



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:32 AM GMT

PDB ID : 2R4E  
Title : Crystal structure of Escherichia coli Glycerol-3-phosphate Dehydrogenase in complex with DHAP  
Authors : Yeh, J.I.; Du, S.; Chinte, U.  
Deposited on : 2007-08-31  
Resolution : 2.10 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

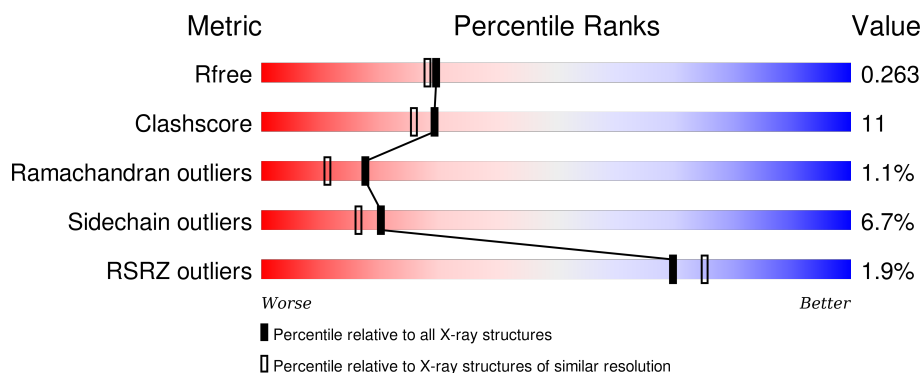
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	501	<div> <div>2%</div> <div>79%</div> <div>17%</div> <div>• •</div> </div>
1	B	501	<div> <div>2%</div> <div>75%</div> <div>19%</div> <div>• • •</div> </div>

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
2	BOG	A	1950	-	-	-	X
2	BOG	A	1952	-	-	-	X
2	BOG	B	1949	-	-	-	X
2	BOG	B	1950	-	-	-	X
3	PO4	A	1953	-	-	-	X
3	PO4	A	1954	-	-	-	X
3	PO4	B	1951	-	-	-	X
3	PO4	B	1952	-	-	-	X
4	FAD	A	600	X	-	-	X
4	FAD	B	600	-	-	-	X
5	13P	A	1955	-	-	-	X
5	13P	B	7067	-	-	X	X
6	EDO	A	1960	-	-	-	X
6	EDO	A	1961	-	-	-	X
6	EDO	B	1957	-	-	-	X
6	EDO	B	1958	-	-	-	X
6	EDO	B	1961	-	-	X	-
7	IMD	A	1957	-	-	-	X

## 2 Entry composition [i](#)

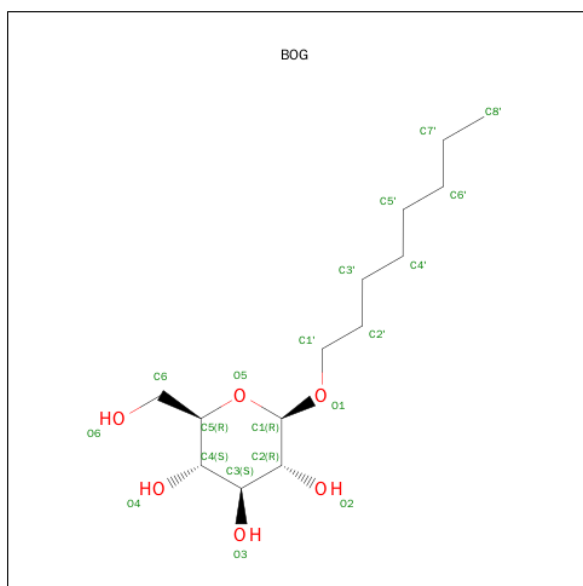
There are 9 unique types of molecules in this entry. The entry contains 8532 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Aerobic glycerol-3-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	0	0
			3953	2510	703	727	13			
1	B	494	Total	C	N	O	S	0	0	0
			3953	2510	703	727	13			

- Molecule 2 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula:  $C_{14}H_{28}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			20	14	6		
2	A	1	Total	C	O	0	0
			20	14	6		
2	B	1	Total	C	O	0	0
			20	14	6		
2	B	1	Total	C	O	0	0
			20	14	6		

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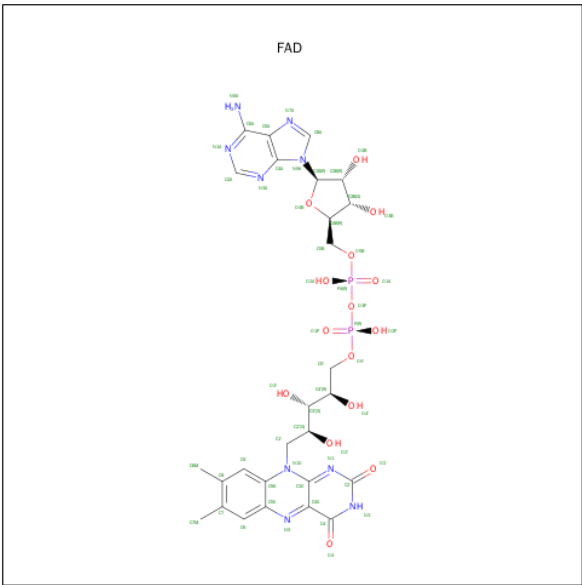
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			20	14	6		
2	A	1	Total	C	O	0	0
			20	14	6		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



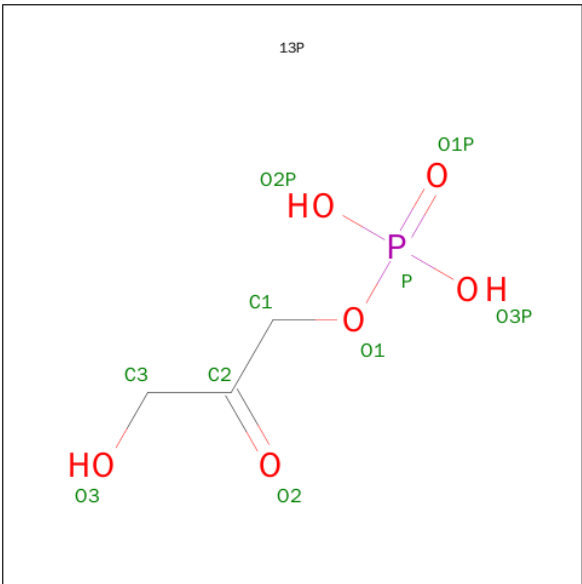
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 5 is 1,3-DIHYDROXYACETONEPHOSPHATE (three-letter code: 13P) (formula: C<sub>3</sub>H<sub>7</sub>O<sub>6</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	P	0	0
			10	3	6	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	O	P	0	0
			10	3	6	1		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



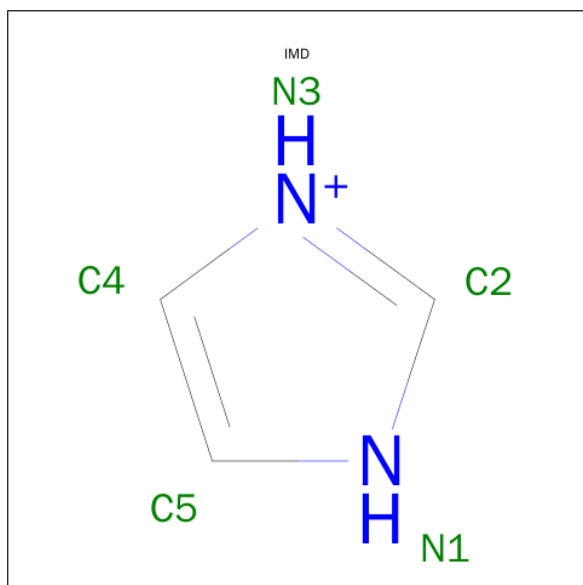
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

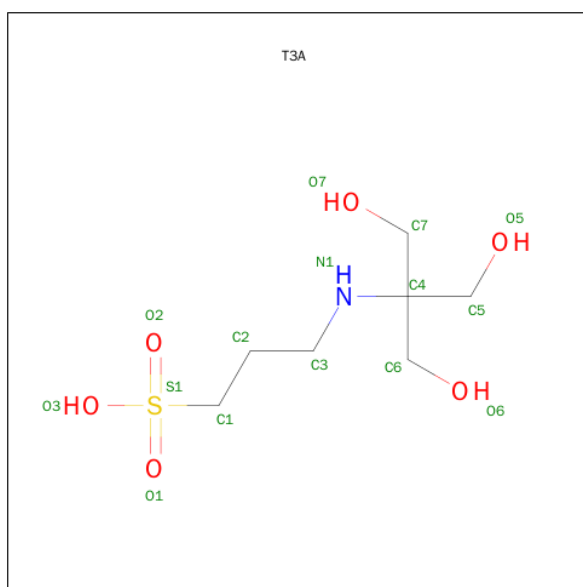
- Molecule 7 is IMIDAZOLE (three-letter code: IMD) (formula:  $C_3H_5N_2$ ).



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

- Molecule 8 is N-(TRIS(HYDROXYMETHYL)METHYL)-3-AMINOPROPANESULFONIC ACID (three-letter code: T3A) (formula:  $C_7H_{17}NO_6S$ ).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	S	0	0
			15	7	1	6	1		
8	B	1	Total	C	N	O	S	0	0
			15	7	1	6	1		

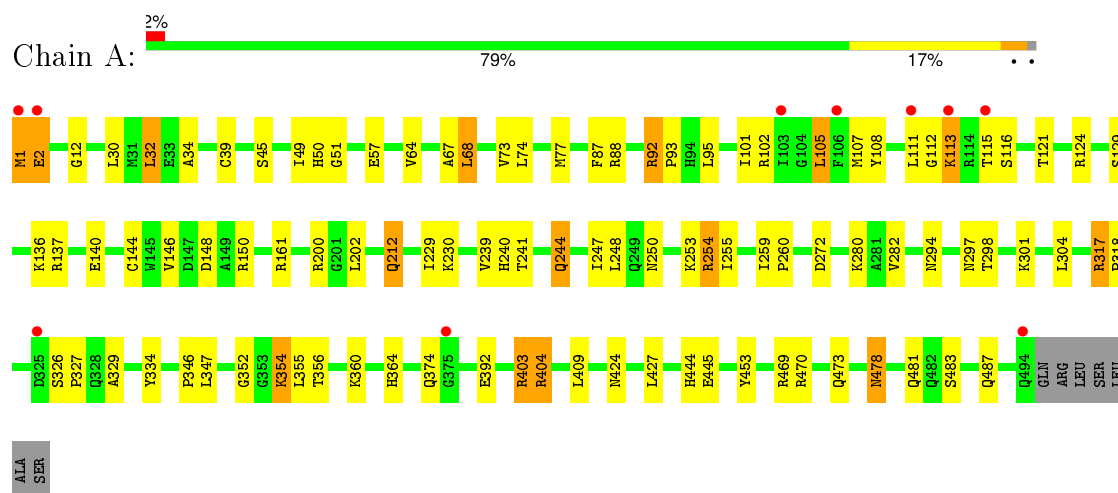
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	131	Total	O	0	0
			131	131		
9	B	132	Total	O	0	0
			132	132		

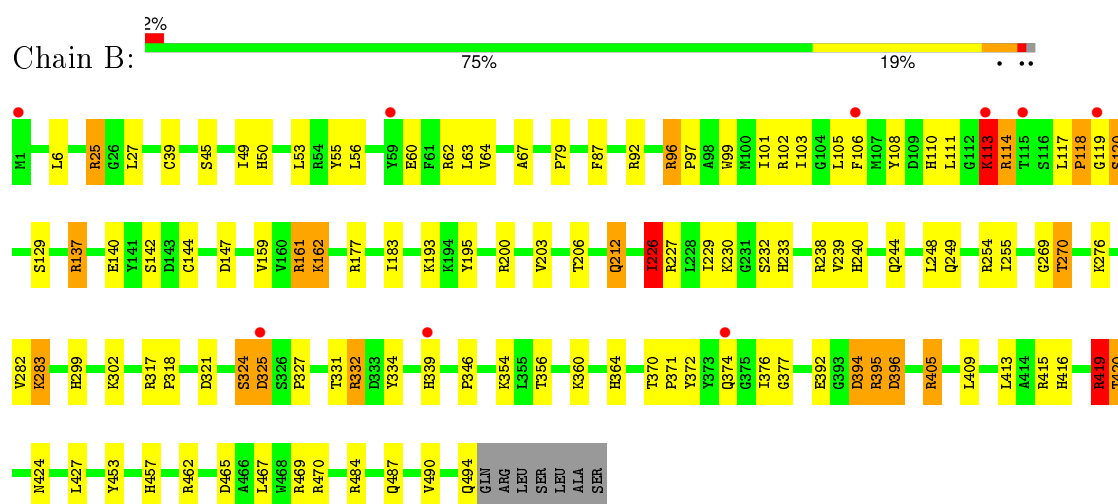
### 3 Residue-property plots [i](#)

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: Aerobic glycerol-3-phosphate dehydrogenase



- Molecule 1: Aerobic glycerol-3-phosphate dehydrogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.85Å 113.82Å 193.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.10 10.00 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.9 (10.00-2.10) 99.5 (10.00-2.05)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.47 (at 2.06Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.198 , 0.256 0.205 , 0.263	Depositor DCC
$R_{free}$ test set	3629 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.3	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 34.7	EDS
Estimated twinning fraction	0.470 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 77396 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8532	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IMD, PO4, EDO, T3A, 13P, FAD, BOG

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	1.08	1/4048 (0.0%)	0.95	5/5482 (0.1%)
1	B	1.07	0/4048	0.99	9/5482 (0.2%)
All	All	1.07	1/8096 (0.0%)	0.97	14/10964 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	329	ALA	CA-CB	5.64	1.64	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	B	96	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	254	ARG	NE-CZ-NH2	5.74	123.17	120.30
1	B	409	LEU	CB-CG-CD1	-5.70	101.30	111.00
1	B	183	ILE	CG1-CB-CG2	-5.67	98.92	111.40
1	B	462	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	A	317	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	A	92	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	B	25	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	B	467	LEU	CB-CG-CD1	-5.21	102.14	111.00
1	B	113	LYS	N-CA-C	5.17	124.97	111.00
1	B	419	ARG	CG-CD-NE	5.14	122.61	111.80
1	B	147	ASP	CB-CG-OD1	5.13	122.92	118.30
1	A	148	ASP	CB-CG-OD1	5.06	122.86	118.30

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	3953	0	3903	74	0
1	B	3953	0	3903	108	0
2	A	80	0	112	11	0
2	B	40	0	56	3	0
3	A	10	0	0	1	0
3	B	15	0	0	2	0
4	A	53	0	29	6	0
4	B	53	0	30	6	0
5	A	10	0	5	3	0
5	B	10	0	5	4	0
6	A	24	0	36	3	0
6	B	28	0	42	5	0
7	A	5	0	5	1	0
7	B	5	0	5	0	0
8	A	15	0	17	1	0
8	B	15	0	17	1	0
9	A	131	0	0	5	0
9	B	132	0	0	7	0
All	All	8532	0	8165	186	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (186) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:GLY:HA3	1:A:68:LEU:HD13	1.30	1.10
1:B:395:ARG:O	1:B:396:ASP:HB2	1.54	1.05
1:B:484:ARG:NH1	1:B:487:GLN:HE21	1.54	1.04
1:B:50:HIS:CE1	1:B:354:LYS:HZ1	1.75	1.03
1:B:50:HIS:HE1	1:B:354:LYS:NZ	1.58	1.01
1:A:57:GLU:HG3	2:A:1950:BOG:O2	1.64	0.97
1:B:50:HIS:CE1	1:B:354:LYS:NZ	2.30	0.97
1:B:484:ARG:HH11	1:B:487:GLN:NE2	1.65	0.93
1:A:297:ASN:HD21	1:A:304:LEU:H	1.19	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ARG:HH22	2:A:1949:BOG:H5	1.37	0.89
1:A:50:HIS:HE1	1:A:354:LYS:HZ1	1.16	0.89
1:B:324:SER:O	1:B:325:ASP:HB2	1.74	0.84
1:B:50:HIS:HE1	1:B:354:LYS:HZ1	0.87	0.83
1:A:57:GLU:CG	2:A:1950:BOG:O2	2.26	0.82
1:A:51:GLY:CA	1:A:68:LEU:HD13	2.09	0.82
1:B:117:LEU:O	1:B:118:PRO:O	1.96	0.81
1:B:113:LYS:HB3	1:B:114:ARG:HA	1.62	0.81
1:B:416:HIS:O	1:B:420:THR:HG23	1.79	0.81
1:A:50:HIS:HE1	1:A:354:LYS:NZ	1.78	0.80
1:A:101:ILE:HA	2:A:1950:BOG:H61	1.63	0.80
1:A:50:HIS:CE1	1:A:354:LYS:NZ	2.50	0.80
1:A:73:VAL:O	1:A:77:MET:HG3	1.81	0.80
1:A:12:GLY:HA3	4:A:600:FAD:O2A	1.82	0.79
1:B:395:ARG:O	1:B:396:ASP:CB	2.28	0.79
1:B:376:ILE:HG12	1:B:377:GLY:N	1.98	0.77
1:B:376:ILE:HG12	1:B:377:GLY:H	1.48	0.76
1:A:107:MET:O	1:A:111:LEU:HB2	1.84	0.76
1:B:137:ARG:HH11	1:B:137:ARG:HG2	1.51	0.75
1:B:394:ASP:OD1	1:B:395:ARG:O	2.05	0.75
1:B:25:ARG:HD3	1:B:377:GLY:HA2	1.67	0.74
1:B:118:PRO:CB	1:B:119:GLY:HA3	2.18	0.73
1:B:113:LYS:CB	1:B:114:ARG:HA	2.19	0.72
1:A:254:ARG:HH11	5:A:1955:13P:H12	1.55	0.72
1:B:484:ARG:HH11	1:B:487:GLN:HE21	0.80	0.71
1:B:324:SER:O	1:B:325:ASP:CB	2.39	0.70
1:B:484:ARG:NH1	1:B:487:GLN:NE2	2.29	0.70
1:A:93:PRO:CB	2:A:1952:BOG:H5	2.21	0.70
9:A:7185:HOH:O	1:B:457:HIS:HE1	1.73	0.70
1:A:161:ARG:HB2	6:A:1962:EDO:O1	1.92	0.70
1:B:137:ARG:HH11	1:B:137:ARG:CG	2.06	0.69
1:A:102:ARG:NH1	2:A:1949:BOG:O5	2.25	0.69
1:B:394:ASP:C	1:B:394:ASP:OD1	2.30	0.69
1:B:161:ARG:HB2	6:B:1961:EDO:O2	1.93	0.68
1:B:50:HIS:CE1	1:B:354:LYS:CE	2.77	0.68
1:B:212:GLN:HB2	3:B:1952:PO4:O1	1.94	0.67
1:B:117:LEU:C	1:B:118:PRO:O	2.33	0.66
1:A:294:ASN:O	1:A:298:THR:HG23	1.95	0.66
1:B:96:ARG:HH11	1:B:249:GLN:HE21	1.41	0.65
1:A:51:GLY:HA3	1:A:68:LEU:CD1	2.18	0.65
6:A:1962:EDO:H12	8:A:7066:T3A:O3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:PRO:HB2	2:A:1952:BOG:H5	1.80	0.64
6:B:1961:EDO:H21	8:B:7066:T3A:O3	1.98	0.64
1:A:478:ASN:ND2	1:A:481:GLN:H	1.95	0.63
1:A:487:GLN:HG2	9:A:7137:HOH:O	1.98	0.62
1:B:114:ARG:HG2	1:B:114:ARG:O	1.98	0.61
1:A:200:ARG:O	1:A:346:PRO:HD2	2.00	0.61
1:A:50:HIS:CE1	1:A:354:LYS:HZ1	2.04	0.61
6:B:1959:EDO:H12	9:B:7168:HOH:O	2.00	0.60
1:B:79:PRO:O	1:B:395:ARG:HD2	2.02	0.60
1:B:317:ARG:HG3	4:B:600:FAD:HM83	1.83	0.60
1:B:119:GLY:O	1:B:120:SER:HB3	2.01	0.60
1:B:27:LEU:HD21	1:B:376:ILE:HG13	1.83	0.60
1:A:102:ARG:NH1	2:A:1949:BOG:H62	2.17	0.60
1:B:118:PRO:HB3	1:B:119:GLY:HA3	1.84	0.60
1:A:254:ARG:HH11	5:A:1955:13P:C1	2.14	0.60
1:B:193:LYS:HE2	1:B:195:TYR:CE1	2.37	0.59
1:B:254:ARG:HH21	5:B:7067:13P:H12	1.67	0.59
1:B:55:TYR:CZ	1:B:332:ARG:HD2	2.37	0.59
1:A:317:ARG:HG3	4:A:600:FAD:HM83	1.83	0.59
1:B:339:HIS:HD2	9:B:7089:HOH:O	1.86	0.58
1:A:50:HIS:CE1	1:A:354:LYS:HZ3	2.20	0.58
1:B:55:TYR:CE1	1:B:332:ARG:HD2	2.37	0.58
1:A:150:ARG:HD2	1:A:470:ARG:O	2.04	0.57
1:A:49:ILE:HB	1:A:144:CYS:HB2	1.87	0.56
1:B:161:ARG:CB	6:B:1961:EDO:O2	2.53	0.56
1:B:113:LYS:HB3	1:B:114:ARG:CA	2.36	0.55
1:B:415:ARG:HG2	1:B:419:ARG:HD2	1.89	0.55
1:B:118:PRO:CB	1:B:119:GLY:CA	2.84	0.55
1:A:445:GLU:HB2	7:A:1957:IMD:H5	1.89	0.55
1:B:161:ARG:HG3	1:B:162:LYS:HD3	1.89	0.54
1:B:49:ILE:HB	1:B:144:CYS:HB2	1.89	0.54
1:A:105:LEU:HD13	2:A:1950:BOG:O6	2.07	0.54
1:A:241:THR:O	1:A:241:THR:HG22	2.06	0.54
1:A:239:VAL:HG23	1:A:240:HIS:CD2	2.42	0.54
1:A:317:ARG:HG3	4:A:600:FAD:C8M	2.38	0.53
1:B:299:HIS:HE1	9:B:7078:HOH:O	1.92	0.53
1:B:102:ARG:NH1	2:B:1949:BOG:O2	2.42	0.52
1:B:427:LEU:HD12	9:B:7159:HOH:O	2.08	0.52
1:B:87:PHE:O	1:B:140:GLU:HA	2.09	0.52
1:B:405:ARG:HD3	3:B:1951:PO4:O3	2.10	0.52
1:A:241:THR:O	1:A:241:THR:CG2	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:ASN:HB3	1:A:453:TYR:OH	2.09	0.52
1:B:96:ARG:HB2	1:B:249:GLN:HE22	1.76	0.51
1:A:230:LYS:HD3	1:A:282:VAL:HG23	1.93	0.51
1:B:229:ILE:HD12	1:B:327:PRO:HB3	1.91	0.51
1:B:137:ARG:NH1	1:B:137:ARG:HG2	2.24	0.51
1:B:465:ASP:O	1:B:470:ARG:HG2	2.12	0.51
1:A:137:ARG:NH2	2:A:1949:BOG:H5	2.18	0.50
1:A:88:ARG:NE	1:A:244:GLN:HG3	2.26	0.50
1:B:317:ARG:HG3	4:B:600:FAD:C8M	2.41	0.50
1:A:112:GLY:O	1:A:113:LYS:HB2	2.12	0.50
4:A:600:FAD:O2A	4:A:600:FAD:H4B	2.11	0.49
1:A:1:MET:HA	1:A:2:GLU:HG3	1.93	0.49
1:B:67:ALA:HB1	1:B:356:THR:HG21	1.94	0.49
1:A:50:HIS:HD2	9:A:7189:HOH:O	1.95	0.49
1:B:394:ASP:O	1:B:394:ASP:OD1	2.31	0.49
1:A:50:HIS:O	1:A:356:THR:HG21	2.13	0.49
1:B:370:THR:O	1:B:371:PRO:C	2.51	0.48
1:B:118:PRO:HB2	1:B:119:GLY:HA3	1.96	0.48
1:A:39:CYS:HA	1:A:469:ARG:HD3	1.96	0.48
1:A:67:ALA:HB1	1:A:356:THR:HG21	1.96	0.48
1:B:101:ILE:HD12	2:B:1950:BOG:H61	1.96	0.48
1:A:478:ASN:HD22	1:A:481:GLN:H	1.61	0.48
1:B:45:SER:HA	4:B:600:FAD:C6	2.44	0.48
1:A:34:ALA:HB3	6:A:1956:EDO:H11	1.96	0.47
1:A:202:LEU:HD23	1:A:347:LEU:HD13	1.95	0.47
1:B:254:ARG:HH21	5:B:7067:13P:C1	2.27	0.47
1:B:25:ARG:HB3	1:B:377:GLY:H	1.80	0.47
1:A:478:ASN:HD22	1:A:478:ASN:C	2.18	0.47
1:B:114:ARG:NH1	1:B:118:PRO:O	2.48	0.47
1:A:212:GLN:HB2	3:A:1954:PO4:O4	2.15	0.46
1:B:101:ILE:CD1	2:B:1950:BOG:H61	2.44	0.46
1:A:301:LYS:CE	9:A:7091:HOH:O	2.62	0.46
1:B:490:VAL:O	1:B:494:GLN:HB2	2.15	0.46
1:B:200:ARG:O	1:B:346:PRO:HD2	2.16	0.46
1:B:45:SER:HB2	4:B:600:FAD:C4X	2.46	0.46
1:A:229:ILE:HD12	1:A:327:PRO:HB3	1.97	0.46
1:B:60:GLU:O	1:B:64:VAL:HG23	2.16	0.46
1:B:50:HIS:CE1	1:B:354:LYS:HE2	2.51	0.45
1:B:50:HIS:O	1:B:356:THR:HG21	2.15	0.45
1:B:92:ARG:HD2	1:B:299:HIS:CE1	2.51	0.45
1:A:93:PRO:HB3	2:A:1952:BOG:H3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:ASN:HB3	1:B:453:TYR:OH	2.15	0.45
1:B:360:LYS:HA	1:B:360:LYS:HD2	1.71	0.45
1:B:226:ILE:HD11	1:B:318:PRO:CB	2.46	0.45
1:A:30:LEU:HG	1:A:32:LEU:HD13	1.98	0.45
1:A:404:ARG:NH2	1:B:162:LYS:O	2.50	0.45
1:B:395:ARG:CZ	1:B:419:ARG:HG2	2.47	0.45
5:B:7067:13P:O3P	5:B:7067:13P:H31	2.15	0.45
1:B:332:ARG:HH11	5:B:7067:13P:P	2.40	0.45
1:B:226:ILE:HD11	1:B:318:PRO:HB2	1.99	0.44
1:B:283:LYS:HE2	1:B:283:LYS:HB2	1.55	0.44
1:B:60:GLU:OE1	1:B:331:THR:OG1	2.24	0.44
1:B:230:LYS:HD3	1:B:282:VAL:HG23	2.00	0.44
1:B:39:CYS:HA	1:B:469:ARG:HD3	2.00	0.44
1:B:120:SER:HA	1:B:140:GLU:O	2.16	0.44
1:B:193:LYS:HE2	1:B:195:TYR:CZ	2.52	0.44
1:B:162:LYS:HD2	1:B:162:LYS:HA	1.71	0.43
1:B:370:THR:O	1:B:372:TYR:N	2.51	0.43
1:A:49:ILE:HD11	1:A:146:VAL:HB	2.00	0.43
1:A:360:LYS:HA	1:A:360:LYS:HD2	1.72	0.43
1:A:297:ASN:HD22	1:A:297:ASN:HA	1.67	0.43
1:B:419:ARG:HH11	1:B:419:ARG:CG	2.31	0.43
1:A:248:LEU:O	1:A:255:ILE:HA	2.17	0.43
1:B:334:TYR:OH	1:B:364:HIS:CD2	2.72	0.43
1:A:444:HIS:HD2	1:A:473:GLN:OE1	2.02	0.43
1:A:64:VAL:O	1:A:68:LEU:HB2	2.19	0.43
1:B:233:HIS:CD2	1:B:269:GLY:HA3	2.53	0.43
1:A:318:PRO:O	1:A:352:GLY:HA2	2.19	0.43
1:A:129:SER:HB2	9:A:7108:HOH:O	2.19	0.42
1:B:6:LEU:HD11	1:B:203:VAL:HG23	2.01	0.42
1:A:403:ARG:NH1	1:A:409:LEU:O	2.45	0.42
1:B:129:SER:HB2	9:B:7094:HOH:O	2.19	0.42
1:A:87:PHE:O	1:A:140:GLU:HA	2.19	0.41
1:B:232:SER:O	1:B:270:THR:CG2	2.68	0.41
1:B:248:LEU:O	1:B:255:ILE:HA	2.19	0.41
1:B:346:PRO:HG3	1:B:372:TYR:CG	2.55	0.41
1:B:97:PRO:HB2	1:B:99:TRP:CD1	2.55	0.41
1:B:239:VAL:HG23	1:B:240:HIS:CD2	2.55	0.41
1:B:117:LEU:HD22	1:B:142:SER:HB3	2.03	0.41
1:B:161:ARG:HB2	6:B:1961:EDO:HO2	1.85	0.41
1:A:92:ARG:HD3	1:A:95:LEU:HD12	2.03	0.41
1:A:12:GLY:CA	4:A:600:FAD:O2A	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:TYR:HH	1:A:364:HIS:CE1	2.37	0.41
1:B:106:PHE:O	1:B:110:HIS:HD2	2.04	0.41
1:B:177:ARG:HD2	9:B:7105:HOH:O	2.20	0.41
1:B:45:SER:HA	4:B:600:FAD:C5X	2.51	0.41
1:A:45:SER:HA	4:A:600:FAD:C6	2.50	0.41
1:A:254:ARG:NH1	5:A:1955:13P:H12	2.31	0.41
1:B:114:ARG:CG	1:B:114:ARG:O	2.68	0.41
1:B:206:THR:HA	4:B:600:FAD:H52A	2.03	0.41
1:B:299:HIS:CE1	9:B:7078:HOH:O	2.70	0.41
1:A:247:ILE:HD13	1:A:247:ILE:HG21	1.87	0.41
1:A:259:ILE:HA	1:A:260:PRO:HD3	1.96	0.41
1:B:227:ARG:HG2	1:B:321:ASP:CB	2.51	0.40
1:A:354:LYS:HE3	1:A:354:LYS:HB3	1.68	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	492/501 (98%)	471 (96%)	18 (4%)	3 (1%)	30	24
1	B	492/501 (98%)	462 (94%)	22 (4%)	8 (2%)	12	6
All	All	984/1002 (98%)	933 (95%)	40 (4%)	11 (1%)	17	11

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	THR
1	A	374	GLN
1	B	113	LYS
1	B	118	PRO
1	B	325	ASP

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Mol	Chain	Res	Type
1	B	374	GLN
1	B	396	ASP
1	B	226	ILE
1	B	120	SER
1	A	113	LYS
1	B	159	VAL

### 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	413/419 (99%)	387 (94%)	26 (6%)	22	18
1	B	413/419 (99%)	384 (93%)	29 (7%)	19	15
All	All	826/838 (99%)	771 (93%)	55 (7%)	20	16

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	GLU
1	A	32	LEU
1	A	68	LEU
1	A	74	LEU
1	A	105	LEU
1	A	108	TYR
1	A	116	SER
1	A	121	THR
1	A	124	ARG
1	A	136	LYS
1	A	212	GLN
1	A	244	GLN
1	A	250	ASN
1	A	253	LYS
1	A	272	ASP
1	A	280	LYS

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Mol	Chain	Res	Type
1	A	326	SER
1	A	354	LYS
1	A	355	LEU
1	A	392	GLU
1	A	403	ARG
1	A	404	ARG
1	A	427	LEU
1	A	478	ASN
1	A	483	SER
1	B	53	LEU
1	B	56	LEU
1	B	62	ARG
1	B	63	LEU
1	B	103	ILE
1	B	105	LEU
1	B	108	TYR
1	B	111	LEU
1	B	114	ARG
1	B	137	ARG
1	B	161	ARG
1	B	162	LYS
1	B	212	GLN
1	B	226	ILE
1	B	238	ARG
1	B	244	GLN
1	B	270	THR
1	B	276	LYS
1	B	283	LYS
1	B	302	LYS
1	B	324	SER
1	B	332	ARG
1	B	392	GLU
1	B	394	ASP
1	B	395	ARG
1	B	405	ARG
1	B	413	LEU
1	B	419	ARG
1	B	420	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	50	HIS
1	A	110	HIS
1	A	128	ASN
1	A	212	GLN
1	A	242	GLN
1	A	250	ASN
1	A	290	ASN
1	A	297	ASN
1	A	444	HIS
1	A	473	GLN
1	A	478	ASN
1	A	482	GLN
1	B	50	HIS
1	B	110	HIS
1	B	212	GLN
1	B	244	GLN
1	B	249	GLN
1	B	299	HIS
1	B	364	HIS
1	B	424	ASN
1	B	457	HIS
1	B	473	GLN
1	B	487	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 ⓘ

32 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	BOG	A	1949	-	20,20,20	0.95	1 (5%)	25,25,25	1.75	6 (24%)
2	BOG	A	1950	-	20,20,20	0.45	0	25,25,25	0.62	0
2	BOG	A	1951	-	20,20,20	0.95	1 (5%)	25,25,25	0.99	1 (4%)
2	BOG	A	1952	-	20,20,20	0.82	1 (5%)	25,25,25	1.22	3 (12%)
3	PO4	A	1953	-	4,4,4	0.35	0	6,6,6	0.27	0
3	PO4	A	1954	-	4,4,4	0.45	0	6,6,6	0.29	0
5	13P	A	1955	-	9,9,9	5.33	6 (66%)	9,12,12	4.13	4 (44%)
6	EDO	A	1956	-	3,3,3	0.72	0	2,2,2	0.43	0
7	IMD	A	1957	-	3,5,5	0.50	0	4,5,5	0.59	0
6	EDO	A	1958	-	3,3,3	1.09	0	2,2,2	0.49	0
6	EDO	A	1959	-	3,3,3	0.56	0	2,2,2	0.58	0
6	EDO	A	1960	-	3,3,3	0.52	0	2,2,2	0.11	0
6	EDO	A	1961	-	3,3,3	0.66	0	2,2,2	0.62	0
6	EDO	A	1962	-	3,3,3	0.86	0	2,2,2	0.73	0
4	FAD	A	600	-	48,58,58	1.60	5 (10%)	54,89,89	2.23	9 (16%)
8	T3A	A	7066	-	13,14,14	0.85	0	17,19,19	2.22	5 (29%)
2	BOG	B	1949	-	20,20,20	0.87	1 (5%)	25,25,25	1.41	2 (8%)
2	BOG	B	1950	-	20,20,20	0.59	0	25,25,25	1.35	4 (16%)
3	PO4	B	1951	-	4,4,4	0.50	0	6,6,6	0.27	0
3	PO4	B	1952	-	4,4,4	0.36	0	6,6,6	0.32	0
3	PO4	B	1953	-	4,4,4	0.36	0	6,6,6	0.28	0
6	EDO	B	1954	-	3,3,3	0.75	0	2,2,2	1.58	1 (50%)
6	EDO	B	1955	-	3,3,3	0.84	0	2,2,2	1.52	0
6	EDO	B	1956	-	3,3,3	0.48	0	2,2,2	0.28	0
6	EDO	B	1957	-	3,3,3	0.96	0	2,2,2	0.75	0
6	EDO	B	1958	-	3,3,3	0.87	0	2,2,2	0.51	0
6	EDO	B	1959	-	3,3,3	0.49	0	2,2,2	0.47	0
7	IMD	B	1960	-	3,5,5	0.66	0	4,5,5	0.43	0
6	EDO	B	1961	-	3,3,3	0.73	0	2,2,2	0.78	0
4	FAD	B	600	-	48,58,58	1.21	4 (8%)	54,89,89	2.45	9 (16%)
8	T3A	B	7066	-	13,14,14	0.72	0	17,19,19	2.68	7 (41%)
5	13P	B	7067	-	9,9,9	5.30	6 (66%)	9,12,12	3.80	4 (44%)

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	BOG	A	1949	-	-	0/11/31/31	0/1/1/1
2	BOG	A	1950	-	-	0/11/31/31	0/1/1/1
2	BOG	A	1951	-	-	0/11/31/31	0/1/1/1
2	BOG	A	1952	-	-	0/11/31/31	0/1/1/1
3	PO4	A	1953	-	-	0/0/0/0	0/0/0/0
3	PO4	A	1954	-	-	0/0/0/0	0/0/0/0
5	13P	A	1955	-	-	0/7/8/8	0/0/0/0
6	EDO	A	1956	-	-	0/1/1/1	0/0/0/0
7	IMD	A	1957	-	-	0/0/0/0	0/1/1/1
6	EDO	A	1958	-	-	0/1/1/1	0/0/0/0
6	EDO	A	1959	-	-	0/1/1/1	0/0/0/0
6	EDO	A	1960	-	-	0/1/1/1	0/0/0/0
6	EDO	A	1961	-	-	0/1/1/1	0/0/0/0
6	EDO	A	1962	-	-	0/1/1/1	0/0/0/0
4	FAD	A	600	-	1/1/9/9	0/30/50/50	0/6/6/6
8	T3A	A	7066	-	-	0/18/18/18	0/0/0/0
2	BOG	B	1949	-	-	0/11/31/31	0/1/1/1
2	BOG	B	1950	-	-	0/11/31/31	0/1/1/1
3	PO4	B	1951	-	-	0/0/0/0	0/0/0/0
3	PO4	B	1952	-	-	0/0/0/0	0/0/0/0
3	PO4	B	1953	-	-	0/0/0/0	0/0/0/0
6	EDO	B	1954	-	-	0/1/1/1	0/0/0/0
6	EDO	B	1955	-	-	0/1/1/1	0/0/0/0
6	EDO	B	1956	-	-	0/1/1/1	0/0/0/0
6	EDO	B	1957	-	-	0/1/1/1	0/0/0/0
6	EDO	B	1958	-	-	0/1/1/1	0/0/0/0
6	EDO	B	1959	-	-	0/1/1/1	0/0/0/0
7	IMD	B	1960	-	-	0/0/0/0	0/1/1/1
6	EDO	B	1961	-	-	0/1/1/1	0/0/0/0
4	FAD	B	600	-	-	0/30/50/50	0/6/6/6
8	T3A	B	7066	-	-	0/18/18/18	0/0/0/0
5	13P	B	7067	-	-	0/7/8/8	0/0/0/0

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	600	FAD	O2B-C2B	-7.45	1.25	1.43
5	A	1955	13P	P-O1	2.34	1.68	1.60
4	A	600	FAD	C2A-N1A	2.40	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	600	FAD	C2A-N1A	2.41	1.38	1.33
2	A	1952	BOG	O1-C1	2.45	1.44	1.40
5	B	7067	13P	P-O1	2.55	1.68	1.60
2	A	1949	BOG	O1-C1	2.56	1.44	1.40
4	A	600	FAD	C4-N3	2.85	1.38	1.33
4	B	600	FAD	C4-N3	2.92	1.38	1.33
2	A	1951	BOG	O1-C1	2.97	1.45	1.40
5	B	7067	13P	O3-C3	3.07	1.51	1.41
2	B	1949	BOG	O1-C1	3.08	1.45	1.40
4	B	600	FAD	C4X-N5	3.27	1.38	1.33
4	A	600	FAD	C4X-N5	3.28	1.38	1.33
5	B	7067	13P	C3-C2	3.48	1.59	1.50
4	A	600	FAD	C2A-N3A	3.56	1.38	1.32
4	B	600	FAD	C2A-N3A	3.57	1.38	1.32
5	A	1955	13P	O3-C3	3.66	1.53	1.41
5	A	1955	13P	C3-C2	3.91	1.61	1.50
5	B	7067	13P	O2-C2	5.41	1.31	1.21
5	A	1955	13P	C1-C2	5.42	1.61	1.50
5	B	7067	13P	C1-C2	5.69	1.61	1.50
5	A	1955	13P	O2-C2	6.14	1.33	1.21
5	A	1955	13P	O1-C1	12.16	1.51	1.43
5	B	7067	13P	O1-C1	12.68	1.51	1.43

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	600	FAD	N3A-C2A-N1A	-11.30	120.24	128.89
4	B	600	FAD	N3A-C2A-N1A	-11.30	120.24	128.89
5	A	1955	13P	O3P-P-O1	-8.01	83.49	106.56
5	B	7067	13P	O3P-P-O1	-7.23	85.75	106.56
5	A	1955	13P	O1-P-O1P	-5.10	94.16	107.14
4	A	600	FAD	P-O3P-PA	-4.36	120.49	132.73
4	B	600	FAD	P-O3P-PA	-4.35	120.50	132.73
8	B	7066	T3A	C3-C2-C1	-3.86	105.93	112.24
4	A	600	FAD	C2B-C1B-N9A	-3.16	109.47	114.29
4	B	600	FAD	C2B-C1B-N9A	-3.13	109.51	114.29
8	A	7066	T3A	C5-C4-N1	-2.96	100.55	109.19
5	B	7067	13P	O1-P-O1P	-2.95	99.63	107.14
2	A	1949	BOG	O1-C1-C2	-2.94	104.32	108.04
8	B	7066	T3A	O3-S1-O2	-2.86	104.94	111.61
4	B	600	FAD	C4X-C4-N3	-2.71	119.88	123.59
4	A	600	FAD	C4X-C4-N3	-2.68	119.92	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1952	BOG	C4-C3-C2	-2.58	105.98	110.79
2	B	1950	BOG	C3-C4-C5	-2.53	105.79	110.20
8	B	7066	T3A	C7-C4-C6	-2.26	105.41	110.14
6	B	1954	EDO	O1-C1-C2	-2.21	96.68	112.54
2	B	1950	BOG	O1-C1-C2	2.02	110.59	108.04
8	B	7066	T3A	C6-C4-C5	2.06	114.45	110.14
2	A	1952	BOG	C1-O5-C5	2.10	117.81	113.75
2	B	1949	BOG	O5-C5-C6	2.12	111.71	106.36
2	B	1950	BOG	O4-C4-C5	2.18	115.01	109.24
4	A	600	FAD	C4B-O4B-C1B	2.28	112.22	109.72
2	A	1949	BOG	C3-C4-C5	2.30	114.21	110.20
2	A	1949	BOG	O6-C6-C5	2.30	118.94	111.33
4	B	600	FAD	C4B-O4B-C1B	2.33	112.28	109.72
8	A	7066	T3A	C7-C4-N1	2.47	116.41	109.19
2	A	1949	BOG	C1-C2-C3	2.57	115.04	109.97
4	B	600	FAD	C4X-N5-C5X	2.72	119.89	116.76
4	A	600	FAD	C4X-N5-C5X	2.78	119.96	116.76
8	A	7066	T3A	C6-C4-C5	2.84	116.09	110.14
2	A	1951	BOG	O1-C1-C2	3.03	111.86	108.04
4	B	600	FAD	C5X-C9A-N10	3.16	120.02	117.62
4	A	600	FAD	C5X-C9A-N10	3.21	120.06	117.62
2	A	1952	BOG	O5-C5-C4	3.41	116.08	109.68
2	B	1950	BOG	C1-C2-C3	3.42	116.71	109.97
8	B	7066	T3A	O2-S1-C1	3.62	110.00	106.91
2	A	1949	BOG	C1-O5-C5	3.63	120.78	113.75
2	A	1949	BOG	C1'-O1-C1	3.88	120.72	113.94
8	A	7066	T3A	O1-S1-C1	4.18	110.47	106.91
8	B	7066	T3A	C3-N1-C4	4.39	122.61	116.07
8	A	7066	T3A	C3-N1-C4	5.10	123.67	116.07
4	A	600	FAD	O2B-C2B-C3B	5.12	128.47	111.83
5	A	1955	13P	O3P-P-O1P	5.16	127.20	110.58
2	B	1949	BOG	O1-C1-C2	5.24	114.66	108.04
5	B	7067	13P	O3P-P-O1P	5.47	128.20	110.58
4	B	600	FAD	C4-N3-C2	5.60	120.09	115.25
4	A	600	FAD	C4-N3-C2	5.66	120.14	115.25
5	A	1955	13P	O2P-P-O1	5.72	123.04	106.56
5	B	7067	13P	O2P-P-O1	5.87	123.47	106.56
8	B	7066	T3A	O1-S1-C1	6.47	112.43	106.91
4	B	600	FAD	O2B-C2B-C3B	9.09	141.40	111.83

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	600	FAD	C2B

There are no torsion outliers.

There are no ring outliers.

19 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1949	BOG	4	0
2	A	1950	BOG	4	0
2	A	1952	BOG	3	0
3	A	1954	PO4	1	0
5	A	1955	13P	3	0
6	A	1956	EDO	1	0
7	A	1957	IMD	1	0
6	A	1962	EDO	2	0
4	A	600	FAD	6	0
8	A	7066	T3A	1	0
2	B	1949	BOG	1	0
2	B	1950	BOG	2	0
3	B	1951	PO4	1	0
3	B	1952	PO4	1	0
6	B	1959	EDO	1	0
6	B	1961	EDO	4	0
4	B	600	FAD	6	0
8	B	7066	T3A	1	0
5	B	7067	13P	4	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	494/501 (98%)	0.11	10 (2%) 68 73	16, 33, 53, 78	0
1	B	494/501 (98%)	0.11	9 (1%) 71 76	16, 33, 53, 75	0
All	All	988/1002 (98%)	0.11	19 (1%) 70 75	16, 33, 53, 78	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	5.5
1	B	1	MET	4.6
1	A	2	GLU	4.4
1	A	106	PHE	4.2
1	A	111	LEU	3.6
1	B	59	TYR	3.4
1	A	113	LYS	3.1
1	B	119	GLY	3.0
1	B	106	PHE	2.8
1	B	115	THR	2.7
1	A	115	THR	2.5
1	B	113	LYS	2.4
1	A	494	GLN	2.3
1	A	325	ASP	2.3
1	B	325	ASP	2.2
1	B	374	GLN	2.2
1	A	375	GLY	2.1
1	A	103	ILE	2.1
1	B	339	HIS	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
2	BOG	A	1950	20/20	0.63	0.55	11.97	110,112,114,114	0
3	PO4	A	1953	5/5	0.91	0.34	10.22	92,92,93,93	0
6	EDO	A	1961	4/4	0.53	0.47	10.19	52,57,57,59	0
3	PO4	A	1954	5/5	0.88	0.24	9.41	70,71,74,76	0
2	BOG	A	1952	20/20	0.61	0.44	9.29	103,105,106,106	0
2	BOG	B	1950	20/20	0.65	0.52	9.20	116,117,119,119	0
7	IMD	A	1957	5/5	0.85	0.18	5.94	59,60,61,62	0
3	PO4	B	1951	5/5	0.92	0.23	5.25	75,76,77,78	0
3	PO4	B	1952	5/5	0.86	0.23	4.75	70,71,75,75	0
5	13P	B	7067	10/10	0.89	0.21	4.09	28,40,45,45	0
2	BOG	B	1949	20/20	0.78	0.27	3.65	60,66,69,70	0
5	13P	A	1955	10/10	0.87	0.19	3.28	28,38,43,44	0
4	FAD	B	600	53/53	0.91	0.17	3.17	15,19,22,25	0
6	EDO	A	1960	4/4	0.88	0.17	3.02	35,41,44,49	0
4	FAD	A	600	53/53	0.90	0.16	2.20	17,20,24,35	0
6	EDO	B	1958	4/4	0.79	0.22	2.10	48,50,51,53	0
6	EDO	B	1957	4/4	0.90	0.14	2.08	25,35,38,40	0
8	T3A	A	7066	15/15	0.93	0.15	1.90	23,37,44,49	0
6	EDO	B	1954	4/4	0.92	0.15	1.80	35,39,40,44	0
6	EDO	A	1956	4/4	0.88	0.19	1.56	50,50,52,53	0
6	EDO	A	1958	4/4	0.95	0.13	1.38	24,33,36,38	0
6	EDO	A	1962	4/4	0.76	0.18	1.37	43,44,45,50	0
2	BOG	A	1949	20/20	0.81	0.24	1.31	58,64,73,74	0
6	EDO	B	1961	4/4	0.86	0.17	1.19	46,47,47,50	0
8	T3A	B	7066	15/15	0.96	0.13	0.38	24,39,45,47	0
6	EDO	B	1959	4/4	0.85	0.18	-	55,57,57,58	0
6	EDO	A	1959	4/4	0.88	0.13	-	38,44,44,47	0
7	IMD	B	1960	5/5	0.92	0.16	-	59,59,62,62	0
3	PO4	B	1953	5/5	0.83	0.16	-	109,109,109,110	0
2	BOG	A	1951	20/20	0.54	0.31	-	92,95,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	EDO	B	1956	4/4	0.82	0.15	-	42,44,44,49	0
6	EDO	B	1955	4/4	0.90	0.15	-	57,58,60,61	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.