



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:26 am GMT

PDB ID : 2X6T  
Title : AGME BOUND TO ADP-B-MANNOSE  
Authors : Kowatz, T.; Morrison, J.P.; Tanner, M.E.; Naismith, J.H.  
Deposited on : 2010-02-21  
Resolution : 2.36 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

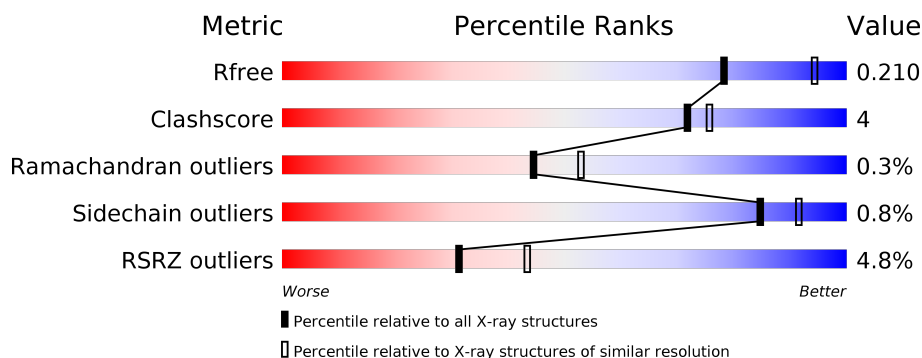
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.36 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))
$R_{free}$	100719	1522 (2.38-2.34)
Clashscore	112137	1626 (2.38-2.34)
Ramachandran outliers	110173	1605 (2.38-2.34)
Sidechain outliers	110143	1606 (2.38-2.34)
RSRZ outliers	101464	1528 (2.38-2.34)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	357	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>6%</div> <div>14%</div> </div> </div>
1	B	357	<div> <div>6%</div> <div> <div></div> <div>82%</div> <div>•</div> <div>14%</div> </div> </div>
1	C	357	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>•</div> <div>14%</div> </div> </div>
1	D	357	<div> <div>7%</div> <div> <div></div> <div>81%</div> <div>5%</div> <div>14%</div> </div> </div>
1	E	357	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>• •</div> <div>14%</div> </div> </div>
1	F	357	<div> <div>7%</div> <div> <div></div> <div>82%</div> <div>•</div> <div>14%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	357	
1	H	357	
1	I	357	
1	J	357	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	1310	-	-	X	X
3	GOL	B	1310	-	-	X	X
3	GOL	C	1310	-	-	X	X
3	GOL	D	1310	-	-	X	X
3	GOL	E	1310	-	-	X	X
3	GOL	F	1310	-	-	X	X
3	GOL	G	1310	-	-	X	X
3	GOL	H	1310	-	-	X	X
3	GOL	I	1310	-	-	X	X
3	GOL	J	1310	-	-	X	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 26879 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 ADP-L-GLYCERO-D-MANNO-HEPTOSE-6-EPIMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2440	1566	396	469	9			
1	B	307	Total	C	N	O	S	0	0	0
			2440	1566	396	469	9			
1	C	307	Total	C	N	O	S	0	0	0
			2440	1566	396	469	9			
1	D	307	Total	C	N	O	S	0	0	0
			2440	1566	396	469	9			
1	E	307	Total	C	N	O	S	0	0	0
			2440	1566	396	469	9			
1	F	307	Total	C	N	O	S	0	0	0
			2440	1566	396	469	9			
1	G	308	Total	C	N	O	S	0	0	0
			2451	1572	400	470	9			
1	H	307	Total	C	N	O	S	0	0	0
			2440	1566	396	469	9			
1	I	307	Total	C	N	O	S	0	0	0
			2440	1566	396	469	9			
1	J	307	Total	C	N	O	S	0	0	0
			2440	1566	396	469	9			

There are 10 discrepancies between the modelled and reference sequences:

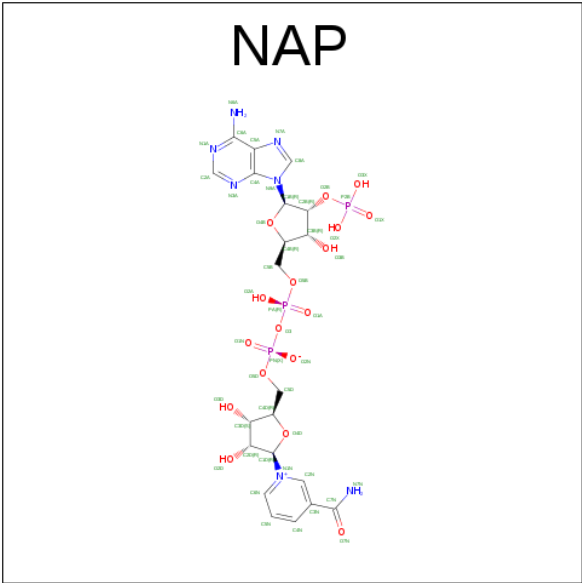
Chain	Residue	Modelled	Actual	Comment	Reference
A	140	PHE	TYR	ENGINEERED MUTATION	UNP P67911
B	140	PHE	TYR	ENGINEERED MUTATION	UNP P67911
C	140	PHE	TYR	ENGINEERED MUTATION	UNP P67911
D	140	PHE	TYR	ENGINEERED MUTATION	UNP P67911
E	140	PHE	TYR	ENGINEERED MUTATION	UNP P67911
F	140	PHE	TYR	ENGINEERED MUTATION	UNP P67911
G	140	PHE	TYR	ENGINEERED MUTATION	UNP P67911
H	140	PHE	TYR	ENGINEERED MUTATION	UNP P67911
I	140	PHE	TYR	ENGINEERED MUTATION	UNP P67911

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Chain	Residue	Modelled	Actual	Comment	Reference
J	140	PHE	TYR	ENGINEERED MUTATION	UNP P67911

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



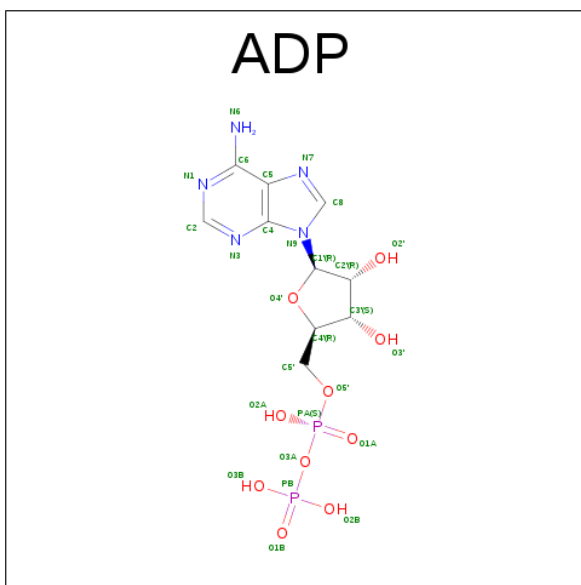
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	H	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	I	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	J	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



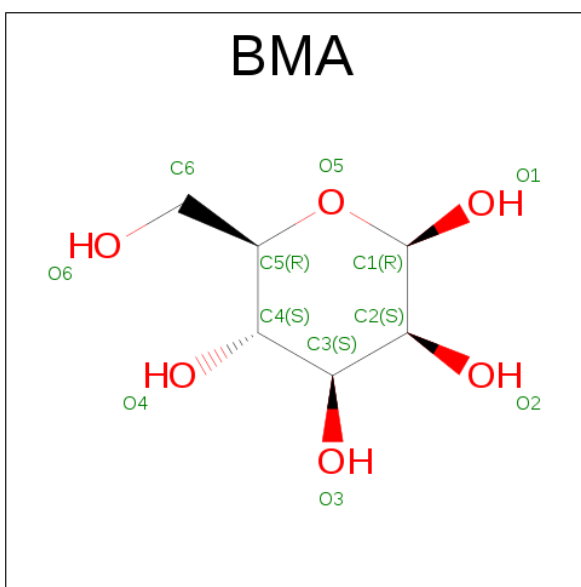
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		
3	I	1	Total	C	O	0	0
			6	3	3		
3	J	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
4	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
4	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
4	D	1	Total 27	C 10	N 5	O 10	P 2	0	0
4	E	1	Total 27	C 10	N 5	O 10	P 2	0	0
4	F	1	Total 27	C 10	N 5	O 10	P 2	0	0
4	G	1	Total 27	C 10	N 5	O 10	P 2	0	0
4	H	1	Total 27	C 10	N 5	O 10	P 2	0	0
4	I	1	Total 27	C 10	N 5	O 10	P 2	0	0
4	J	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 5 is SUGAR (BETA-D-MANNOSE) (three-letter code: BMA) (formula:  $\text{C}_6\text{H}_{12}\text{O}_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		
5	C	1	Total	C	O	0	0
			11	6	5		
5	D	1	Total	C	O	0	0
			11	6	5		
5	E	1	Total	C	O	0	0
			11	6	5		
5	F	1	Total	C	O	0	0
			11	6	5		
5	G	1	Total	C	O	0	0
			11	6	5		
5	H	1	Total	C	O	0	0
			11	6	5		
5	I	1	Total	C	O	0	0
			11	6	5		
5	J	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	2	Total	Cl	0	0
			2	2		

- Molecule 7 is water.

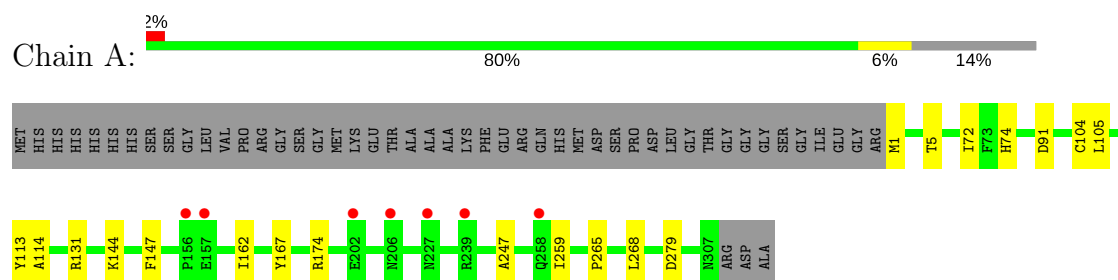


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	186	Total 186	O 186	0	0
7	B	143	Total 143	O 143	0	0
7	C	168	Total 168	O 168	0	0
7	D	115	Total 115	O 115	0	0
7	E	158	Total 158	O 158	0	0
7	F	130	Total 130	O 130	0	0
7	G	176	Total 176	O 176	0	0
7	H	169	Total 169	O 169	0	0
7	I	146	Total 146	O 146	0	0
7	J	155	Total 155	O 155	0	0

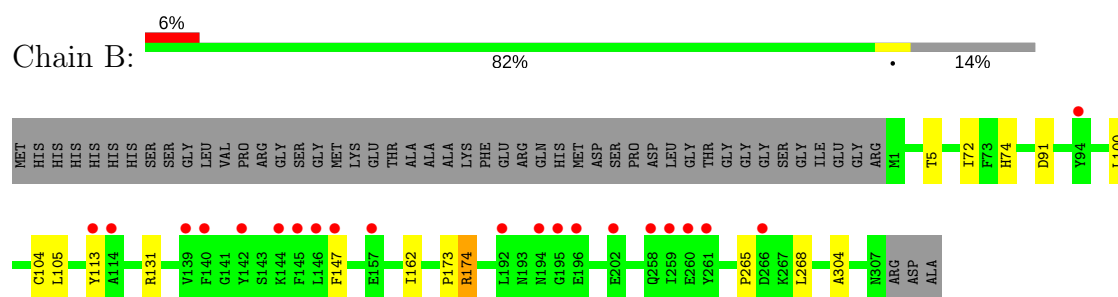
### 3 Residue-property plots [i](#)

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.

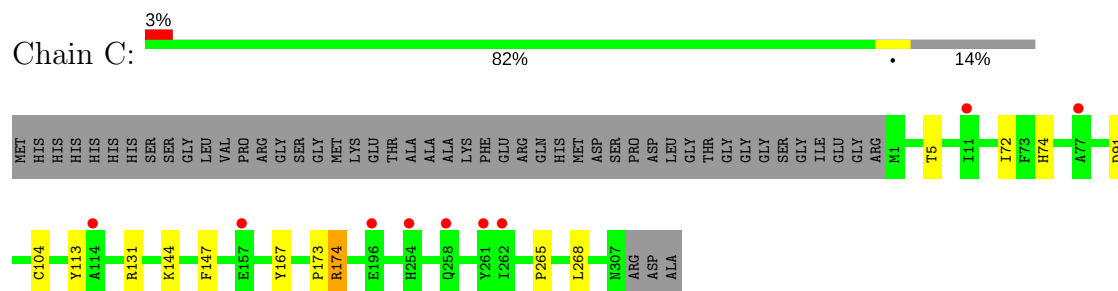
#### • Molecule 1: ADP-L-GLYCERO-D-MANNO-HEPTOSE-6-EPIMERASE



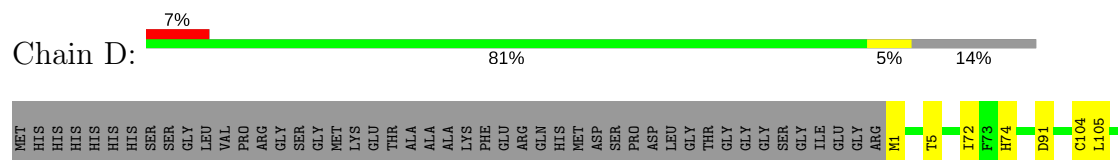
#### • Molecule 1: ADP-L-GLYCERO-D-MANNO-HEPTOSE-6-EPIMERASE

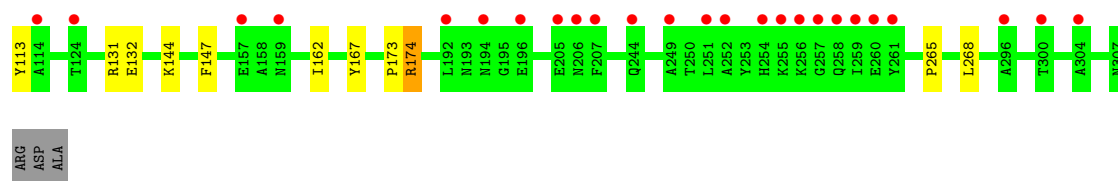


#### • Molecule 1: ADP-L-GLYCERO-D-MANNO-HEPTOSE-6-EPIMERASE

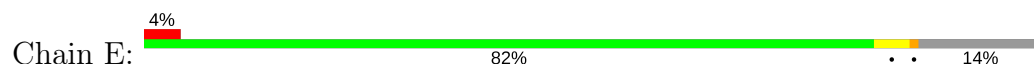


#### • Molecule 1: ADP-L-GLYCERO-D-MANNO-HEPTOSE-6-EPIMERASE

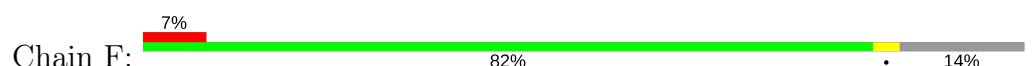




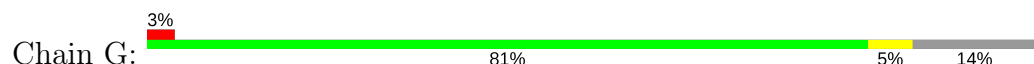
• Molecule 1: ADP-L-GLYCERO-D-MANNO-HEPTOSE-6-EPIMERASE



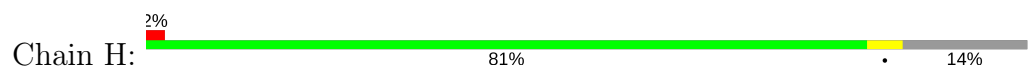
• Molecule 1: ADP-L-GLYCERO-D-MANNO-HEPTOSE-6-EPIMERASE



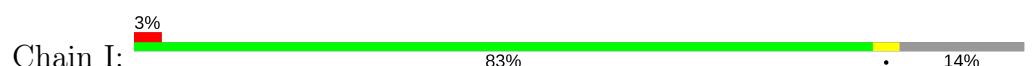
• Molecule 1: ADP-L-GLYCERO-D-MANNO-HEPTOSE-6-EPIMERASE

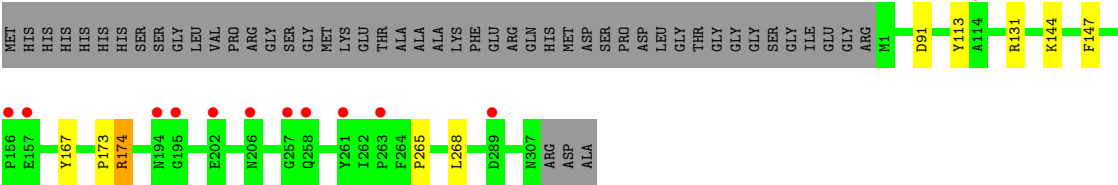


• Molecule 1: ADP-L-GLYCERO-D-MANNO-HEPTOSE-6-EPIMERASE

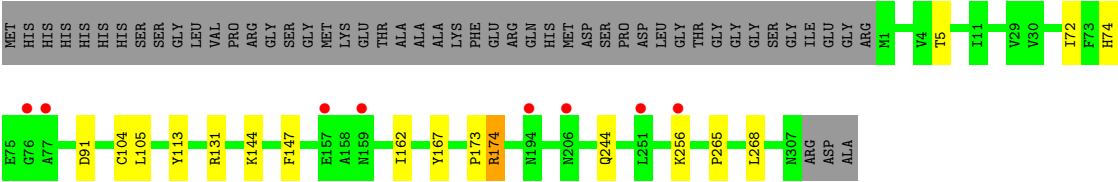
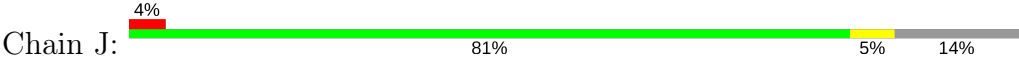


• Molecule 1: ADP-L-GLYCERO-D-MANNO-HEPTOSE-6-EPIMERASE





● Molecule 1: ADP-L-GLYCERO-D-MANNO-HEPTOSE-6-EPIMERASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	341.99Å 60.79Å 191.79Å 90.00° 91.41° 90.00°	Depositor
Resolution (Å)	38.69 – 2.36 38.68 – 2.36	Depositor EDS
% Data completeness (in resolution range)	99.3 (38.69-2.36) 99.2 (38.68-2.36)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.58 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.4.0067	Depositor
R, $R_{free}$	0.189 , 0.209 0.192 , 0.210	Depositor DCC
$R_{free}$ test set	8156 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.3	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 41.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	26879	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, NAP, BMA, 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	0.38	0/2498	0.50	0/3377
1	B	0.35	0/2498	0.48	0/3377
1	C	0.36	0/2498	0.48	0/3377
1	D	0.33	0/2498	0.47	0/3377
1	E	0.36	0/2498	0.48	0/3377
1	F	0.34	0/2498	0.47	0/3377
1	G	0.39	1/2509 (0.0%)	0.51	1/3391 (0.0%)
1	H	0.35	0/2498	0.48	0/3377
1	I	0.36	0/2498	0.48	0/3377
1	J	0.37	1/2498 (0.0%)	0.48	0/3377
All	All	0.36	2/24991 (0.0%)	0.48	1/33784 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	256	LYS	CB-CG	-5.88	1.36	1.52
1	G	297	GLU	CB-CG	-5.45	1.41	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	297	GLU	OE1-CD-OE2	-5.06	117.23	123.30

There are no chirality outliers.

There are no planarity outliers.

## 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	2440	0	2337	19	1
1	B	2440	0	2337	16	0
1	C	2440	0	2337	16	0
1	D	2440	0	2337	20	1
1	E	2440	0	2337	18	0
1	F	2440	0	2337	16	0
1	G	2451	0	2350	12	1
1	H	2440	0	2337	21	0
1	I	2440	0	2337	14	0
1	J	2440	0	2337	18	0
2	A	48	0	25	4	0
2	B	48	0	25	2	0
2	C	48	0	25	3	0
2	D	48	0	25	4	0
2	E	48	0	25	3	0
2	F	48	0	25	4	0
2	G	48	0	25	4	0
2	H	48	0	25	4	0
2	I	48	0	25	3	0
2	J	48	0	25	4	0
3	A	6	0	8	12	0
3	B	6	0	8	7	0
3	C	6	0	8	12	0
3	D	6	0	8	13	0
3	E	6	0	8	11	0
3	F	6	0	8	11	0
3	G	6	0	8	5	0
3	H	6	0	8	10	0
3	I	6	0	8	11	0
3	J	6	0	8	12	0
4	A	27	0	12	0	0
4	B	27	0	12	0	0
4	C	27	0	12	0	0
4	D	27	0	12	0	0
4	E	27	0	12	0	0
4	F	27	0	12	0	0
4	G	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	27	0	12	0	0
4	I	27	0	12	0	0
4	J	27	0	12	0	0
5	A	11	0	10	3	0
5	B	11	0	10	2	0
5	C	11	0	10	2	0
5	D	11	0	10	3	0
5	E	11	0	10	3	0
5	F	11	0	10	3	0
5	G	11	0	10	3	0
5	H	11	0	10	3	0
5	I	11	0	10	2	0
5	J	11	0	10	3	0
6	G	2	0	0	0	0
7	A	186	0	0	1	0
7	B	143	0	0	0	0
7	C	168	0	0	1	0
7	D	115	0	0	2	0
7	E	158	0	0	1	0
7	F	130	0	0	1	0
7	G	176	0	0	1	0
7	H	169	0	0	0	0
7	I	146	0	0	0	0
7	J	155	0	0	2	0
All	All	26879	0	23933	195	2

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 4.

All (195) 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:J:144:LYS:HA	3:J:1310:GOL:H31	1.26	1.18
1:C:144:LYS:HA	3:C:1310:GOL:H31	1.24	1.10
1:A:144:LYS:HA	3:A:1310:GOL:H31	1.33	1.08
1:I:144:LYS:HA	3:I:1310:GOL:H31	1.33	1.08
1:H:144:LYS:HA	3:H:1310:GOL:H31	1.34	1.07
1:D:144:LYS:HA	3:D:1310:GOL:H31	1.37	1.02
1:F:144:LYS:HA	3:F:1310:GOL:H31	1.45	0.95
1:B:304:ALA:CB	1:H:132:GLU:OE1	2.18	0.90
1:C:147:PHE:HB3	3:C:1310:GOL:H32	1.50	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:147:PHE:HB3	3:F:1310:GOL:H32	1.53	0.89
1:E:144:LYS:HA	3:E:1310:GOL:H12	1.55	0.89
1:B:147:PHE:HB3	3:B:1310:GOL:H32	1.56	0.88
1:H:147:PHE:HB3	3:H:1310:GOL:H32	1.55	0.87
1:A:147:PHE:HB3	3:A:1310:GOL:H32	1.55	0.86
1:J:147:PHE:HB3	3:J:1310:GOL:H32	1.56	0.86
1:I:147:PHE:HB3	3:I:1310:GOL:H32	1.59	0.85
1:D:147:PHE:HB3	3:D:1310:GOL:H32	1.58	0.85
1:B:304:ALA:HB1	1:H:132:GLU:OE1	1.78	0.83
2:F:1308:NAP:C4N	5:F:1321:BMA:H61	2.09	0.82
2:H:1308:NAP:C4N	5:H:1321:BMA:H61	2.09	0.82
2:J:1308:NAP:C4N	5:J:1321:BMA:H61	2.09	0.81
1:I:147:PHE:CB	3:I:1310:GOL:H32	2.12	0.80
1:H:147:PHE:CB	3:H:1310:GOL:H32	2.13	0.79
2:D:1308:NAP:C4N	5:D:1321:BMA:H61	2.12	0.78
1:J:147:PHE:CB	3:J:1310:GOL:H32	2.12	0.78
1:J:144:LYS:CD	3:J:1310:GOL:H2	2.13	0.78
1:C:147:PHE:CB	3:C:1310:GOL:H32	2.12	0.78
2:B:1308:NAP:C4N	5:B:1321:BMA:H61	2.13	0.77
2:H:1308:NAP:C5N	5:H:1321:BMA:H61	2.15	0.76
1:A:147:PHE:CB	3:A:1310:GOL:H32	2.14	0.76
1:F:147:PHE:CB	3:F:1310:GOL:H32	2.15	0.75
1:A:144:LYS:HD3	3:A:1310:GOL:H2	1.66	0.75
1:D:147:PHE:CB	3:D:1310:GOL:H32	2.15	0.75
1:A:144:LYS:CD	3:A:1310:GOL:H2	2.18	0.74
2:B:1308:NAP:C5N	5:B:1321:BMA:H61	2.18	0.74
1:C:144:LYS:HD3	3:C:1310:GOL:H2	1.70	0.73
2:G:1308:NAP:C4N	5:G:1321:BMA:H61	2.19	0.72
1:J:144:LYS:HD3	3:J:1310:GOL:H2	1.69	0.72
1:E:147:PHE:HB3	3:E:1310:GOL:H11	1.72	0.72
1:C:144:LYS:CD	3:C:1310:GOL:H2	2.20	0.71
2:A:1308:NAP:C4N	5:A:1321:BMA:H61	2.21	0.71
1:D:144:LYS:HD3	3:D:1310:GOL:H2	1.72	0.70
2:C:1308:NAP:C4N	5:C:1321:BMA:H61	2.21	0.70
1:F:144:LYS:HD3	3:F:1310:GOL:H2	1.73	0.70
2:E:1308:NAP:C4N	5:E:1321:BMA:H61	2.22	0.70
3:J:1310:GOL:O2	7:J:2155:HOH:O	2.01	0.70
1:D:265:PRO:HG2	1:D:268:LEU:HD12	1.75	0.69
1:D:144:LYS:CD	3:D:1310:GOL:H2	2.22	0.69
2:F:1308:NAP:C5N	5:F:1321:BMA:H61	2.22	0.69
1:E:147:PHE:CB	3:E:1310:GOL:H11	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:265:PRO:HG2	1:G:268:LEU:HD12	1.76	0.68
1:F:144:LYS:CD	3:F:1310:GOL:H2	2.25	0.67
1:H:144:LYS:CD	3:H:1310:GOL:H2	2.25	0.67
2:D:1308:NAP:C5N	5:D:1321:BMA:H61	2.24	0.67
1:J:265:PRO:HG2	1:J:268:LEU:HD12	1.77	0.67
1:H:265:PRO:HG2	1:H:268:LEU:HD12	1.76	0.66
1:B:265:PRO:HG2	1:B:268:LEU:HD12	1.75	0.66
1:C:265:PRO:HG2	1:C:268:LEU:HD12	1.78	0.66
1:A:265:PRO:HG2	1:A:268:LEU:HD12	1.77	0.66
1:I:265:PRO:HG2	1:I:268:LEU:HD12	1.76	0.66
1:G:147:PHE:CB	3:G:1310:GOL:H12	2.26	0.65
1:H:144:LYS:HD3	3:H:1310:GOL:H2	1.78	0.64
2:C:1308:NAP:C5N	5:C:1321:BMA:H61	2.28	0.64
1:I:144:LYS:HD3	3:I:1310:GOL:H2	1.79	0.64
1:E:144:LYS:HD3	3:E:1310:GOL:H12	1.79	0.64
1:F:265:PRO:HG2	1:F:268:LEU:HD12	1.78	0.63
1:I:144:LYS:CD	3:I:1310:GOL:H2	2.28	0.63
1:E:265:PRO:HG2	1:E:268:LEU:HD12	1.79	0.62
1:B:147:PHE:CD2	3:B:1310:GOL:H11	2.34	0.62
1:D:147:PHE:HD2	3:D:1310:GOL:H11	1.64	0.62
2:I:1308:NAP:C4N	5:I:1321:BMA:H61	2.30	0.61
1:F:147:PHE:HD2	3:F:1310:GOL:H11	1.66	0.60
1:F:144:LYS:HD3	3:F:1310:GOL:H31	1.82	0.59
1:D:144:LYS:HD3	3:D:1310:GOL:H31	1.85	0.59
1:C:144:LYS:HA	3:C:1310:GOL:C3	2.16	0.59
1:B:113:TYR:CE1	3:B:1310:GOL:H31	2.38	0.59
2:G:1308:NAP:C5N	5:G:1321:BMA:H61	2.32	0.58
1:A:144:LYS:HD3	3:A:1310:GOL:C2	2.33	0.58
1:A:147:PHE:HD2	3:A:1310:GOL:H11	1.67	0.58
2:J:1308:NAP:C5N	5:J:1321:BMA:H61	2.31	0.58
1:A:144:LYS:HD3	3:A:1310:GOL:H31	1.86	0.58
1:H:144:LYS:HD3	3:H:1310:GOL:H31	1.86	0.58
1:C:144:LYS:HD3	3:C:1310:GOL:H31	1.86	0.57
1:J:147:PHE:HD2	3:J:1310:GOL:H11	1.69	0.57
1:C:147:PHE:HD2	3:C:1310:GOL:H11	1.69	0.57
1:C:144:LYS:HD3	3:C:1310:GOL:C2	2.35	0.56
2:E:1308:NAP:C5N	5:E:1321:BMA:H61	2.35	0.56
1:H:147:PHE:HD2	3:H:1310:GOL:H11	1.70	0.56
1:J:144:LYS:HD3	3:J:1310:GOL:C2	2.35	0.56
1:B:304:ALA:HB2	1:H:132:GLU:CD	2.27	0.55
1:C:144:LYS:HD3	3:C:1310:GOL:C3	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:144:LYS:HD3	3:J:1310:GOL:C3	2.36	0.55
1:I:147:PHE:HD2	3:I:1310:GOL:H11	1.72	0.55
1:A:144:LYS:HD3	3:A:1310:GOL:C3	2.37	0.54
1:H:144:LYS:HD3	3:H:1310:GOL:C3	2.37	0.54
1:I:144:LYS:HD3	3:I:1310:GOL:C3	2.39	0.53
1:D:144:LYS:HD3	3:D:1310:GOL:C3	2.39	0.53
1:G:147:PHE:HB2	3:G:1310:GOL:H12	1.89	0.53
1:H:113:TYR:CE1	3:H:1310:GOL:H11	2.43	0.53
1:F:144:LYS:HA	3:F:1310:GOL:C3	2.28	0.52
1:E:147:PHE:CD2	3:E:1310:GOL:H32	2.44	0.52
1:F:144:LYS:HD3	3:F:1310:GOL:C2	2.40	0.52
1:B:304:ALA:CB	1:H:132:GLU:CD	2.78	0.52
1:I:144:LYS:HD3	3:I:1310:GOL:H31	1.92	0.52
1:D:144:LYS:HD3	3:D:1310:GOL:C2	2.39	0.51
2:H:1308:NAP:C5N	5:H:1321:BMA:C6	2.88	0.51
1:A:167:TYR:HB2	2:A:1308:NAP:C5N	2.40	0.51
1:E:144:LYS:HD3	3:E:1310:GOL:C2	2.41	0.51
1:G:167:TYR:HB2	2:G:1308:NAP:C5N	2.41	0.50
1:E:144:LYS:HD3	3:E:1310:GOL:C1	2.40	0.50
1:G:113:TYR:CD1	3:G:1310:GOL:H32	2.47	0.50
1:G:147:PHE:HB3	3:G:1310:GOL:H12	1.93	0.50
1:F:144:LYS:HD3	3:F:1310:GOL:C3	2.42	0.50
1:C:113:TYR:CE1	3:C:1310:GOL:H11	2.46	0.50
1:I:144:LYS:HD3	3:I:1310:GOL:C2	2.42	0.49
1:J:113:TYR:CE1	3:J:1310:GOL:H11	2.47	0.48
1:D:113:TYR:CE1	3:D:1310:GOL:H11	2.48	0.48
1:J:144:LYS:HD2	3:J:1310:GOL:H2	1.91	0.48
3:C:1310:GOL:O2	7:C:2168:HOH:O	2.15	0.47
1:A:144:LYS:HA	3:A:1310:GOL:C3	2.23	0.47
1:I:167:TYR:HB2	2:I:1308:NAP:C5N	2.44	0.47
1:H:144:LYS:HD3	3:H:1310:GOL:C2	2.42	0.47
1:C:167:TYR:HB2	2:C:1308:NAP:C5N	2.44	0.47
1:F:113:TYR:CE1	3:F:1310:GOL:H11	2.49	0.47
1:J:105:LEU:HD11	1:J:162:ILE:HD11	1.97	0.47
1:B:147:PHE:HD2	3:B:1310:GOL:C3	2.29	0.46
2:F:1308:NAP:C5N	5:F:1321:BMA:C6	2.93	0.46
1:E:144:LYS:HD3	3:E:1310:GOL:H2	1.98	0.46
2:D:1308:NAP:C5N	5:D:1321:BMA:C6	2.93	0.45
1:A:1:MET:N	7:A:2001:HOH:O	2.36	0.45
2:G:1308:NAP:C5N	5:G:1321:BMA:C6	2.94	0.45
1:H:105:LEU:HD11	1:H:162:ILE:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:105:LEU:HD11	1:G:162:ILE:HD11	1.99	0.45
2:J:1308:NAP:C5N	5:J:1321:BMA:C6	2.94	0.45
1:D:167:TYR:HB2	2:D:1308:NAP:C5N	2.47	0.45
1:D:1:MET:N	7:D:2001:HOH:O	2.46	0.45
1:J:167:TYR:HB2	2:J:1308:NAP:C5N	2.47	0.45
1:F:87:LYS:NZ	7:F:2040:HOH:O	2.47	0.44
1:H:167:TYR:HB2	2:H:1308:NAP:C5N	2.47	0.44
1:F:167:TYR:HB2	2:F:1308:NAP:C5N	2.48	0.44
1:J:144:LYS:HD3	3:J:1310:GOL:H31	1.99	0.44
1:G:144:LYS:HD3	3:G:1310:GOL:H2	2.00	0.44
1:B:113:TYR:HE1	3:B:1310:GOL:H31	1.82	0.44
2:A:1308:NAP:C5N	5:A:1321:BMA:H61	2.47	0.44
1:B:173:PRO:O	1:B:174:ARG:HB2	2.17	0.43
1:J:5:THR:OG1	1:J:74:HIS:HA	2.18	0.43
1:H:72:ILE:HD12	1:H:104:CYS:SG	2.59	0.43
2:A:1308:NAP:C5N	5:A:1321:BMA:C6	2.96	0.43
1:D:144:LYS:HA	3:D:1310:GOL:C3	2.27	0.43
1:F:173:PRO:O	1:F:174:ARG:HB2	2.18	0.43
1:G:1:MET:N	7:G:2001:HOH:O	2.52	0.43
1:I:113:TYR:CE1	3:I:1310:GOL:H11	2.53	0.43
1:E:173:PRO:O	1:E:174:ARG:HB2	2.18	0.43
1:J:173:PRO:O	1:J:174:ARG:HB2	2.19	0.43
2:E:1308:NAP:C5N	5:E:1321:BMA:C6	2.96	0.43
1:C:72:ILE:HD12	1:C:104:CYS:SG	2.58	0.42
1:B:147:PHE:CD2	3:B:1310:GOL:C1	2.99	0.42
1:B:147:PHE:HD2	3:B:1310:GOL:H31	1.84	0.42
1:E:144:LYS:CD	3:E:1310:GOL:H2	2.50	0.42
1:A:114:ALA:O	3:A:1310:GOL:H12	2.20	0.42
1:A:247:ALA:HB1	1:A:259:ILE:HD11	2.02	0.42
1:E:147:PHE:CD2	3:E:1310:GOL:C3	3.02	0.42
1:I:147:PHE:HB2	3:I:1310:GOL:H32	1.96	0.42
1:E:144:LYS:NZ	3:E:1310:GOL:H2	2.35	0.42
1:C:173:PRO:O	1:C:174:ARG:HB2	2.20	0.42
1:D:105:LEU:HD11	1:D:162:ILE:HD11	2.02	0.42
1:A:113:TYR:CE1	3:A:1310:GOL:H11	2.55	0.41
1:I:173:PRO:O	1:I:174:ARG:HB2	2.21	0.41
1:J:244:GLN:NE2	7:J:2104:HOH:O	2.47	0.41
1:A:5:THR:OG1	1:A:74:HIS:HA	2.20	0.41
1:J:72:ILE:HD12	1:J:104:CYS:SG	2.60	0.41
1:D:147:PHE:HB2	3:D:1310:GOL:H32	2.00	0.41
3:D:1310:GOL:O2	7:D:2114:HOH:O	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:THR:OG1	1:B:74:HIS:HA	2.20	0.41
1:F:105:LEU:HD11	1:F:162:ILE:HD11	2.01	0.41
1:D:173:PRO:O	1:D:174:ARG:HB2	2.21	0.41
1:D:5:THR:OG1	1:D:74:HIS:HA	2.21	0.41
1:A:72:ILE:HD12	1:A:104:CYS:SG	2.60	0.41
1:B:72:ILE:HD12	1:B:104:CYS:SG	2.61	0.41
1:E:5:THR:OG1	1:E:74:HIS:HA	2.21	0.41
1:E:87:LYS:O	1:E:91:ASP:HB2	2.21	0.41
1:A:105:LEU:HD11	1:A:162:ILE:HD11	2.02	0.41
1:E:204:SER:HA	1:E:207:PHE:CD2	2.56	0.41
1:E:1:MET:N	7:E:2001:HOH:O	2.50	0.40
1:H:105:LEU:HD21	1:H:154:ILE:CG2	2.51	0.40
1:C:5:THR:OG1	1:C:74:HIS:HA	2.21	0.40
1:D:132:GLU:CD	1:D:132:GLU:H	2.24	0.40
1:E:72:ILE:HD12	1:E:104:CYS:SG	2.61	0.40
1:D:72:ILE:HD12	1:D:104:CYS:SG	2.62	0.40
1:G:204:SER:HA	1:G:207:PHE:CD2	2.56	0.40
1:G:89:MET:O	1:G:93:ASN:HB2	2.21	0.40
1:B:105:LEU:HD11	1:B:162:ILE:HD11	2.04	0.40
1:H:173:PRO:O	1:H:174:ARG:HB2	2.22	0.40
2:I:1308:NAP:C5N	5:I:1321:BMA:H61	2.51	0.40
1:G:90:MET:HG3	1:H:33:LEU:HD12	2.04	0.40

All (2) 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	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:GLU:OE1	1:D:132:GLU:OE1[2_554]	1.75	0.45
1:A:279:ASP:OD2	1:G:297:GLU:OE2[4_545]	2.13	0.07

## 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	305/357 (85%)	296 (97%)	8 (3%)	1 (0%)	44	53
1	B	305/357 (85%)	296 (97%)	8 (3%)	1 (0%)	44	53
1	C	305/357 (85%)	296 (97%)	8 (3%)	1 (0%)	44	53
1	D	305/357 (85%)	296 (97%)	8 (3%)	1 (0%)	44	53
1	E	305/357 (85%)	296 (97%)	8 (3%)	1 (0%)	44	53
1	F	305/357 (85%)	296 (97%)	8 (3%)	1 (0%)	44	53
1	G	306/357 (86%)	297 (97%)	8 (3%)	1 (0%)	44	53
1	H	305/357 (85%)	296 (97%)	8 (3%)	1 (0%)	44	53
1	I	305/357 (85%)	296 (97%)	8 (3%)	1 (0%)	44	53
1	J	305/357 (85%)	296 (97%)	8 (3%)	1 (0%)	44	53
All	All	3051/3570 (86%)	2961 (97%)	80 (3%)	10 (0%)	44	53

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	174	ARG
1	B	174	ARG
1	C	174	ARG
1	D	174	ARG
1	E	174	ARG
1	F	174	ARG
1	G	174	ARG
1	H	174	ARG
1	I	174	ARG
1	J	174	ARG

### 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	255/292 (87%)	253 (99%)	2 (1%)	85	91
1	B	255/292 (87%)	252 (99%)	3 (1%)	75	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	255/292 (87%)	253 (99%)	2 (1%)	85	91
1	D	255/292 (87%)	253 (99%)	2 (1%)	85	91
1	E	255/292 (87%)	253 (99%)	2 (1%)	85	91
1	F	255/292 (87%)	253 (99%)	2 (1%)	85	91
1	G	256/292 (88%)	254 (99%)	2 (1%)	85	91
1	H	255/292 (87%)	253 (99%)	2 (1%)	85	91
1	I	255/292 (87%)	253 (99%)	2 (1%)	85	91
1	J	255/292 (87%)	253 (99%)	2 (1%)	85	91
All	All	2551/2920 (87%)	2530 (99%)	21 (1%)	85	91

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	ASP
1	A	131	ARG
1	B	91	ASP
1	B	100	LEU
1	B	131	ARG
1	C	91	ASP
1	C	131	ARG
1	D	91	ASP
1	D	131	ARG
1	E	91	ASP
1	E	131	ARG
1	F	91	ASP
1	F	131	ARG
1	G	91	ASP
1	G	131	ARG
1	H	91	ASP
1	H	131	ARG
1	I	91	ASP
1	I	131	ARG
1	J	91	ASP
1	J	131	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	277	GLN
1	J	244	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 42 ligands modelled in this entry, 2 are monoatomic - leaving 40 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	NAP	A	1308	-	44,52,52	1.66	4 (9%)	51,80,80	1.72	4 (7%)
3	GOL	A	1310	-	5,5,5	0.63	0	5,5,5	1.08	0
4	ADP	A	1320	5	25,29,29	1.08	2 (8%)	24,45,45	1.89	2 (8%)
5	BMA	A	1321	4	11,11,12	0.50	0	13,15,17	1.13	1 (7%)
2	NAP	B	1308	-	44,52,52	1.71	4 (9%)	51,80,80	1.67	5 (9%)
3	GOL	B	1310	-	5,5,5	0.29	0	5,5,5	0.96	0
4	ADP	B	1320	5	25,29,29	1.06	2 (8%)	24,45,45	1.85	2 (8%)
5	BMA	B	1321	4	11,11,12	0.54	0	13,15,17	0.74	0
2	NAP	C	1308	-	44,52,52	1.72	5 (11%)	51,80,80	1.62	4 (7%)
3	GOL	C	1310	-	5,5,5	0.54	0	5,5,5	1.13	1 (20%)
4	ADP	C	1320	5	25,29,29	1.07	2 (8%)	24,45,45	1.78	2 (8%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	BMA	C	1321	4	11,11,12	0.46	0	13,15,17	0.85	0
2	NAP	D	1308	-	44,52,52	1.67	4 (9%)	51,80,80	1.70	4 (7%)
3	GOL	D	1310	-	5,5,5	0.64	0	5,5,5	1.13	1 (20%)
4	ADP	D	1320	5	25,29,29	1.14	2 (8%)	24,45,45	1.76	2 (8%)
5	BMA	D	1321	4	11,11,12	0.48	0	13,15,17	0.62	0
2	NAP	E	1308	-	44,52,52	1.66	4 (9%)	51,80,80	1.56	2 (3%)
3	GOL	E	1310	-	5,5,5	0.22	0	5,5,5	0.96	0
4	ADP	E	1320	5	25,29,29	1.09	2 (8%)	24,45,45	1.77	2 (8%)
5	BMA	E	1321	4	11,11,12	0.50	0	13,15,17	0.72	0
2	NAP	F	1308	-	44,52,52	1.67	4 (9%)	51,80,80	1.76	2 (3%)
3	GOL	F	1310	-	5,5,5	0.54	0	5,5,5	1.01	0
4	ADP	F	1320	5	25,29,29	1.10	2 (8%)	24,45,45	1.76	1 (4%)
5	BMA	F	1321	4	11,11,12	0.45	0	13,15,17	0.83	1 (7%)
2	NAP	G	1308	-	44,52,52	1.66	4 (9%)	51,80,80	1.64	2 (3%)
3	GOL	G	1310	-	5,5,5	0.39	0	5,5,5	0.84	0
4	ADP	G	1320	5	25,29,29	1.05	2 (8%)	24,45,45	1.86	2 (8%)
5	BMA	G	1321	4	11,11,12	0.56	0	13,15,17	1.06	1 (7%)
2	NAP	H	1308	-	44,52,52	1.65	4 (9%)	51,80,80	1.66	3 (5%)
3	GOL	H	1310	-	5,5,5	0.52	0	5,5,5	1.16	1 (20%)
4	ADP	H	1320	5	25,29,29	1.09	2 (8%)	24,45,45	1.76	2 (8%)
5	BMA	H	1321	4	11,11,12	0.55	0	13,15,17	0.77	0
2	NAP	I	1308	-	44,52,52	1.67	4 (9%)	51,80,80	1.62	2 (3%)
3	GOL	I	1310	-	5,5,5	0.57	0	5,5,5	1.07	0
4	ADP	I	1320	5	25,29,29	1.11	2 (8%)	24,45,45	1.74	1 (4%)
5	BMA	I	1321	4	11,11,12	0.49	0	13,15,17	0.85	0
2	NAP	J	1308	-	44,52,52	1.68	4 (9%)	51,80,80	1.68	1 (1%)
3	GOL	J	1310	-	5,5,5	0.57	0	5,5,5	0.76	0
4	ADP	J	1320	5	25,29,29	1.07	2 (8%)	24,45,45	1.85	2 (8%)
5	BMA	J	1321	4	11,11,12	0.46	0	13,15,17	0.62	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	NAP	A	1308	-	-	0/27/67/67	0/5/5/5
3	GOL	A	1310	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	A	1320	5	-	0/12/32/32	0/3/3/3
5	BMA	A	1321	4	-	0/2/19/22	0/1/1/1
2	NAP	B	1308	-	-	0/27/67/67	0/5/5/5
3	GOL	B	1310	-	-	0/4/4/4	0/0/0/0
4	ADP	B	1320	5	-	0/12/32/32	0/3/3/3
5	BMA	B	1321	4	-	0/2/19/22	0/1/1/1
2	NAP	C	1308	-	-	0/27/67/67	0/5/5/5
3	GOL	C	1310	-	-	0/4/4/4	0/0/0/0
4	ADP	C	1320	5	-	0/12/32/32	0/3/3/3
5	BMA	C	1321	4	-	0/2/19/22	0/1/1/1
2	NAP	D	1308	-	-	0/27/67/67	0/5/5/5
3	GOL	D	1310	-	-	0/4/4/4	0/0/0/0
4	ADP	D	1320	5	-	0/12/32/32	0/3/3/3
5	BMA	D	1321	4	-	0/2/19/22	0/1/1/1
2	NAP	E	1308	-	-	0/27/67/67	0/5/5/5
3	GOL	E	1310	-	-	0/4/4/4	0/0/0/0
4	ADP	E	1320	5	-	0/12/32/32	0/3/3/3
5	BMA	E	1321	4	-	0/2/19/22	0/1/1/1
2	NAP	F	1308	-	-	0/27/67/67	0/5/5/5
3	GOL	F	1310	-	-	0/4/4/4	0/0/0/0
4	ADP	F	1320	5	-	0/12/32/32	0/3/3/3
5	BMA	F	1321	4	-	0/2/19/22	0/1/1/1
2	NAP	G	1308	-	-	0/27/67/67	0/5/5/5
3	GOL	G	1310	-	-	0/4/4/4	0/0/0/0
4	ADP	G	1320	5	-	0/12/32/32	0/3/3/3
5	BMA	G	1321	4	-	0/2/19/22	0/1/1/1
2	NAP	H	1308	-	-	0/27/67/67	0/5/5/5
3	GOL	H	1310	-	-	0/4/4/4	0/0/0/0
4	ADP	H	1320	5	-	0/12/32/32	0/3/3/3
5	BMA	H	1321	4	-	0/2/19/22	0/1/1/1
2	NAP	I	1308	-	-	0/27/67/67	0/5/5/5
3	GOL	I	1310	-	-	0/4/4/4	0/0/0/0
4	ADP	I	1320	5	-	0/12/32/32	0/3/3/3
5	BMA	I	1321	4	-	0/2/19/22	0/1/1/1
2	NAP	J	1308	-	-	0/27/67/67	0/5/5/5
3	GOL	J	1310	-	-	0/4/4/4	0/0/0/0
4	ADP	J	1320	5	-	0/12/32/32	0/3/3/3
5	BMA	J	1321	4	-	0/2/19/22	0/1/1/1

All (61) bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	1320	ADP	C8-N7	-2.63	1.29	1.34
4	G	1320	ADP	C8-N7	-2.51	1.30	1.34
4	C	1320	ADP	C8-N7	-2.47	1.30	1.34
4	B	1320	ADP	C8-N7	-2.39	1.30	1.34
4	J	1320	ADP	C8-N7	-2.36	1.30	1.34
4	D	1320	ADP	C8-N7	-2.35	1.30	1.34
4	A	1320	ADP	C8-N7	-2.23	1.30	1.34
4	F	1320	ADP	C8-N7	-2.18	1.30	1.34
4	H	1320	ADP	C8-N7	-2.15	1.30	1.34
4	E	1320	ADP	C8-N7	-2.04	1.30	1.34
2	C	1308	NAP	O4B-C1B	2.03	1.44	1.41
2	F	1308	NAP	C2A-N1A	2.29	1.38	1.33
2	E	1308	NAP	C2A-N1A	2.30	1.38	1.33
2	G	1308	NAP	C2A-N1A	2.38	1.38	1.33
2	A	1308	NAP	C2A-N1A	2.40	1.38	1.33
2	H	1308	NAP	C2A-N1A	2.42	1.38	1.33
2	J	1308	NAP	C2A-N1A	2.42	1.38	1.33
2	I	1308	NAP	C2A-N1A	2.44	1.38	1.33
2	B	1308	NAP	C2A-N1A	2.52	1.38	1.33
4	G	1320	ADP	O4'-C1'	2.59	1.44	1.41
2	D	1308	NAP	C2A-N1A	2.63	1.38	1.33
2	C	1308	NAP	C2A-N1A	2.68	1.38	1.33
4	C	1320	ADP	O4'-C1'	2.69	1.45	1.41
4	B	1320	ADP	O4'-C1'	2.71	1.45	1.41
2	D	1308	NAP	P2B-O2B	2.86	1.64	1.59
4	A	1320	ADP	O4'-C1'	2.86	1.45	1.41
4	D	1320	ADP	O4'-C1'	2.95	1.45	1.41
4	I	1320	ADP	O4'-C1'	2.96	1.45	1.41
2	A	1308	NAP	P2B-O2B	2.99	1.64	1.59
2	J	1308	NAP	P2B-O2B	3.00	1.64	1.59
4	E	1320	ADP	O4'-C1'	3.02	1.45	1.41
4	F	1320	ADP	O4'-C1'	3.08	1.45	1.41
4	J	1320	ADP	O4'-C1'	3.12	1.45	1.41
4	H	1320	ADP	O4'-C1'	3.15	1.45	1.41
2	H	1308	NAP	C2A-N3A	3.16	1.37	1.32
2	G	1308	NAP	C2A-N3A	3.23	1.37	1.32
2	C	1308	NAP	P2B-O2B	3.24	1.65	1.59
2	G	1308	NAP	P2B-O2B	3.26	1.65	1.59
2	F	1308	NAP	P2B-O2B	3.27	1.65	1.59
2	A	1308	NAP	C2A-N3A	3.35	1.37	1.32
2	D	1308	NAP	C2A-N3A	3.42	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	1308	NAP	P2B-O2B	3.43	1.65	1.59
2	H	1308	NAP	P2B-O2B	3.46	1.65	1.59
2	I	1308	NAP	C2A-N3A	3.52	1.38	1.32
2	E	1308	NAP	P2B-O2B	3.56	1.65	1.59
2	B	1308	NAP	C2A-N3A	3.57	1.38	1.32
2	E	1308	NAP	C2A-N3A	3.64	1.38	1.32
2	B	1308	NAP	P2B-O2B	3.66	1.66	1.59
2	F	1308	NAP	C2A-N3A	3.66	1.38	1.32
2	J	1308	NAP	C2A-N3A	3.84	1.38	1.32
2	C	1308	NAP	C2A-N3A	3.97	1.38	1.32
2	E	1308	NAP	O7N-C7N	8.18	1.41	1.24
2	F	1308	NAP	O7N-C7N	8.40	1.41	1.24
2	H	1308	NAP	O7N-C7N	8.41	1.41	1.24
2	G	1308	NAP	O7N-C7N	8.49	1.41	1.24
2	J	1308	NAP	O7N-C7N	8.52	1.41	1.24
2	C	1308	NAP	O7N-C7N	8.58	1.41	1.24
2	A	1308	NAP	O7N-C7N	8.58	1.41	1.24
2	D	1308	NAP	O7N-C7N	8.60	1.41	1.24
2	I	1308	NAP	O7N-C7N	8.61	1.41	1.24
2	B	1308	NAP	O7N-C7N	8.63	1.42	1.24

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1308	NAP	N3A-C2A-N1A	-10.16	120.01	128.86
2	A	1308	NAP	N3A-C2A-N1A	-10.12	120.04	128.86
2	J	1308	NAP	N3A-C2A-N1A	-10.05	120.11	128.86
2	F	1308	NAP	N3A-C2A-N1A	-9.95	120.19	128.86
2	I	1308	NAP	N3A-C2A-N1A	-9.83	120.30	128.86
2	H	1308	NAP	N3A-C2A-N1A	-9.78	120.34	128.86
2	G	1308	NAP	N3A-C2A-N1A	-9.66	120.44	128.86
2	E	1308	NAP	N3A-C2A-N1A	-9.24	120.81	128.86
2	B	1308	NAP	N3A-C2A-N1A	-9.23	120.82	128.86
2	C	1308	NAP	N3A-C2A-N1A	-9.17	120.87	128.86
4	A	1320	ADP	N3-C2-N1	-8.50	121.45	128.86
4	B	1320	ADP	N3-C2-N1	-8.21	121.71	128.86
4	G	1320	ADP	N3-C2-N1	-8.12	121.78	128.86
4	J	1320	ADP	N3-C2-N1	-8.09	121.81	128.86
4	C	1320	ADP	N3-C2-N1	-7.74	122.12	128.86
4	D	1320	ADP	N3-C2-N1	-7.71	122.14	128.86
4	H	1320	ADP	N3-C2-N1	-7.67	122.18	128.86
4	F	1320	ADP	N3-C2-N1	-7.64	122.21	128.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	1320	ADP	N3-C2-N1	-7.57	122.26	128.86
4	E	1320	ADP	N3-C2-N1	-7.57	122.26	128.86
4	E	1320	ADP	C4-C5-N7	-2.66	106.84	109.41
4	H	1320	ADP	C4-C5-N7	-2.44	107.05	109.41
4	J	1320	ADP	C4-C5-N7	-2.42	107.07	109.41
2	C	1308	NAP	C1B-N9A-C4A	-2.32	122.63	126.64
2	E	1308	NAP	C4A-C5A-N7A	-2.26	107.23	109.41
2	B	1308	NAP	C4A-C5A-N7A	-2.23	107.25	109.41
2	C	1308	NAP	C4A-C5A-N7A	-2.22	107.27	109.41
2	G	1308	NAP	C4A-C5A-N7A	-2.20	107.28	109.41
2	I	1308	NAP	C1B-N9A-C4A	-2.18	122.86	126.64
2	H	1308	NAP	C1B-N9A-C4A	-2.18	122.86	126.64
2	A	1308	NAP	O4B-C1B-C2B	-2.18	102.78	106.59
4	C	1320	ADP	C4-C5-N7	-2.15	107.33	109.41
2	B	1308	NAP	C1B-N9A-C4A	-2.13	122.95	126.64
4	D	1320	ADP	C4-C5-N7	-2.11	107.37	109.41
2	D	1308	NAP	C1B-N9A-C4A	-2.09	123.02	126.64
2	A	1308	NAP	C4A-C5A-N7A	-2.09	107.39	109.41
5	A	1321	BMA	C3-C4-C5	-2.07	106.56	110.22
2	A	1308	NAP	C1B-N9A-C4A	-2.07	123.06	126.64
4	B	1320	ADP	C4-C5-N7	-2.06	107.42	109.41
4	G	1320	ADP	C4-C5-N7	-2.06	107.42	109.41
2	D	1308	NAP	C4A-C5A-N7A	-2.05	107.42	109.41
5	F	1321	BMA	C6-C5-C4	-2.04	108.22	113.00
4	A	1320	ADP	C4-C5-N7	-2.01	107.47	109.41
3	D	1310	GOL	O1-C1-C2	2.01	120.22	110.07
2	B	1308	NAP	O3B-C3B-C2B	2.04	116.97	111.18
3	H	1310	GOL	O1-C1-C2	2.08	120.56	110.07
3	C	1310	GOL	O1-C1-C2	2.11	120.71	110.07
2	H	1308	NAP	O3X-P2B-O2B	2.27	116.34	106.00
2	C	1308	NAP	C3N-C7N-N7N	2.30	120.40	117.77
5	G	1321	BMA	C1-O5-C5	2.31	115.35	112.17
2	B	1308	NAP	C3N-C7N-N7N	2.44	120.56	117.77
2	D	1308	NAP	C3N-C7N-N7N	2.44	120.56	117.77
2	F	1308	NAP	C3N-C7N-N7N	3.50	121.77	117.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

30 monomers are involved in 139 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1308	NAP	4	0
3	A	1310	GOL	12	0
5	A	1321	BMA	3	0
2	B	1308	NAP	2	0
3	B	1310	GOL	7	0
5	B	1321	BMA	2	0
2	C	1308	NAP	3	0
3	C	1310	GOL	12	0
5	C	1321	BMA	2	0
2	D	1308	NAP	4	0
3	D	1310	GOL	13	0
5	D	1321	BMA	3	0
2	E	1308	NAP	3	0
3	E	1310	GOL	11	0
5	E	1321	BMA	3	0
2	F	1308	NAP	4	0
3	F	1310	GOL	11	0
5	F	1321	BMA	3	0
2	G	1308	NAP	4	0
3	G	1310	GOL	5	0
5	G	1321	BMA	3	0
2	H	1308	NAP	4	0
3	H	1310	GOL	10	0
5	H	1321	BMA	3	0
2	I	1308	NAP	3	0
3	I	1310	GOL	11	0
5	I	1321	BMA	2	0
2	J	1308	NAP	4	0
3	J	1310	GOL	12	0
5	J	1321	BMA	3	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	307/357 (85%)	0.25	7 (2%) 61 71	27, 29, 30, 32	0
1	B	307/357 (85%)	0.42	21 (6%) 18 26	27, 29, 30, 32	0
1	C	307/357 (85%)	0.33	9 (2%) 52 63	27, 29, 30, 32	0
1	D	307/357 (85%)	0.47	25 (8%) 13 18	27, 29, 30, 32	0
1	E	307/357 (85%)	0.34	16 (5%) 28 40	27, 29, 30, 32	0
1	F	307/357 (85%)	0.47	24 (7%) 14 20	27, 29, 30, 32	0
1	G	308/357 (86%)	0.33	12 (3%) 40 52	27, 29, 30, 34	0
1	H	307/357 (85%)	0.28	7 (2%) 61 71	27, 29, 30, 32	0
1	I	307/357 (85%)	0.29	12 (3%) 40 52	27, 29, 30, 32	0
1	J	307/357 (85%)	0.35	13 (4%) 37 49	27, 29, 30, 32	0
All	All	3071/3570 (86%)	0.35	146 (4%) 31 43	27, 29, 30, 34	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	258	GLN	5.7
1	F	254	HIS	5.5
1	D	251	LEU	5.3
1	D	194	ASN	5.1
1	F	206	ASN	4.8
1	F	194	ASN	4.7
1	H	258	GLN	4.6
1	D	258	GLN	4.3
1	B	146	LEU	3.9
1	A	156	PRO	3.9
1	D	196	GLU	3.9
1	I	195	GLY	3.8
1	B	258	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	254	HIS	3.7
1	F	202	GLU	3.7
1	H	261	TYR	3.7
1	D	124	THR	3.6
1	D	256	LYS	3.6
1	E	157	GLU	3.6
1	F	251	LEU	3.6
1	I	202	GLU	3.5
1	J	206	ASN	3.4
1	A	206	ASN	3.4
1	D	252	ALA	3.4
1	F	257	GLY	3.3
1	J	157	GLU	3.3
1	F	258	GLN	3.3
1	F	261	TYR	3.3
1	D	206	ASN	3.2
1	D	260	GLU	3.2
1	D	205	GLU	3.2
1	E	252	ALA	3.2
1	J	11	ILE	3.1
1	J	29	VAL	3.1
1	F	157	GLU	3.1
1	E	254	HIS	3.0
1	B	157	GLU	3.0
1	F	195	GLY	3.0
1	D	259	ILE	3.0
1	B	192	LEU	3.0
1	B	147	PHE	3.0
1	J	159	ASN	3.0
1	H	205	GLU	2.9
1	F	201	PHE	2.9
1	F	207	PHE	2.9
1	E	255	LYS	2.9
1	C	262	ILE	2.8
1	B	261	TYR	2.8
1	E	250	THR	2.8
1	I	289	ASP	2.8
1	A	258	GLN	2.8
1	F	204	SER	2.8
1	B	140	PHE	2.7
1	D	244	GLN	2.7
1	H	203	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	262	ILE	2.7
1	C	254	HIS	2.7
1	E	251	LEU	2.7
1	J	30	VAL	2.7
1	B	195	GLY	2.6
1	C	258	GLN	2.6
1	B	114	ALA	2.6
1	F	259	ILE	2.6
1	I	257	GLY	2.6
1	E	300	THR	2.5
1	J	4	VAL	2.5
1	E	201	PHE	2.5
1	F	256	LYS	2.5
1	B	194	ASN	2.5
1	G	157	GLU	2.5
1	E	206	ASN	2.5
1	G	4	VAL	2.5
1	G	11	ILE	2.5
1	G	124	THR	2.4
1	E	253	TYR	2.4
1	B	260	GLU	2.4
1	H	157	GLU	2.4
1	E	256	LYS	2.4
1	D	159	ASN	2.4
1	B	94	TYR	2.4
1	F	205	GLU	2.4
1	E	194	ASN	2.4
1	F	247	ALA	2.4
1	E	202	GLU	2.4
1	F	196	GLU	2.4
1	I	157	GLU	2.4
1	C	196	GLU	2.4
1	G	29	VAL	2.4
1	H	206	ASN	2.4
1	B	113	TYR	2.3
1	J	256	LYS	2.3
1	G	30	VAL	2.3
1	C	157	GLU	2.3
1	D	249	ALA	2.3
1	G	301	GLU	2.3
1	I	206	ASN	2.3
1	D	304	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	300	THR	2.3
1	E	124	THR	2.3
1	B	266	ASP	2.3
1	B	259	ILE	2.3
1	I	114	ALA	2.3
1	B	139	VAL	2.2
1	D	157	GLU	2.2
1	G	114	ALA	2.2
1	E	235	LEU	2.2
1	H	67	GLY	2.2
1	F	159	ASN	2.2
1	G	12	GLY	2.2
1	D	261	TYR	2.2
1	B	145	PHE	2.2
1	D	207	PHE	2.2
1	D	257	GLY	2.2
1	J	77	ALA	2.2
1	J	194	ASN	2.2
1	I	263	PRO	2.2
1	D	296	ALA	2.2
1	E	266	ASP	2.2
1	B	144	LYS	2.1
1	I	194	ASN	2.1
1	D	192	LEU	2.1
1	G	206	ASN	2.1
1	J	76	GLY	2.1
1	B	142	TYR	2.1
1	B	196	GLU	2.1
1	B	202	GLU	2.1
1	C	77	ALA	2.1
1	D	114	ALA	2.1
1	F	23	GLY	2.1
1	A	202	GLU	2.1
1	I	261	TYR	2.1
1	A	157	GLU	2.1
1	G	205	GLU	2.1
1	F	285	ALA	2.1
1	I	156	PRO	2.1
1	C	261	TYR	2.1
1	A	239	ARG	2.0
1	C	11	ILE	2.0
1	F	192	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	227	ASN	2.0
1	F	227	ASN	2.0
1	D	255	LYS	2.0
1	F	255	LYS	2.0
1	J	251	LEU	2.0
1	J	5	THR	2.0
1	C	114	ALA	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. 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, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	I	1310	6/6	0.63	0.49	8.84	50,51,52,52	0
3	GOL	D	1310	6/6	0.76	0.40	7.48	42,42,43,44	0
3	GOL	J	1310	6/6	0.74	0.42	7.34	48,49,50,50	0
3	GOL	C	1310	6/6	0.73	0.44	6.73	46,48,48,49	0
3	GOL	H	1310	6/6	0.71	0.44	6.50	44,47,48,48	0
3	GOL	F	1310	6/6	0.82	0.35	5.48	45,47,47,48	0
3	GOL	E	1310	6/6	0.71	0.38	5.42	44,45,46,47	0
3	GOL	B	1310	6/6	0.68	0.42	4.31	45,46,48,49	0
3	GOL	A	1310	6/6	0.86	0.27	4.30	41,43,43,44	0
3	GOL	G	1310	6/6	0.83	0.30	3.30	42,44,44,45	0
5	BMA	F	1321	11/12	0.93	0.15	-0.13	37,38,40,42	0
5	BMA	E	1321	11/12	0.89	0.14	-0.26	34,35,37,38	0
4	ADP	I	1320	27/27	0.95	0.12	-0.43	27,30,32,34	0
2	NAP	H	1308	48/48	0.95	0.16	-0.44	28,31,36,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAP	F	1308	48/48	0.94	0.14	-0.46	27,31,38,42	0
2	NAP	E	1308	48/48	0.94	0.15	-0.46	25,31,37,41	0
5	BMA	G	1321	11/12	0.93	0.15	-0.47	32,34,37,37	0
4	ADP	E	1320	27/27	0.94	0.13	-0.49	27,30,32,34	0
4	ADP	B	1320	27/27	0.96	0.13	-0.50	26,29,31,33	0
2	NAP	J	1308	48/48	0.95	0.16	-0.59	26,30,36,39	0
5	BMA	I	1321	11/12	0.93	0.12	-0.63	34,35,37,39	0
5	BMA	H	1321	11/12	0.93	0.15	-0.64	32,34,37,39	0
5	BMA	D	1321	11/12	0.92	0.13	-0.66	34,35,37,38	0
5	BMA	C	1321	11/12	0.94	0.15	-0.67	33,35,37,39	0
2	NAP	G	1308	48/48	0.95	0.17	-0.67	27,31,38,41	0
4	ADP	J	1320	27/27	0.97	0.11	-0.69	27,29,31,31	0
2	NAP	B	1308	48/48	0.94	0.14	-0.71	25,31,35,41	0
4	ADP	D	1320	27/27	0.92	0.13	-0.72	28,30,31,34	0
2	NAP	I	1308	48/48	0.95	0.14	-0.74	26,31,37,40	0
5	BMA	J	1321	11/12	0.95	0.11	-0.76	33,35,37,39	0
4	ADP	F	1320	27/27	0.91	0.13	-0.76	29,31,33,35	0
2	NAP	D	1308	48/48	0.95	0.14	-0.81	27,31,36,37	0
5	BMA	B	1321	11/12	0.95	0.12	-0.85	34,35,37,39	0
2	NAP	C	1308	48/48	0.95	0.15	-0.89	26,30,37,40	0
4	ADP	H	1320	27/27	0.96	0.12	-0.89	27,29,30,32	0
4	ADP	A	1320	27/27	0.97	0.12	-0.92	25,30,33,34	0
2	NAP	A	1308	48/48	0.95	0.16	-0.95	27,30,36,39	0
4	ADP	C	1320	27/27	0.97	0.11	-1.08	27,29,31,31	0
4	ADP	G	1320	27/27	0.97	0.10	-1.39	27,29,31,32	0
5	BMA	A	1321	11/12	0.92	0.14	-1.67	34,36,40,42	0
6	CL	G	1313	1/1	0.95	0.08	-	65,65,65,65	0
6	CL	G	1312	1/1	0.98	0.36	-	60,60,60,60	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.