1	Total	C	N	O	P	0	1
			39	16	5	16	2		

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	1
			62	32	9	19	2		
4	B	1	Total	C	N	O	P	0	1
			62	32	9	19	2		

- Molecule 5 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



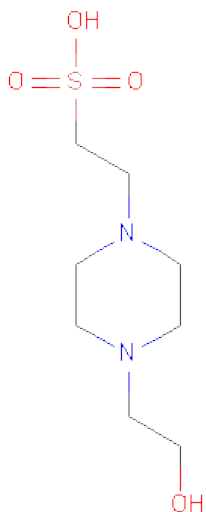
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			3	1	2		
5	A	1	Total	C	O	0	0
			3	1	2		

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

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINEETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

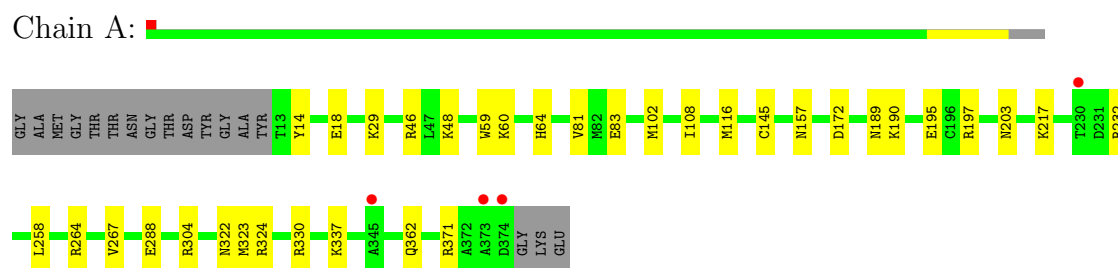
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	466	Total	O	0	0
			466	466		
7	B	478	Total	O	0	0
			478	478		

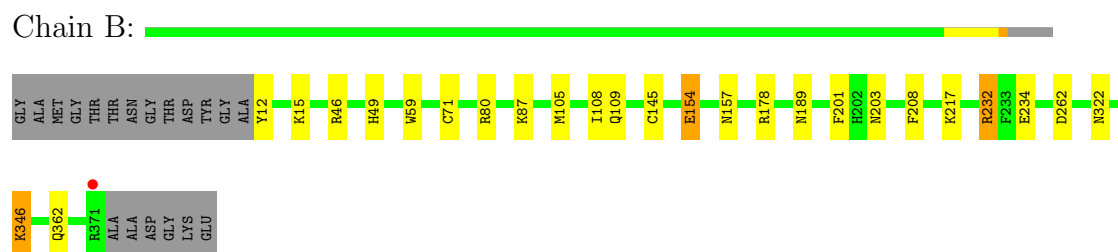
3 Residue-property plots i

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: GDP-MANNOSE-3', 5'-EPIMERASE



- Molecule 1: GDP-MANNOSE-3', 5'-EPIMERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.28Å 82.46Å 65.88Å 90.00° 98.77° 90.00°	Depositor
Resolution (Å)	64.55 – 1.50 23.30 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (64.55-1.50) 99.9 (23.30-1.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.81 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.118 , 0.167 0.131 , 0.174	Depositor DCC
R_{free} test set	5247 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	11.5	Xtriage
Anisotropy	0.531	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 46.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 105046 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7269	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.27% 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: FMT, EPE, GKE, GKD, NAD

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	0.96	1/3120 (0.0%)	0.95	5/4193 (0.1%)
1	B	0.94	1/3092 (0.0%)	0.92	7/4157 (0.2%)
All	All	0.95	2/6212 (0.0%)	0.94	12/8350 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	71	CYS	CB-SG	-5.46	1.73	1.81
1	A	330	ARG	CG-CD	5.14	1.64	1.51

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	ARG	NE-CZ-NH1	9.65	125.12	120.30
1	B	178	ARG	NE-CZ-NH1	9.30	124.95	120.30
1	A	116	MET	CG-SD-CE	-8.62	86.41	100.20
1	B	80	ARG	NE-CZ-NH2	-6.75	116.92	120.30
1	B	178	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	B	46	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	B	208	PHE	CB-CG-CD2	-5.61	116.88	120.80
1	A	197	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	B	208	PHE	CB-CG-CD1	5.26	124.48	120.80
1	B	201	PHE	CB-CG-CD2	-5.13	117.21	120.80
1	A	304	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	A	330	ARG	NE-CZ-NH1	5.08	122.84	120.30

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	3000	0	0	34	0
1	B	2976	0	0	27	0
2	A	39	0	0	1	0
2	B	39	0	0	3	0
3	A	39	0	0	8	0
3	B	39	0	0	4	0
4	A	62	0	0	4	0
4	B	62	0	0	0	0
5	A	27	0	0	1	0
5	B	27	0	0	3	0
6	A	15	0	0	0	0
7	A	466	0	0	16	1
7	B	478	0	0	15	1
All	All	7269	0	0	63	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 11.

All (63) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:232[B]:ARG:NH2	7:B:2301:HOH:O	1.62	1.28
1:B:105[A]:MET:CE	2:B:1372[A]:GKE:O2G	2.10	0.99
1:A:14:TYR:CD2	1:A:323[B]:MET:CE	2.47	0.95
1:A:217[B]:LYS:NZ	3:A:1374[B]:GKD:C4G	2.37	0.88
1:B:232[A]:ARG:NH1	7:B:2303:HOH:O	2.05	0.88
1:A:217[B]:LYS:NZ	3:A:1374[B]:GKD:C3G	2.37	0.87
1:A:217[B]:LYS:NZ	3:A:1374[B]:GKD:O3G	2.12	0.81
1:B:145:CYS:SG	2:B:1372[A]:GKE:O4G	2.42	0.78
1:A:322:ASN:OD1	7:A:2374:HOH:O	2.04	0.77
1:B:217[B]:LYS:NZ	3:B:1374[B]:GKD:C5G	2.48	0.76
1:A:83[B]:GLU:OE2	7:A:2117:HOH:O	2.04	0.75
1:B:262[B]:ASP:CB	7:B:2317:HOH:O	2.34	0.75
1:A:190:LYS:NZ	7:A:2231:HOH:O	2.20	0.74
1:A:217[B]:LYS:NZ	3:A:1374[B]:GKD:C2G	2.52	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:217[B]:LYS:CE	3:A:1374[B]:GKD:C3G	2.69	0.70
1:A:264[B]:ARG:CZ	7:A:2299:HOH:O	2.40	0.69
1:A:371[A]:ARG:NH1	7:A:2432:HOH:O	2.27	0.66
1:B:362:GLN:NE2	7:B:2440:HOH:O	2.28	0.65
1:A:217[A]:LYS:NZ	4:A:1378[A]:NAD:O7N	2.31	0.64
1:B:262[B]:ASP:OD1	7:B:2319:HOH:O	2.16	0.63
1:B:157:ASN:O	7:B:2228:HOH:O	2.16	0.62
1:A:145:CYS:SG	2:A:1372[A]:GKE:O4G	2.58	0.62
1:A:264[B]:ARG:NH2	7:A:2299:HOH:O	2.31	0.61
1:A:14:TYR:CE2	1:A:323[B]:MET:CE	2.84	0.60
3:A:1374[B]:GKD:O4G	4:A:1378[B]:NAD:C4N	2.50	0.60
1:A:108:ILE:CG2	1:A:172[B]:ASP:OD2	2.49	0.59
1:B:217[B]:LYS:CE	3:B:1374[B]:GKD:O3G	2.52	0.58
1:A:172[B]:ASP:OD1	7:A:2219:HOH:O	2.17	0.58
1:B:346:LYS:NZ	1:B:346:LYS:CB	2.67	0.57
1:A:371[B]:ARG:NH1	7:A:2430:HOH:O	2.39	0.55
1:B:154:GLU:OE2	7:B:2222:HOH:O	2.19	0.54
1:A:217[B]:LYS:CE	3:A:1374[B]:GKD:C1G	2.85	0.53
1:A:60:LYS:NZ	7:A:2079:HOH:O	2.40	0.53
1:A:258:LEU:CD2	1:A:267[B]:VAL:CG1	2.88	0.52
1:B:12:TYR:N	7:B:2001:HOH:O	2.44	0.51
1:B:217[B]:LYS:NZ	3:B:1374[B]:GKD:C4G	2.74	0.50
1:A:190:LYS:NZ	7:A:2229:HOH:O	2.43	0.50
1:B:346:LYS:CD	7:B:2408:HOH:O	2.58	0.50
1:B:15[B]:LYS:NZ	7:B:2006:HOH:O	2.45	0.49
1:B:232[B]:ARG:NH2	1:B:234:GLU:OE2	2.46	0.49
1:A:157:ASN:O	7:A:2200:HOH:O	2.20	0.48
1:A:217[A]:LYS:CE	4:A:1378[A]:NAD:C7N	2.91	0.48
1:A:29[B]:LYS:NZ	7:A:2044:HOH:O	2.47	0.48
1:A:362:GLN:NE2	5:A:1387:FMT:O1	2.47	0.48
1:B:108[B]:ILE:CD1	7:B:2254:HOH:O	2.62	0.47
1:A:48:LYS:NZ	7:A:2061:HOH:O	2.47	0.47
1:A:217[A]:LYS:CE	4:A:1378[A]:NAD:O7N	2.64	0.46
1:B:49[A]:HIS:CE1	7:B:2067:HOH:O	2.69	0.46
1:B:109:GLN:O	5:B:1380:FMT:C	2.64	0.46
1:A:288:GLU:OE2	1:A:337:LYS:NZ	2.49	0.45
1:A:264[B]:ARG:NH1	7:A:2299:HOH:O	2.47	0.45
1:B:105[A]:MET:CE	2:B:1372[A]:GKE:C2G	2.96	0.44
1:A:195:GLU:OE2	7:A:2241:HOH:O	2.21	0.43
1:A:64:HIS:CE1	7:A:2245:HOH:O	2.72	0.42
1:B:87:LYS:NZ	7:B:2149:HOH:O	2.52	0.42
1:B:232[A]:ARG:NH2	7:B:2300:HOH:O	2.53	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:109:GLN:O	5:B:1380:FMT:O2	2.37	0.41
1:A:217[B]:LYS:CE	3:A:1374[B]:GKD:C2G	2.98	0.41
1:B:217[B]:LYS:NZ	3:B:1374[B]:GKD:C3G	2.84	0.40
1:B:232[B]:ARG:NH1	5:B:1386:FMT:C	2.84	0.40
1:A:81:VAL:CG1	1:A:83[A]:GLU:CG	2.99	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:2365:HOH:O	7:B:2122:HOH:O[1_554]	2.09	0.11

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	379/379 (100%)	370 (98%)	8 (2%)	1 (0%)	50	20
1	B	374/379 (99%)	365 (98%)	8 (2%)	1 (0%)	50	20
All	All	753/758 (99%)	735 (98%)	16 (2%)	2 (0%)	50	20

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	ASN
1	B	203	ASN

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	328/319 (103%)	320 (98%)	8 (2%)	61	25
1	B	325/319 (102%)	317 (98%)	8 (2%)	60	23
All	All	653/638 (102%)	637 (98%)	16 (2%)	69	23

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18[A]	GLU
1	A	18[B]	GLU
1	A	59	TRP
1	A	102[A]	MET
1	A	102[B]	MET
1	A	189	ASN
1	A	232	ARG
1	A	324	ARG
1	B	59	TRP
1	B	154	GLU
1	B	189	ASN
1	B	232[A]	ARG
1	B	232[B]	ARG
1	B	322[A]	ASN
1	B	322[B]	ASN
1	B	346	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

27 ligands are modelled in this entry.

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	GKE	A	1372[A]	-	42,42,42	1.31	4 (9%)	62,65,65	1.67	10 (16%)
3	GKD	A	1374[B]	1	42,42,42	1.26	4 (9%)	62,65,65	1.73	10 (16%)
4	NAD	A	1378[A]	-	19,19,48	1.78	4 (21%)	27,27,73	1.10	1 (3%)
4	NAD	A	1378[B]	-	19,19,48	2.28	1 (5%)	27,27,73	2.35	7 (25%)
5	FMT	A	1381	-	2,2,2	0.86	0	1,1,1	0.67	0
5	FMT	A	1382	-	2,2,2	0.89	0	1,1,1	0.14	0
5	FMT	A	1383	-	2,2,2	0.44	0	1,1,1	0.27	0
5	FMT	A	1384	-	2,2,2	0.73	0	1,1,1	0.37	0
5	FMT	A	1385	-	2,2,2	0.71	0	1,1,1	0.37	0
5	FMT	A	1386	-	2,2,2	0.63	0	1,1,1	0.35	0
5	FMT	A	1387	-	2,2,2	0.49	0	1,1,1	0.15	0
5	FMT	A	1388	-	2,2,2	0.64	0	1,1,1	0.31	0
5	FMT	A	1389	-	2,2,2	0.61	0	1,1,1	0.66	0
6	EPE	A	1390	-	15,15,15	1.01	1 (6%)	20,20,20	1.79	4 (20%)
2	GKE	B	1372[A]	-	42,42,42	1.16	6 (14%)	62,65,65	1.47	7 (11%)
3	GKD	B	1374[B]	1	42,42,42	1.21	6 (14%)	62,65,65	2.18	11 (17%)
4	NAD	B	1375[A]	-	19,19,48	1.43	4 (21%)	27,27,73	1.85	6 (22%)
4	NAD	B	1375[B]	-	19,19,48	2.35	3 (15%)	27,27,73	2.96	6 (22%)
5	FMT	B	1378	-	2,2,2	0.62	0	1,1,1	0.42	0
5	FMT	B	1379	-	2,2,2	0.85	0	1,1,1	0.51	0
5	FMT	B	1380	-	2,2,2	0.43	0	1,1,1	0.14	0
5	FMT	B	1381	-	2,2,2	1.16	0	1,1,1	0.24	0
5	FMT	B	1382	-	2,2,2	0.60	0	1,1,1	0.47	0
5	FMT	B	1383	-	2,2,2	0.74	0	1,1,1	0.36	0
5	FMT	B	1384	-	2,2,2	0.63	0	1,1,1	0.55	0
5	FMT	B	1385	-	2,2,2	0.59	0	1,1,1	0.32	0
5	FMT	B	1386	-	2,2,2	1.13	0	1,1,1	0.75	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GKE	A	1372[A]	-	-	0/23/59/59	0/2/4/4
3	GKD	A	1374[B]	1	-	0/23/59/59	0/2/4/4
4	NAD	A	1378[A]	-	-	0/10/26/62	0/2/2/5
4	NAD	A	1378[B]	-	-	0/10/26/62	0/2/2/5
5	FMT	A	1381	-	-	0/0/0/0	0/0/0/0
5	FMT	A	1382	-	-	0/0/0/0	0/0/0/0
5	FMT	A	1383	-	-	0/0/0/0	0/0/0/0
5	FMT	A	1384	-	-	0/0/0/0	0/0/0/0
5	FMT	A	1385	-	-	0/0/0/0	0/0/0/0
5	FMT	A	1386	-	-	0/0/0/0	0/0/0/0
5	FMT	A	1387	-	-	0/0/0/0	0/0/0/0
5	FMT	A	1388	-	-	0/0/0/0	0/0/0/0
5	FMT	A	1389	-	-	0/0/0/0	0/0/0/0
6	EPE	A	1390	-	-	0/9/19/19	0/1/1/1
2	GKE	B	1372[A]	-	-	0/23/59/59	0/2/4/4
3	GKD	B	1374[B]	1	-	0/23/59/59	0/2/4/4
4	NAD	B	1375[A]	-	-	0/10/26/62	0/2/2/5
4	NAD	B	1375[B]	-	-	0/10/26/62	0/2/2/5
5	FMT	B	1378	-	-	0/0/0/0	0/0/0/0
5	FMT	B	1379	-	-	0/0/0/0	0/0/0/0
5	FMT	B	1380	-	-	0/0/0/0	0/0/0/0
5	FMT	B	1381	-	-	0/0/0/0	0/0/0/0
5	FMT	B	1382	-	-	0/0/0/0	0/0/0/0
5	FMT	B	1383	-	-	0/0/0/0	0/0/0/0
5	FMT	B	1384	-	-	0/0/0/0	0/0/0/0
5	FMT	B	1385	-	-	0/0/0/0	0/0/0/0
5	FMT	B	1386	-	-	0/0/0/0	0/0/0/0

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1378[B]	NAD	C4N-C3N	9.21	1.55	1.39
4	B	1375[B]	NAD	C4N-C3N	8.62	1.54	1.39
2	A	1372[A]	GKE	C4-N9	-4.87	1.30	1.37
3	A	1374[B]	GKD	C4-N9	-4.87	1.30	1.37
4	A	1378[A]	NAD	C2N-N1N	4.74	1.41	1.35
4	B	1375[B]	NAD	O4D-C1D	4.44	1.48	1.41
4	A	1378[A]	NAD	O7N-C7N	4.21	1.34	1.24
2	A	1372[A]	GKE	O1B-C1G	-3.89	1.34	1.42
3	B	1374[B]	GKD	C4-N9	-3.46	1.32	1.37
2	B	1372[A]	GKE	C4-N9	-3.46	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1390	EPE	C10-S	3.36	1.82	1.77
4	B	1375[A]	NAD	C2N-N1N	3.27	1.39	1.35
4	B	1375[A]	NAD	O7N-C7N	2.72	1.30	1.24
2	B	1372[A]	GKE	O1B-C1G	-2.62	1.37	1.42
3	B	1374[B]	GKD	O5G-C5G	-2.54	1.39	1.43
3	B	1374[B]	GKD	C8-N9	2.49	1.40	1.36
2	B	1372[A]	GKE	C8-N9	2.49	1.40	1.36
4	B	1375[A]	NAD	O4D-C1D	2.42	1.45	1.41
4	B	1375[A]	NAD	C6N-N1N	2.37	1.42	1.35
3	B	1374[B]	GKD	O4'-C1'	-2.36	1.37	1.41
2	B	1372[A]	GKE	O4'-C1'	-2.36	1.37	1.41
3	B	1374[B]	GKD	C5-C4	2.34	1.45	1.40
2	B	1372[A]	GKE	C5-C4	2.34	1.45	1.40
2	A	1372[A]	GKE	C6-C5	2.31	1.45	1.41
3	A	1374[B]	GKD	C6-C5	2.31	1.45	1.41
3	A	1374[B]	GKD	C5G-C4G	2.25	1.54	1.52
2	A	1372[A]	GKE	O6-C6	2.22	1.28	1.24
3	A	1374[B]	GKD	O6-C6	2.22	1.28	1.24
4	A	1378[A]	NAD	C6N-N1N	2.08	1.41	1.35
3	B	1374[B]	GKD	C2'-C1'	2.08	1.56	1.53
2	B	1372[A]	GKE	C2'-C1'	2.08	1.56	1.53
4	B	1375[B]	NAD	C3N-C7N	2.05	1.54	1.50
4	A	1378[A]	NAD	C3N-C7N	2.05	1.54	1.50

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1374[B]	GKD	O5G-C1G-O1B	-10.72	97.35	111.36
4	B	1375[B]	NAD	C5N-C4N-C3N	-9.03	108.59	120.32
4	B	1375[B]	NAD	O4D-C1D-N1N	8.63	116.78	107.95
2	A	1372[A]	GKE	C6-C5-N7	7.26	135.12	134.14
3	A	1374[B]	GKD	C6-C5-N7	7.26	135.12	134.14
4	A	1378[B]	NAD	C5N-C4N-C3N	-6.72	111.59	120.32
4	A	1378[B]	NAD	C2D-C1D-N1N	-5.88	103.90	113.86
4	B	1375[B]	NAD	C6N-N1N-C2N	-5.61	115.70	122.04
3	B	1374[B]	GKD	O5G-C5G-C4G	-5.47	106.28	111.46
3	A	1374[B]	GKD	O5G-C1G-O1B	-5.38	104.33	111.36
3	B	1374[B]	GKD	C8-N9-C4	5.04	110.75	106.90
2	B	1372[A]	GKE	C8-N9-C4	5.04	110.75	106.90
2	A	1372[A]	GKE	O4'-C1'-N9	4.69	112.80	108.44
3	A	1374[B]	GKD	O4'-C1'-N9	4.69	112.80	108.44
4	B	1375[A]	NAD	O5D-C5D-C4D	-4.66	106.76	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1374[B]	GKD	O4'-C1'-N9	4.38	112.51	108.44
2	B	1372[A]	GKE	O4'-C1'-N9	4.38	112.51	108.44
6	A	1390	EPE	O3S-S-C10	4.26	111.32	105.93
4	A	1378[A]	NAD	O5D-C5D-C4D	-4.03	107.64	113.28
4	B	1375[A]	NAD	C4D-O4D-C1D	-3.87	105.54	109.75
6	A	1390	EPE	O3S-S-O2S	-3.76	103.64	111.78
4	B	1375[B]	NAD	C2D-C1D-N1N	-3.72	107.56	113.86
3	B	1374[B]	GKD	N3-C4-N9	3.66	132.28	126.91
2	B	1372[A]	GKE	N3-C4-N9	3.66	132.28	126.91
4	A	1378[B]	NAD	O4D-C1D-N1N	3.59	111.63	107.95
3	B	1374[B]	GKD	C6G-C5G-C4G	-3.44	106.52	111.19
4	A	1378[B]	NAD	O5D-C5D-C4D	-3.35	108.59	113.28
4	B	1375[A]	NAD	C2N-C3N-C4N	3.28	122.02	118.31
3	B	1374[B]	GKD	C6-N1-C2	3.13	124.98	119.51
2	B	1372[A]	GKE	C6-N1-C2	3.13	124.98	119.51
2	B	1372[A]	GKE	O5G-C1G-O1B	-3.00	107.44	111.36
4	B	1375[A]	NAD	C3N-C7N-N7N	2.92	121.09	117.77
3	B	1374[B]	GKD	C5-C4-N9	-2.86	103.03	107.16
2	B	1372[A]	GKE	C5-C4-N9	-2.86	103.03	107.16
6	A	1390	EPE	C9-N1-C6	-2.84	103.98	111.32
2	A	1372[A]	GKE	O5G-C1G-O1B	-2.80	107.70	111.36
2	A	1372[A]	GKE	C4-C5-N7	-2.76	107.16	109.52
3	A	1374[B]	GKD	C4-C5-N7	-2.76	107.16	109.52
4	B	1375[B]	NAD	C3D-C2D-C1D	2.70	105.13	100.91
4	B	1375[A]	NAD	O4D-C1D-C2D	-2.68	102.66	106.77
2	A	1372[A]	GKE	O4G-C4G-C3G	2.67	116.33	110.35
4	B	1375[B]	NAD	C6N-N1N-C1D	-2.60	112.89	119.33
3	B	1374[B]	GKD	C8-N9-C1'	-2.57	121.31	126.38
2	B	1372[A]	GKE	C8-N9-C1'	-2.57	121.31	126.38
4	A	1378[B]	NAD	C6N-N1N-C2N	-2.54	119.17	122.04
6	A	1390	EPE	O3S-S-O1S	2.47	117.11	111.78
3	B	1374[B]	GKD	O3G-C3G-C2G	-2.46	104.85	110.13
4	B	1375[A]	NAD	O7N-C7N-C3N	-2.46	116.80	119.58
2	A	1372[A]	GKE	C4'-O4'-C1'	-2.42	107.12	109.75
3	A	1374[B]	GKD	C4'-O4'-C1'	-2.42	107.12	109.75
3	B	1374[B]	GKD	C5G-C4G-C3G	2.40	120.50	113.14
2	A	1372[A]	GKE	C8-N9-C4	2.33	108.67	106.90
3	A	1374[B]	GKD	C8-N9-C4	2.33	108.67	106.90
2	A	1372[A]	GKE	O3G-C3G-C2G	-2.30	105.19	110.35
3	A	1374[B]	GKD	C1G-C2G-C3G	2.30	113.49	109.69
4	A	1378[B]	NAD	C4N-C3N-C7N	-2.25	115.11	121.10
4	A	1378[B]	NAD	C6N-N1N-C1D	-2.23	113.80	119.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1372[A]	GKE	N3-C4-N9	2.19	130.12	126.91
3	A	1374[B]	GKD	N3-C4-N9	2.19	130.12	126.91
3	A	1374[B]	GKD	PB-O3A-PA	2.13	137.93	131.68
2	A	1372[A]	GKE	N1-C2-N3	2.11	124.75	121.78
3	A	1374[B]	GKD	N1-C2-N3	2.11	124.75	121.78

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	362/379 (95%)	-0.33	4 (1%) 77 84	7, 12, 23, 32	0
1	B	360/379 (94%)	-0.36	1 (0%) 91 94	7, 11, 22, 39	0
All	All	722/758 (95%)	-0.34	5 (0%) 84 90	7, 12, 23, 39	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	345	ALA	3.1
1	A	373	ALA	3.0
1	A	230	THR	2.9
1	B	371	ARG	2.5
1	A	374	ASP	2.4

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(\AA^2)	Q<0.9
6	EPE	A	1390	15/15	0.19	8.40	34,35,42,44	0
5	FMT	A	1388	3/3	0.24	8.28	41,41,43,43	0
5	FMT	B	1383	3/3	0.23	8.24	35,35,35,35	0
5	FMT	A	1384	3/3	0.15	6.45	23,23,24,29	0
5	FMT	B	1381	3/3	0.23	6.17	20,20,23,24	0
5	FMT	B	1380	3/3	0.16	5.09	22,22,24,24	0
5	FMT	A	1389	3/3	0.14	4.80	23,23,24,26	0
5	FMT	B	1384	3/3	0.17	4.60	41,41,42,42	0
5	FMT	A	1386	3/3	0.26	4.29	61,61,62,62	0
5	FMT	B	1385	3/3	0.27	4.18	55,55,55,56	0
5	FMT	A	1387	3/3	0.15	2.21	29,29,30,30	0
5	FMT	B	1379	3/3	0.12	1.94	22,22,26,28	0
5	FMT	A	1385	3/3	0.14	1.91	30,30,31,32	0
5	FMT	B	1378	3/3	0.08	1.03	18,18,23,25	0
5	FMT	B	1386	3/3	0.16	0.95	33,33,33,33	0
5	FMT	A	1383	3/3	0.15	0.60	25,25,26,28	0
3	GKD	A	1374[B]	39/39	0.07	-0.19	8,10,25,29	39
2	GKE	A	1372[A]	39/39	0.07	-0.19	7,9,13,13	39
4	NAD	A	1378[B]	18/44	0.06	-0.24	6,8,9,10	18
5	FMT	B	1382	3/3	0.08	-0.25	28,28,28,28	0
4	NAD	A	1378[A]	18/44	0.06	-0.37	4,5,8,11	18
3	GKD	B	1374[B]	39/39	0.07	-0.38	7,9,22,28	39
2	GKE	B	1372[A]	39/39	0.06	-0.47	7,9,12,13	39
5	FMT	A	1382	3/3	0.07	-0.66	18,18,21,21	0
4	NAD	B	1375[B]	18/44	0.05	-0.71	9,11,14,15	18
4	NAD	B	1375[A]	18/44	0.05	-0.72	4,6,7,9	18
5	FMT	A	1381	3/3	0.04	-0.96	14,14,15,16	0

6.5 Other polymers ⓘ

There are no such residues in this entry.