



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 13, 2018 – 06:14 pm GMT

PDB ID : 2R4J  
Title : Crystal structure of Escherichia coli SeMet substituted Glycerol-3-phosphate Dehydrogenase in complex with DHAP  
Authors : Yeh, J.I.; Du, S.; Chinte, U.  
Deposited on : 2007-08-31  
Resolution : 1.96 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

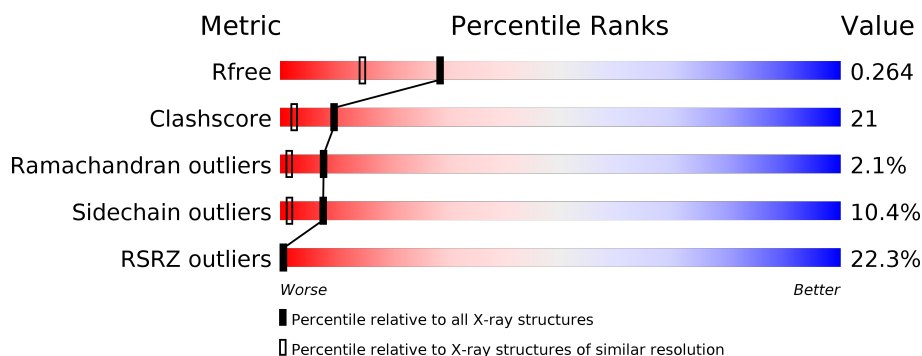
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.96 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))
$R_{free}$	111664	2220 (1.96-1.96)
Clashscore	122126	2333 (1.96-1.96)
Ramachandran outliers	120053	2314 (1.96-1.96)
Sidechain outliers	120020	2314 (1.96-1.96)
RSRZ outliers	108989	2174 (1.96-1.96)

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>22%</div> <div>67%</div> <div>26%</div> <div>5%</div> </div>
1	B	501	<div> <div>22%</div> <div>65%</div> <div>27%</div> <div>6%</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	1949	-	-	-	X
2	BOG	A	1950	-	-	-	X
2	BOG	A	800	-	-	-	X
2	BOG	B	800	-	-	-	X
3	PO4	B	801	-	-	-	X
5	EDO	A	1956	-	-	-	X
5	EDO	A	1957	-	-	X	-
5	EDO	A	1958	-	-	X	-
5	EDO	A	1959	-	-	X	-
5	EDO	B	806	-	-	-	X
5	EDO	B	807	-	-	X	-
5	EDO	B	813	-	-	X	-
5	EDO	B	817	-	-	-	X
6	IMD	A	1960	-	-	X	-
6	IMD	A	1961	-	-	X	-
6	IMD	A	1963	-	-	X	-
6	IMD	A	1966	-	-	X	-
7	13P	B	816	-	-	X	-
8	BCN	A	1969	-	-	-	X
8	BCN	B	820	-	-	-	X
8	BCN	B	821	-	-	-	X
9	TAM	B	812	-	-	X	X

# 2 Entry composition [i](#)

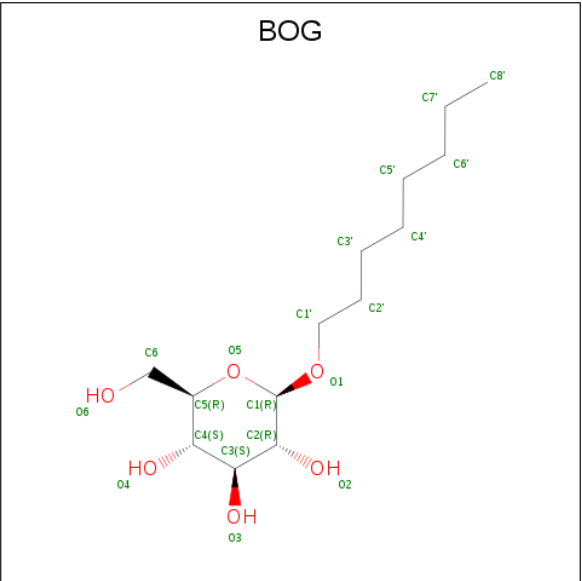
There are 10 unique types of molecules in this entry. The entry contains 8645 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	Se	0	0	0
			3953	2510	703	727	6	7			
1	B	497	Total	C	N	O	S	Se	0	0	0
			3981	2527	710	731	6	7			

- Molecule 2 is B-OCTYLGLUCOSIDE (three-letter code: BOG) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>6</sub>).



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	A	1	Total	C	O	0	0
			20	14	6		
2	A	1	Total	C	O	0	0
			20	14	6		

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

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



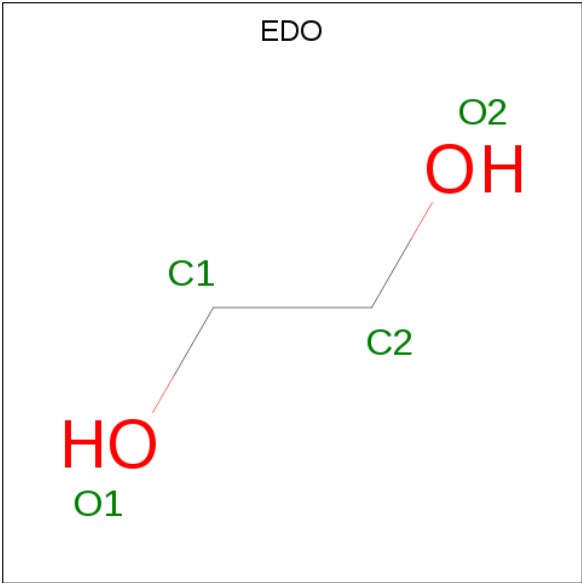
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

- 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 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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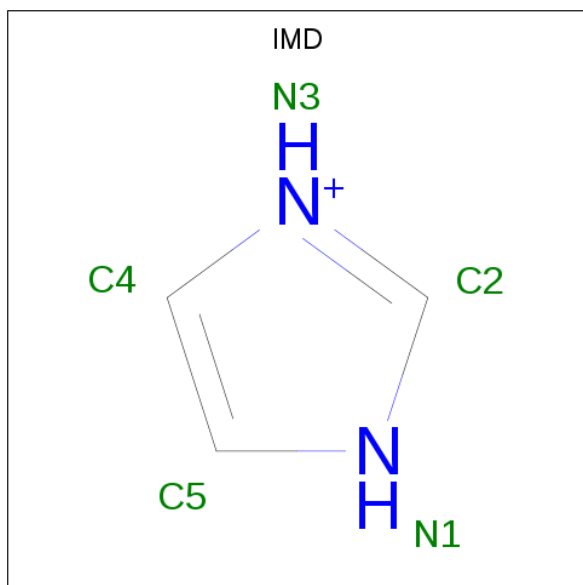
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total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

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

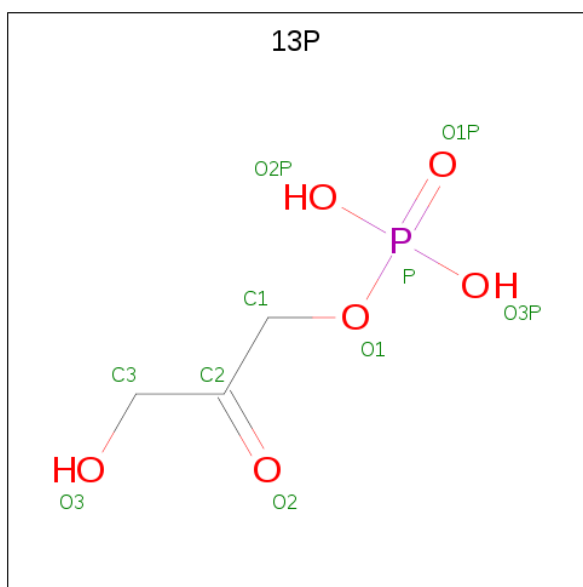
- Molecule 6 is IMIDAZOLE (three-letter code: IMD) (formula:  $C_3H_5N_2$ ).



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

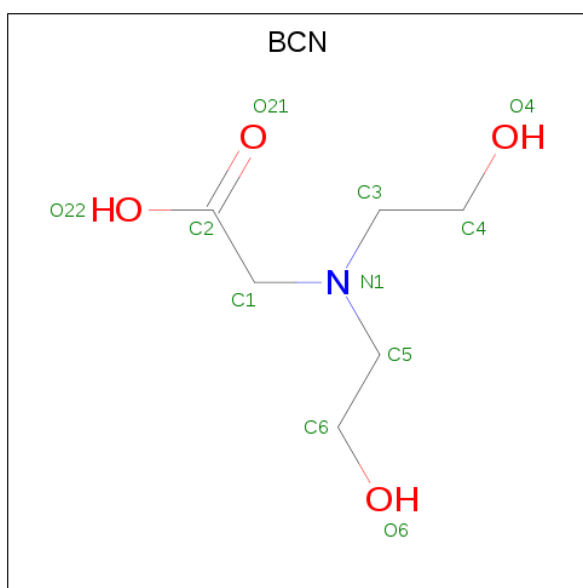
- Molecule 7 is 1,3-DIHYDROXYACETONEPHOSPHATE (three-letter code: 13P) (formula:  $C_3H_7O_6P$ ).





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

- Molecule 8 is BICINE (three-letter code: BCN) (formula:  $C_6H_{13}NO_4$ ).



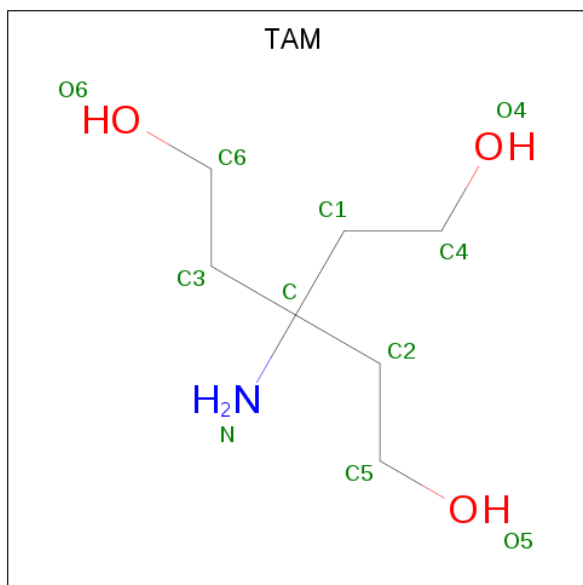
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			11	6	1	4		
8	B	1	Total	C	N	O	0	0
			11	6	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	0	0
			11	6	1	4		

- Molecule 9 is TRIS(HYDROXYETHYL)AMINOMETHANE (three-letter code: TAM) (formula:  $C_7H_{17}NO_3$ ).

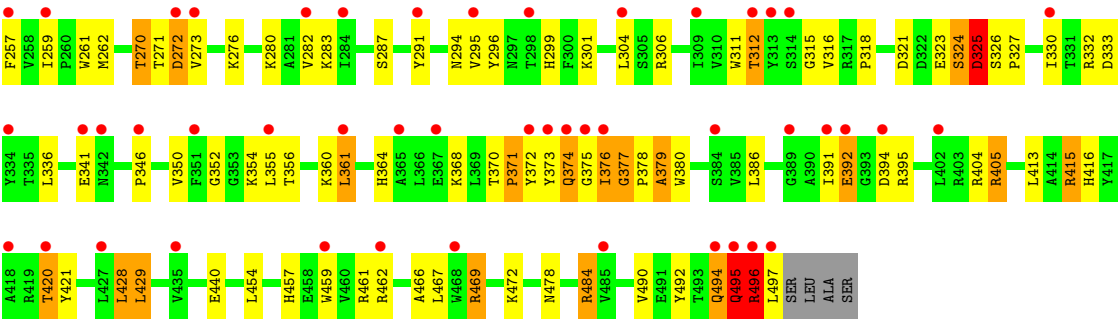


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	N	O	0	0
			11	7	1	3		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	140	Total	O	0	0
			140	140		
10	B	137	Total	O	0	0
			137	137		





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.92Å 114.14Å 193.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.96 40.32 – 1.96	Depositor EDS
% Data completeness (in resolution range)	100.0 (10.00-1.96) 91.0 (40.32-1.96)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	133.85 (at 1.95Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.211 , 0.263 0.220 , 0.264	Depositor DCC
$R_{free}$ test set	4126 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.3	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 31.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.450 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8645	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BCN, IMD, PO4, EDO, 13P, TAM, 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	1.10	4/4041 (0.1%)	1.03	6/5461 (0.1%)
1	B	1.12	2/4069 (0.0%)	1.05	12/5498 (0.2%)
All	All	1.11	6/8110 (0.1%)	1.04	18/10959 (0.2%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	295	VAL	C-O	5.60	1.33	1.23
1	A	447	TYR	CD2-CE2	5.58	1.47	1.39
1	A	165	GLU	CB-CG	5.50	1.62	1.52
1	B	12	GLY	N-CA	-5.27	1.38	1.46
1	A	236	VAL	CB-CG2	5.19	1.63	1.52

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	169	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	247	ILE	CB-CA-C	-5.74	100.11	111.60
1	A	355	LEU	CB-CG-CD1	-5.71	101.28	111.00
1	B	148	ASP	CB-CG-OD1	5.68	123.41	118.30
1	A	355	LEU	CA-CB-CG	5.60	128.17	115.30

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	144	0
1	B	3981	0	3935	177	0
2	A	80	0	112	7	0
2	B	40	0	56	9	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	53	0	31	1	0
4	B	53	0	31	0	0
5	A	44	0	66	28	0
5	B	60	0	90	24	0
6	A	25	0	25	21	0
6	B	5	0	5	1	0
7	A	10	0	5	0	0
7	B	10	0	5	4	0
8	A	11	0	12	1	0
8	B	22	0	24	5	0
9	B	11	0	17	7	0
10	A	140	0	0	9	0
10	B	137	0	0	13	0
All	All	8645	0	8317	347	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 21.

The worst 5 of 347 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:B:27:LEU:HD21	1:B:376:ILE:CD1	1.54	1.37
1:B:374:GLN:CB	1:B:375:GLY:HA3	1.59	1.27
1:B:467:LEU:HA	10:B:938:HOH:O	1.37	1.22
5:B:813:EDO:H22	10:B:869:HOH:O	1.37	1.20
1:B:428:LEU:HD12	1:B:428:LEU:O	1.36	1.20

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%)	456 (93%)	30 (6%)	6 (1%)	14	4
1	B	495/501 (99%)	454 (92%)	26 (5%)	15 (3%)	5	1
All	All	987/1002 (98%)	910 (92%)	56 (6%)	21 (2%)	8	1

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	LYS
1	A	118	PRO
1	B	113	LYS
1	B	118	PRO
1	B	324	SER

### 5.3.2 Protein sidechains [i](#)

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	413/412 (100%)	377 (91%)	36 (9%)	11	3
1	B	416/412 (101%)	366 (88%)	50 (12%)	5	1
All	All	829/824 (101%)	743 (90%)	86 (10%)	8	2

5 of 86 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	4	LYS

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Mol	Chain	Res	Type
1	B	116	SER
1	B	420	THR
1	B	53	LEU
1	B	103	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	424	ASN
1	A	478	ASN
1	B	494	GLN
1	A	444	HIS
1	A	473	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

48 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	0.96	1 (5%)	25,25,25	0.90	1 (4%)
2	BOG	A	1950	-	20,20,20	0.95	1 (5%)	25,25,25	1.67	5 (20%)
3	PO4	A	1951	-	4,4,4	0.61	0	6,6,6	0.60	0
5	EDO	A	1952	-	3,3,3	0.74	0	2,2,2	0.26	0
5	EDO	A	1953	-	3,3,3	0.64	0	2,2,2	0.95	0
5	EDO	A	1954	-	3,3,3	0.59	0	2,2,2	0.27	0
5	EDO	A	1955	-	3,3,3	0.71	0	2,2,2	0.38	0
5	EDO	A	1956	-	3,3,3	0.51	0	2,2,2	0.23	0
5	EDO	A	1957	-	3,3,3	1.12	0	2,2,2	0.88	0
5	EDO	A	1958	-	3,3,3	0.50	0	2,2,2	0.24	0
5	EDO	A	1959	-	3,3,3	0.70	0	2,2,2	0.51	0
6	IMD	A	1960	-	3,5,5	0.34	0	4,5,5	0.92	0
6	IMD	A	1961	-	3,5,5	0.37	0	4,5,5	0.60	0
5	EDO	A	1962	-	3,3,3	0.56	0	2,2,2	0.35	0
6	IMD	A	1963	-	3,5,5	0.52	0	4,5,5	0.49	0
5	EDO	A	1964	-	3,3,3	0.58	0	2,2,2	0.46	0
5	EDO	A	1965	-	3,3,3	0.65	0	2,2,2	0.67	0
6	IMD	A	1966	-	3,5,5	0.41	0	4,5,5	1.12	0
6	IMD	A	1967	-	3,5,5	0.55	0	4,5,5	0.49	0
7	13P	A	1968	-	9,9,9	5.43	6 (66%)	10,12,12	3.94	4 (40%)
8	BCN	A	1969	-	7,10,10	0.77	0	8,11,11	2.60	4 (50%)
4	FAD	A	600	-	51,58,58	1.78	17 (33%)	57,89,89	2.10	14 (24%)
2	BOG	A	700	-	20,20,20	0.75	1 (5%)	25,25,25	1.12	2 (8%)
2	BOG	A	800	-	20,20,20	0.63	1 (5%)	25,25,25	1.54	5 (20%)
4	FAD	B	600	-	51,58,58	2.21	14 (27%)	57,89,89	2.72	18 (31%)
2	BOG	B	700	-	20,20,20	0.80	1 (5%)	25,25,25	1.07	2 (8%)
2	BOG	B	800	-	20,20,20	0.56	0	25,25,25	1.22	2 (8%)
3	PO4	B	801	-	4,4,4	0.39	0	6,6,6	0.86	0
5	EDO	B	802	-	3,3,3	0.98	0	2,2,2	0.89	0
5	EDO	B	803	-	3,3,3	0.84	0	2,2,2	0.81	0
5	EDO	B	804	-	3,3,3	0.53	0	2,2,2	0.90	0
5	EDO	B	805	-	3,3,3	0.55	0	2,2,2	0.68	0
5	EDO	B	806	-	3,3,3	1.11	0	2,2,2	0.38	0
5	EDO	B	807	-	3,3,3	1.02	0	2,2,2	0.63	0
5	EDO	B	808	-	3,3,3	0.86	0	2,2,2	0.35	0
5	EDO	B	809	-	3,3,3	0.61	0	2,2,2	0.42	0
5	EDO	B	810	-	3,3,3	0.60	0	2,2,2	0.43	0
5	EDO	B	811	-	3,3,3	0.34	0	2,2,2	0.80	0
9	TAM	B	812	-	7,10,10	0.73	0	9,12,12	2.75	5 (55%)
5	EDO	B	813	-	3,3,3	0.27	0	2,2,2	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	EDO	B	814	-	3,3,3	0.75	0	2,2,2	0.21	0
5	EDO	B	815	-	3,3,3	0.39	0	2,2,2	0.91	0
7	13P	B	816	-	9,9,9	5.44	6 (66%)	10,12,12	3.64	4 (40%)
5	EDO	B	817	-	3,3,3	0.66	0	2,2,2	0.32	0
5	EDO	B	818	-	3,3,3	0.57	0	2,2,2	0.29	0
6	IMD	B	819	-	3,5,5	0.46	0	4,5,5	0.44	0
8	BCN	B	820	-	7,10,10	0.82	0	8,11,11	3.27	4 (50%)
8	BCN	B	821	-	7,10,10	0.65	0	8,11,11	3.85	4 (50%)

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
3	PO4	A	1951	-	-	0/0/0/0	0/0/0/0
5	EDO	A	1952	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1953	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1954	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1955	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1956	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1957	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1958	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1959	-	-	0/1/1/1	0/0/0/0
6	IMD	A	1960	-	-	0/0/0/0	0/1/1/1
6	IMD	A	1961	-	-	0/0/0/0	0/1/1/1
5	EDO	A	1962	-	-	0/1/1/1	0/0/0/0
6	IMD	A	1963	-	-	0/0/0/0	0/1/1/1
5	EDO	A	1964	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1965	-	-	0/1/1/1	0/0/0/0
6	IMD	A	1966	-	-	0/0/0/0	0/1/1/1
6	IMD	A	1967	-	-	0/0/0/0	0/1/1/1
7	13P	A	1968	-	-	0/7/8/8	0/0/0/0
8	BCN	A	1969	-	-	0/8/10/10	0/0/0/0
4	FAD	A	600	-	-	0/28/50/50	0/6/6/6
2	BOG	A	700	-	-	0/11/31/31	0/1/1/1
2	BOG	A	800	-	-	0/11/31/31	0/1/1/1
4	FAD	B	600	-	-	0/28/50/50	0/6/6/6
2	BOG	B	700	-	-	0/11/31/31	0/1/1/1
2	BOG	B	800	-	-	0/11/31/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PO4	B	801	-	-	0/0/0/0	0/0/0/0
5	EDO	B	802	-	-	0/1/1/1	0/0/0/0
5	EDO	B	803	-	-	0/1/1/1	0/0/0/0
5	EDO	B	804	-	-	0/1/1/1	0/0/0/0
5	EDO	B	805	-	-	0/1/1/1	0/0/0/0
5	EDO	B	806	-	-	0/1/1/1	0/0/0/0
5	EDO	B	807	-	-	0/1/1/1	0/0/0/0
5	EDO	B	808	-	-	0/1/1/1	0/0/0/0
5	EDO	B	809	-	-	0/1/1/1	0/0/0/0
5	EDO	B	810	-	-	0/1/1/1	0/0/0/0
5	EDO	B	811	-	-	0/1/1/1	0/0/0/0
9	TAM	B	812	-	-	0/12/12/12	0/0/0/0
5	EDO	B	813	-	-	0/1/1/1	0/0/0/0
5	EDO	B	814	-	-	0/1/1/1	0/0/0/0
5	EDO	B	815	-	-	0/1/1/1	0/0/0/0
7	13P	B	816	-	-	0/7/8/8	0/0/0/0
5	EDO	B	817	-	-	0/1/1/1	0/0/0/0
5	EDO	B	818	-	-	0/1/1/1	0/0/0/0
6	IMD	B	819	-	-	0/0/0/0	0/1/1/1
8	BCN	B	820	-	-	0/8/10/10	0/0/0/0
8	BCN	B	821	-	-	0/8/10/10	0/0/0/0

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	600	FAD	C4'-C3'	-3.77	1.46	1.53
4	A	600	FAD	C6-C5X	-3.48	1.36	1.41
4	B	600	FAD	C6-C5X	-3.04	1.37	1.41
4	A	600	FAD	O4'-C4'	-2.86	1.37	1.43
4	A	600	FAD	PA-O2A	-2.85	1.41	1.55

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	600	FAD	N3A-C2A-N1A	-8.90	121.25	128.86
7	A	1968	13P	O3P-P-O1	-8.74	83.48	106.73
4	A	600	FAD	N3A-C2A-N1A	-8.07	121.96	128.86
7	B	816	13P	O3P-P-O1	-7.88	85.77	106.73
4	A	600	FAD	O2A-PA-O5B	-4.46	87.04	107.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

36 monomers are involved in 97 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1950	BOG	1	0
5	A	1953	EDO	2	0
5	A	1955	EDO	2	0
5	A	1956	EDO	3	0
5	A	1957	EDO	6	0
5	A	1958	EDO	4	0
5	A	1959	EDO	7	0
6	A	1960	IMD	4	0
6	A	1961	IMD	5	0
5	A	1962	EDO	1	0
6	A	1963	IMD	8	0
5	A	1964	EDO	1	0
5	A	1965	EDO	3	0
6	A	1966	IMD	4	0
8	A	1969	BCN	1	0
4	A	600	FAD	1	0
2	A	700	BOG	1	0
2	A	800	BOG	5	0
2	B	700	BOG	2	0
2	B	800	BOG	7	0
5	B	802	EDO	1	0
5	B	803	EDO	2	0
5	B	804	EDO	1	0
5	B	806	EDO	1	0
5	B	807	EDO	7	0
5	B	808	EDO	2	0
5	B	810	EDO	2	0
5	B	811	EDO	3	0
9	B	812	TAM	7	0
5	B	813	EDO	6	0
5	B	815	EDO	1	0
7	B	816	13P	4	0
5	B	817	EDO	1	0
6	B	819	IMD	1	0
8	B	820	BCN	2	0
8	B	821	BCN	3	0

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	487/501 (97%)	1.40	110 (22%) 0 0	20, 41, 65, 84	0
1	B	490/501 (97%)	1.45	108 (22%) 0 1	19, 41, 66, 98	0
All	All	977/1002 (97%)	1.42	218 (22%) 0 0	19, 41, 66, 98	0

The worst 5 of 218 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	113	LYS	11.3
1	B	494	GLN	9.4
1	B	59	TYR	8.3
1	A	1	MET	8.1
1	B	106	PHE	6.7

### 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BOG	A	800	20/20	0.02	1.71	131,136,138,138	0
2	BOG	A	1949	20/20	0.09	0.55	92,95,97,97	0
2	BOG	A	1950	20/20	0.12	0.67	90,93,94,95	0
8	BCN	A	1969	11/11	0.20	0.59	63,76,79,79	0
5	EDO	B	806	4/4	0.35	0.63	34,45,50,55	0
2	BOG	B	800	20/20	0.42	0.66	133,136,139,140	0
9	TAM	B	812	11/11	0.45	0.49	56,63,66,70	0
5	EDO	B	809	4/4	0.48	0.19	65,66,67,68	0
2	BOG	A	700	20/20	0.51	0.31	86,91,94,94	0
5	EDO	B	807	4/4	0.52	0.22	46,47,50,52	0
5	EDO	A	1964	4/4	0.52	0.20	64,66,66,67	0
8	BCN	B	821	11/11	0.52	0.45	58,64,70,70	0
6	IMD	A	1960	5/5	0.53	0.37	58,58,60,60	0
5	EDO	B	802	4/4	0.56	0.37	38,44,48,50	0
8	BCN	B	820	11/11	0.63	0.47	64,69,72,74	0
5	EDO	B	808	4/4	0.63	0.30	52,56,57,60	0
6	IMD	B	819	5/5	0.66	0.18	78,78,79,81	0
6	IMD	A	1961	5/5	0.67	0.25	73,73,74,74	0
6	IMD	A	1966	5/5	0.68	0.24	70,70,72,72	0
5	EDO	B	818	4/4	0.70	0.21	72,75,75,75	0
5	EDO	B	805	4/4	0.71	0.20	63,64,64,68	0
5	EDO	A	1956	4/4	0.71	0.49	41,44,50,54	0
5	EDO	B	810	4/4	0.71	0.25	53,53,54,58	0
6	IMD	A	1963	5/5	0.76	0.19	42,47,49,50	0
5	EDO	B	814	4/4	0.76	0.22	54,56,56,56	0
5	EDO	B	817	4/4	0.76	0.73	55,62,65,66	0
3	PO4	B	801	5/5	0.76	0.52	68,68,70,71	0
5	EDO	B	804	4/4	0.76	0.22	49,49,51,52	0
5	EDO	A	1957	4/4	0.77	0.17	43,48,48,49	0
5	EDO	A	1954	4/4	0.77	0.16	64,65,65,66	0
5	EDO	A	1965	4/4	0.80	0.24	37,37,42,42	0
5	EDO	B	803	4/4	0.81	0.23	47,49,52,53	0
7	13P	B	816	10/10	0.81	0.24	28,40,45,45	0
5	EDO	A	1952	4/4	0.81	0.23	63,63,64,64	0
5	EDO	B	813	4/4	0.83	0.25	36,39,41,43	0
2	BOG	B	700	20/20	0.83	0.30	63,71,77,79	0
5	EDO	A	1955	4/4	0.83	0.30	38,50,50,52	0
7	13P	A	1968	10/10	0.83	0.23	28,38,43,44	0
5	EDO	A	1953	4/4	0.85	0.22	32,45,46,47	0
5	EDO	A	1962	4/4	0.85	0.16	70,71,72,74	0
6	IMD	A	1967	5/5	0.85	0.19	63,64,65,67	0
5	EDO	B	815	4/4	0.88	0.17	54,57,59,62	0
3	PO4	A	1951	5/5	0.89	0.15	84,84,84,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	FAD	B	600	53/53	0.90	0.15	19,25,29,32	0
5	EDO	A	1959	4/4	0.90	0.14	43,48,49,52	0
5	EDO	B	811	4/4	0.91	0.28	36,43,44,49	0
5	EDO	A	1958	4/4	0.91	0.36	32,34,40,46	0
4	FAD	A	600	53/53	0.92	0.16	18,26,29,36	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.