



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:32 AM 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

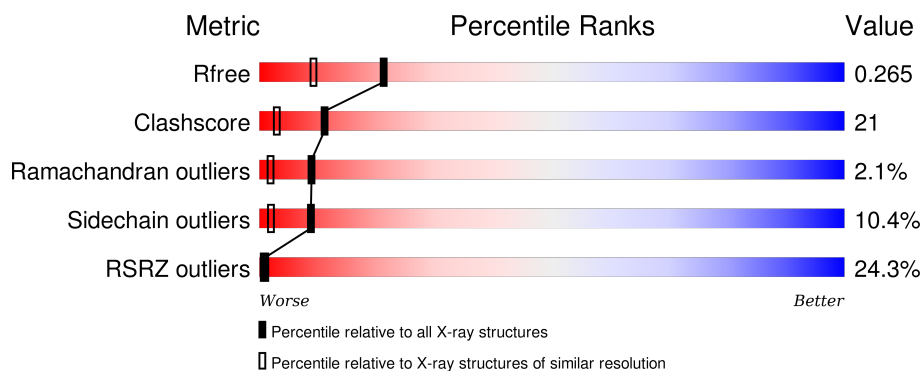
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (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 ≥ 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>24%</div> <div>67%</div> <div>26%</div> <div>5%</div> </div>
1	B	501	<div> <div>23%</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	800	-	-	-	X
2	BOG	B	700	-	-	-	X
2	BOG	B	800	-	-	-	X
3	PO4	B	801	-	-	-	X
5	EDO	A	1952	-	-	-	X
5	EDO	A	1953	-	-	-	X
5	EDO	A	1955	-	-	-	X
5	EDO	A	1956	-	-	-	X
5	EDO	A	1957	-	-	X	X
5	EDO	A	1958	-	-	X	X
5	EDO	A	1959	-	-	X	-
5	EDO	A	1965	-	-	-	X
5	EDO	B	802	-	-	-	X
5	EDO	B	806	-	-	-	X
5	EDO	B	807	-	-	X	-
5	EDO	B	808	-	-	-	X
5	EDO	B	810	-	-	-	X
5	EDO	B	811	-	-	-	X
5	EDO	B	813	-	-	X	-
6	IMD	A	1960	-	-	X	X
6	IMD	A	1961	-	-	X	-
6	IMD	A	1963	-	-	X	-
6	IMD	A	1966	-	-	X	-
7	TAM	B	812	-	-	X	X
8	13P	B	816	-	-	X	-
9	BCN	A	1969	-	-	-	X
9	BCN	B	820	-	-	-	X
9	BCN	B	821	-	-	-	X

2 Entry composition [i](#)

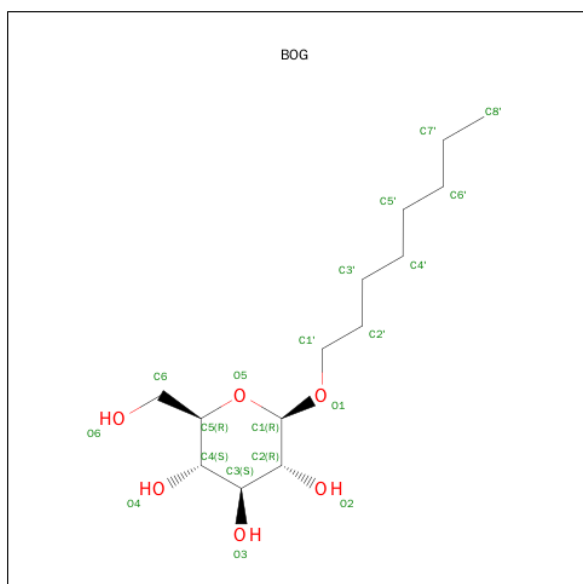
There are 10 unique types of molecules in this entry. The entry contains 8645 atoms, of which 0 are hydrogens and 0 are deuteriums.

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



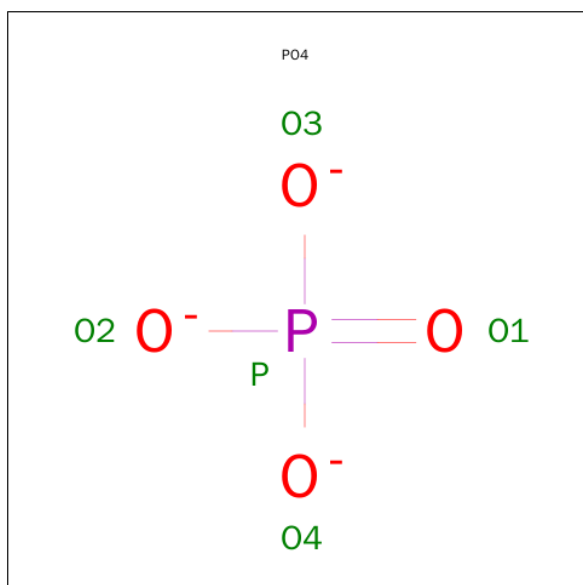
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			20	14	6		
2	A	1	Total	C	O	0	0
			20	14	6		
2	B	1	Total	C	O	0	0
			20	14	6		
2	B	1	Total	C	O	0	0
			20	14	6		

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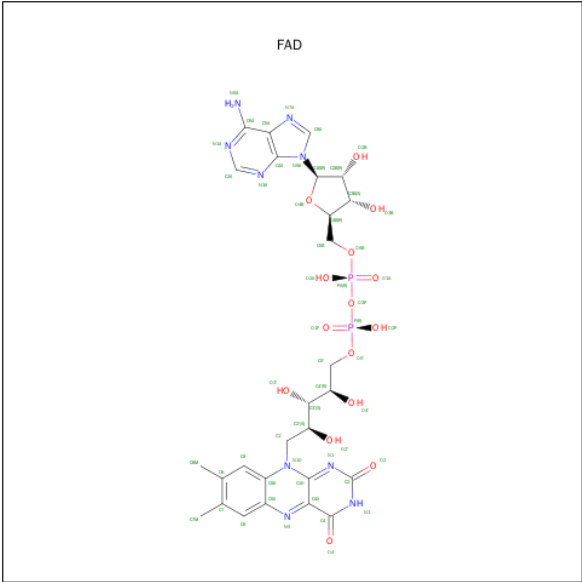
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			20	14	6		
2	A	1	Total	C	O	0	0
			20	14	6		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



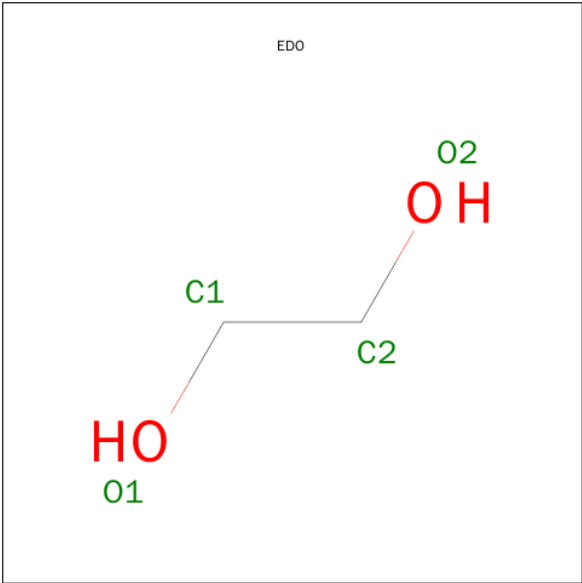
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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: C₂H₆O₂).



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		

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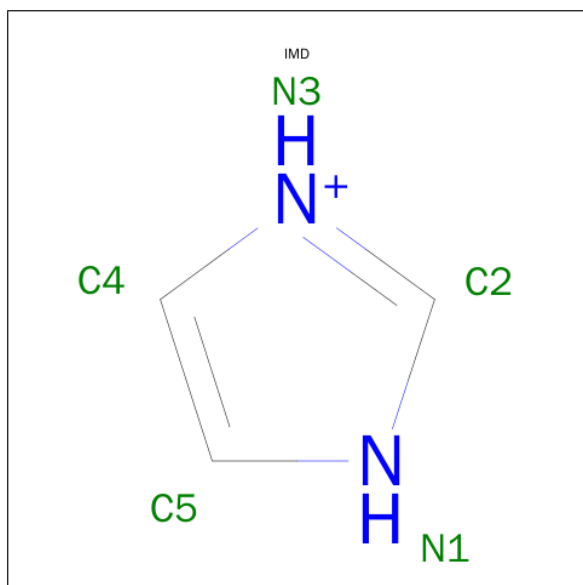
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0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

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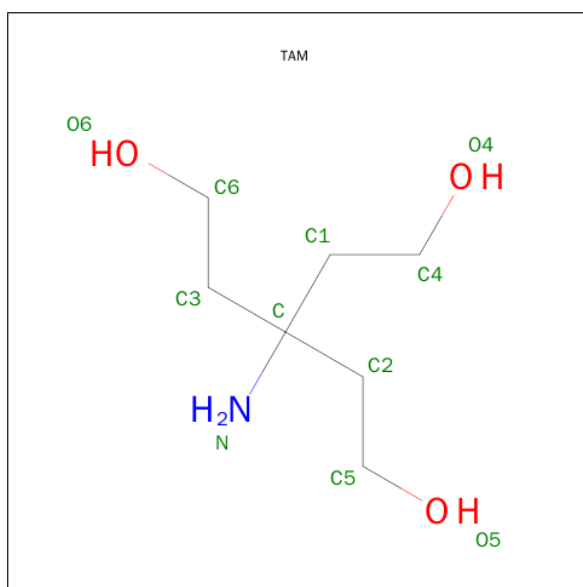
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

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



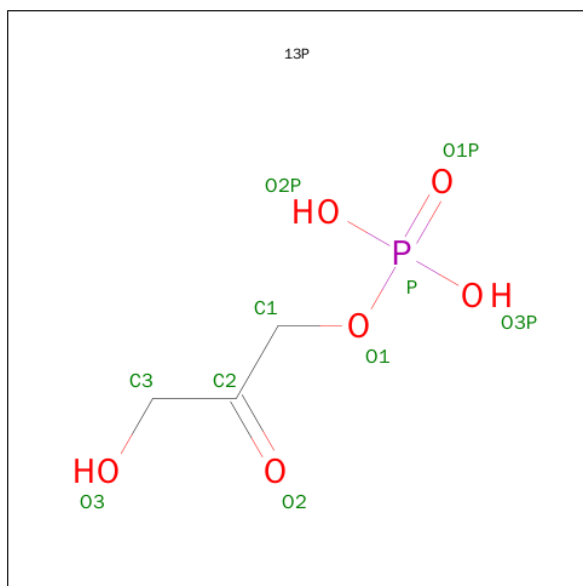
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	N	0	0
			5	3	2		
6	A	1	Total	C	N	0	0
			5	3	2		
6	A	1	Total	C	N	0	0
			5	3	2		
6	A	1	Total	C	N	0	0
			5	3	2		
6	A	1	Total	C	N	0	0
			5	3	2		
6	B	1	Total	C	N	0	0
			5	3	2		

- Molecule 7 is TRIS(HYDROXYETHYL)AMINOMETHANE (three-letter code: TAM) (formula: $C_7H_{17}NO_3$).



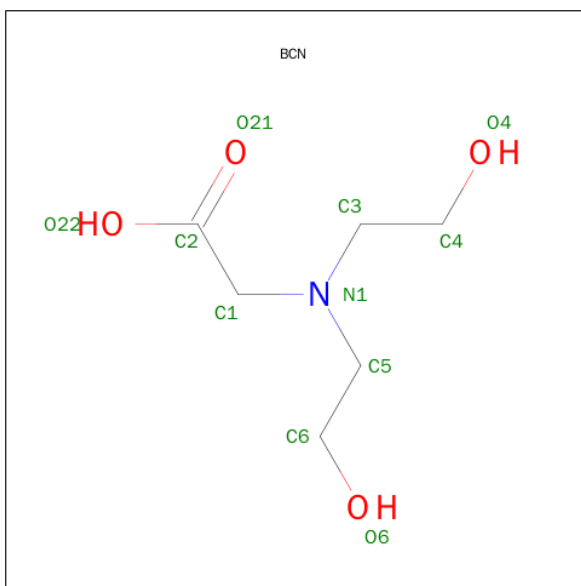
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			11	7	1	3		

- Molecule 8 is 1,3-DIHYDROXYACETONEPHOSPHATE (three-letter code: 13P) (formula: $C_3H_7O_6P$).



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

- Molecule 9 is BICINE (three-letter code: BCN) (formula: $C_6H_{13}NO_4$).



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

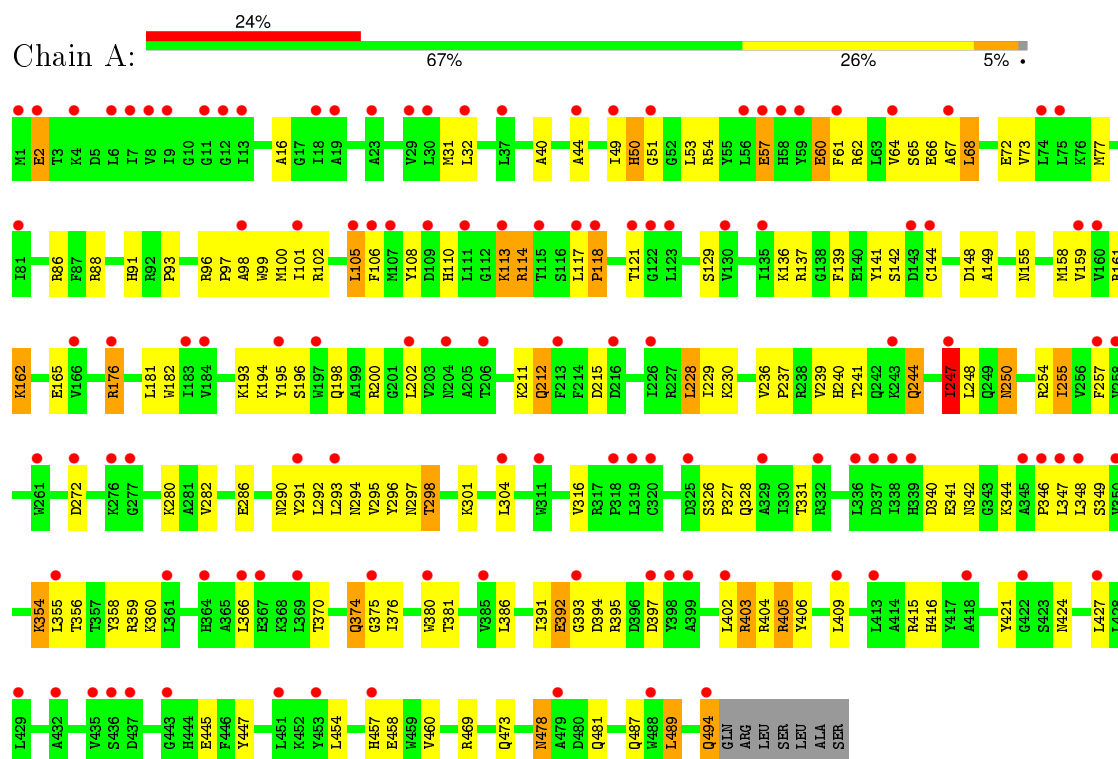
- Molecule 10 is water.

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

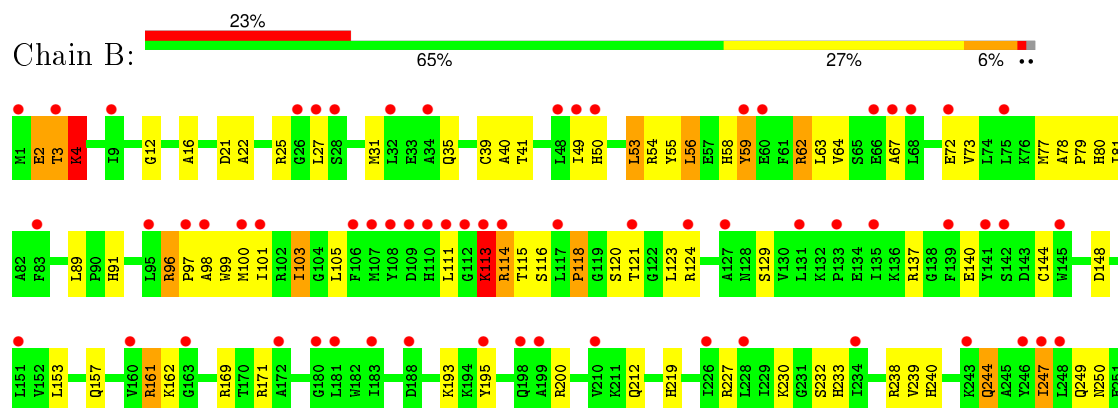
3 Residue-property plots [i](#)

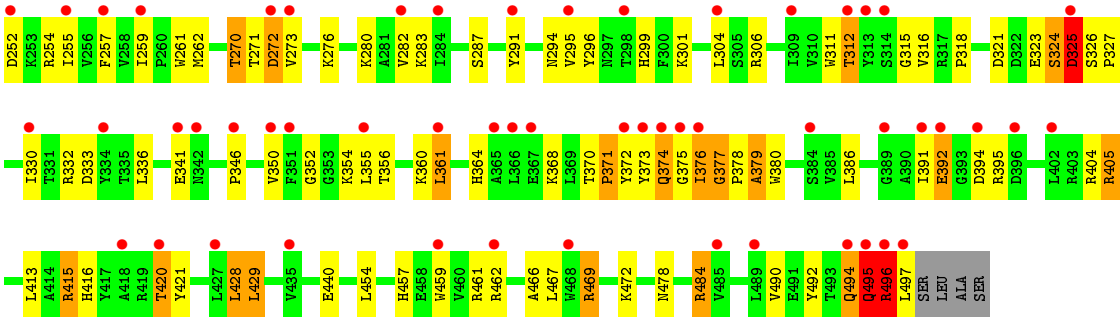
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	133.85 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.211 , 0.263 0.218 , 0.265	Depositor DCC
R_{free} test set	4086 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	33.3	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 31.9	EDS
Estimated twinning fraction	0.450 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 82520 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8645	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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%)

All (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
1	B	466	ALA	CA-CB	5.07	1.63	1.52

All (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
1	B	304	LEU	CB-CG-CD1	-5.58	101.52	111.00
1	B	429	LEU	CA-CB-CG	5.55	128.06	115.30
1	A	86	ARG	NE-CZ-NH1	-5.51	117.54	120.30
1	B	153	LEU	CB-CG-CD1	-5.42	101.79	111.00
1	B	113	LYS	N-CA-C	5.40	125.58	111.00
1	B	96	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	B	469	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	228	LEU	CA-CB-CG	-5.28	103.16	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	489	LEU	CA-CB-CG	5.28	127.44	115.30
1	B	53	LEU	CB-CG-CD1	-5.19	102.17	111.00
1	B	96	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	B	283	LYS	CB-CA-C	-5.13	100.15	110.40
1	B	462	ARG	NE-CZ-NH1	5.08	122.84	120.30

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	B	11	0	17	7	0
8	A	10	0	5	0	0
8	B	10	0	5	4	0
9	A	11	0	12	1	0
9	B	22	0	24	5	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.

All (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
5:A:1959:EDO:H21	6:A:1963:IMD:H5	1.22	1.17
1:A:237:PRO:HG3	6:A:1966:IMD:N3	1.60	1.16
1:B:361:LEU:O	1:B:361:LEU:HD12	1.44	1.14
1:A:51:GLY:HA3	1:A:68:LEU:HD13	1.29	1.12
1:A:374:GLN:CB	1:A:375:GLY:HA3	1.78	1.12
1:A:237:PRO:HG3	6:A:1966:IMD:HN3	1.02	1.11
1:A:341:GLU:CG	1:A:342:ASN:H	1.63	1.11
1:B:374:GLN:HB2	1:B:375:GLY:CA	1.79	1.10
1:A:374:GLN:HB2	1:A:375:GLY:HA3	1.28	1.10
5:A:1957:EDO:H11	6:A:1960:IMD:H5	1.29	1.10
1:A:237:PRO:CG	6:A:1966:IMD:HN3	1.66	1.07
5:B:807:EDO:H11	5:B:808:EDO:O1	1.55	1.06
1:B:50:HIS:CE1	1:B:354:LYS:NZ	2.24	1.06
1:A:341:GLU:HG3	1:A:342:ASN:N	1.65	1.05
1:B:27:LEU:HD21	1:B:376:ILE:HD12	1.13	1.05
1:B:361:LEU:HD12	1:B:361:LEU:C	1.77	1.04
5:A:1959:EDO:H21	6:A:1963:IMD:C5	1.86	1.04
1:B:50:HIS:CE1	1:B:354:LYS:HZ3	1.75	1.03
1:A:158:MSE:CE	1:A:161:ARG:HD2	1.87	1.03
1:B:113:LYS:HB3	1:B:114:ARG:HA	1.41	1.02
1:B:50:HIS:HE1	1:B:354:LYS:NZ	1.58	1.01
1:A:158:MSE:HE1	1:A:161:ARG:HD2	1.02	0.99
1:B:428:LEU:HD12	1:B:428:LEU:C	1.82	0.98
1:A:294:ASN:O	1:A:298:THR:HG23	1.62	0.97
5:A:1959:EDO:C2	6:A:1963:IMD:H5	1.95	0.97
1:A:176:ARG:HH11	1:A:176:ARG:HG2	1.29	0.96
1:A:341:GLU:HG3	1:A:342:ASN:H	0.81	0.95
1:B:62:ARG:HD3	1:B:333:ASP:OD2	1.66	0.95
1:A:158:MSE:HE1	1:A:161:ARG:CD	1.96	0.95
5:A:1957:EDO:C1	6:A:1960:IMD:H5	1.97	0.93
1:B:73:VAL:HG12	1:B:77:MSE:CE	1.96	0.93
1:A:297:ASN:HD21	1:A:304:LEU:H	1.05	0.93
1:A:457:HIS:C	6:A:1963:IMD:H4	1.89	0.93
1:B:467:LEU:HD23	10:B:938:HOH:O	1.68	0.92
1:B:50:HIS:CE1	1:B:354:LYS:CE	2.53	0.91
1:B:27:LEU:CD2	1:B:376:ILE:HD12	2.00	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:TYR:OH	1:A:247:ILE:CD1	2.21	0.88
1:B:376:ILE:HG23	1:B:376:ILE:O	1.70	0.88
1:B:374:GLN:HB2	1:B:375:GLY:HA3	0.88	0.88
1:B:315:GLY:HA2	5:B:813:EDO:H11	1.56	0.88
1:B:73:VAL:HG12	1:B:77:MSE:HE1	1.55	0.87
1:B:27:LEU:CD2	1:B:376:ILE:CD1	2.49	0.85
1:A:51:GLY:HA3	1:A:68:LEU:CD1	2.06	0.84
1:A:176:ARG:CG	1:A:176:ARG:HH11	1.91	0.83
1:B:315:GLY:CA	5:B:813:EDO:H11	2.09	0.83
1:B:212:GLN:HG2	5:B:810:EDO:H22	1.59	0.82
1:A:445:GLU:HB2	6:A:1960:IMD:H2	1.61	0.82
1:A:158:MSE:HA	1:A:158:MSE:HE3	1.61	0.82
1:B:323:GLU:O	1:B:324:SER:HB3	1.80	0.82
1:B:27:LEU:HD11	1:B:376:ILE:HD11	1.60	0.82
1:B:374:GLN:CB	1:B:375:GLY:CA	2.43	0.82
1:A:478:ASN:ND2	1:A:481:GLN:H	1.78	0.80
1:A:487:GLN:HG2	10:A:2079:HOH:O	1.80	0.80
5:B:807:EDO:H11	5:B:808:EDO:HO1	1.47	0.80
1:A:374:GLN:CB	1:A:375:GLY:CA	2.59	0.80
1:B:161:ARG:HB2	7:B:812:TAM:O5	1.81	0.79
1:A:141:TYR:OH	1:A:247:ILE:HD11	1.82	0.79
1:B:50:HIS:HE1	1:B:354:LYS:CE	1.93	0.79
1:B:59:TYR:CE2	2:B:800:BOG:H5'2	2.17	0.79
1:A:392:GLU:CA	1:A:392:GLU:OE1	2.30	0.78
1:B:416:HIS:O	1:B:420:THR:HG23	1.83	0.78
1:A:280:LYS:HA	1:A:280:LYS:HE2	1.65	0.78
1:B:56:LEU:HD13	1:B:64:VAL:HG21	1.66	0.78
1:B:361:LEU:C	1:B:361:LEU:CD1	2.52	0.77
1:B:262:MSE:HE2	5:B:807:EDO:H12	1.67	0.77
1:B:113:LYS:CB	1:B:114:ARG:HA	2.12	0.75
1:A:392:GLU:HA	1:A:392:GLU:OE1	1.84	0.75
1:B:364:HIS:HB2	10:B:885:HOH:O	1.86	0.75
1:A:254:ARG:HD2	1:A:328:GLN:HB3	1.68	0.74
1:B:316:VAL:H	5:B:813:EDO:C1	2.00	0.74
1:B:361:LEU:O	1:B:361:LEU:CD1	2.30	0.74
1:B:157:GLN:HG2	7:B:812:TAM:N	2.01	0.74
1:B:27:LEU:HD21	1:B:376:ILE:HD11	1.67	0.74
1:A:96:ARG:NE	2:A:800:BOG:H5	2.02	0.73
1:B:114:ARG:HG2	1:B:114:ARG:O	1.88	0.73
1:A:374:GLN:HB3	1:A:375:GLY:HA3	1.71	0.72
1:B:324:SER:O	1:B:325:ASP:HB2	1.87	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:LEU:HD12	1:B:364:HIS:HD2	1.52	0.72
1:B:324:SER:OG	1:B:325:ASP:N	2.23	0.72
1:B:376:ILE:CG2	1:B:376:ILE:O	2.38	0.71
1:B:99:TRP:O	1:B:103:ILE:HG12	1.90	0.71
1:A:202:LEU:HD23	1:A:347:LEU:HD13	1.71	0.71
1:A:424:ASN:ND2	6:A:1961:IMD:H4	2.06	0.70
1:B:129:SER:O	1:B:301:LYS:HE2	1.91	0.69
1:A:176:ARG:NH1	1:A:176:ARG:HG2	2.06	0.69
1:B:299:HIS:HE1	10:B:882:HOH:O	1.75	0.68
1:B:50:HIS:CE1	1:B:354:LYS:HE2	2.28	0.68
1:B:113:LYS:HB3	1:B:114:ARG:CA	2.20	0.68
1:B:114:ARG:NH1	1:B:118:PRO:O	2.26	0.68
1:A:53:LEU:HG	2:A:800:BOG:H2	1.76	0.68
1:B:72:GLU:OE2	1:B:114:ARG:HB2	1.93	0.68
1:A:370:THR:HG23	1:A:376:ILE:HG21	1.76	0.68
1:B:378:PRO:O	1:B:379:ALA:O	2.12	0.67
1:A:406:TYR:HE1	10:A:2045:HOH:O	1.76	0.67
5:B:806:EDO:H21	10:B:958:HOH:O	1.95	0.67
1:B:250:ASN:ND2	1:B:291:TYR:CZ	2.63	0.67
1:B:405:ARG:HG3	10:B:894:HOH:O	1.93	0.67
1:B:461:ARG:NH1	10:B:942:HOH:O	2.29	0.66
5:A:1958:EDO:C2	10:A:2097:HOH:O	2.44	0.66
1:B:496:ARG:O	1:B:497:LEU:HG	1.96	0.66
1:B:336:LEU:HD12	1:B:364:HIS:CD2	2.30	0.66
1:A:254:ARG:NE	1:A:272:ASP:OD2	2.27	0.65
1:A:392:GLU:N	1:A:392:GLU:OE1	2.30	0.65
1:B:492:TYR:HB2	6:B:819:IMD:H4	1.79	0.65
1:A:51:GLY:CA	1:A:68:LEU:HD13	2.17	0.65
1:B:2:GLU:O	1:B:4:LYS:HB2	1.97	0.65
1:A:290:ASN:HA	5:A:1956:EDO:H12	1.79	0.64
1:B:301:LYS:NZ	10:B:933:HOH:O	2.29	0.64
1:A:181:LEU:HD23	10:A:2063:HOH:O	1.98	0.64
1:B:428:LEU:CD1	1:B:428:LEU:C	2.58	0.64
1:B:161:ARG:HB2	7:B:812:TAM:HO5	1.63	0.63
1:A:50:HIS:NE2	1:A:354:LYS:NZ	2.44	0.62
1:B:273:VAL:HG13	9:B:820:BCN:H32	1.80	0.62
1:B:428:LEU:CD1	1:B:428:LEU:O	2.30	0.62
1:A:403:ARG:NH1	1:A:409:LEU:O	2.28	0.62
1:A:117:LEU:O	1:A:118:PRO:O	2.17	0.62
1:A:93:PRO:HB3	2:A:1950:BOG:H2	1.82	0.61
1:B:373:TYR:HB2	1:B:376:ILE:HD13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ARG:HA	2:A:800:BOG:O6	2.01	0.61
1:B:287:SER:CB	9:B:821:BCN:H62	2.30	0.61
1:B:73:VAL:CG1	1:B:77:MSE:HE1	2.30	0.61
1:B:239:VAL:HG12	1:B:240:HIS:CD2	2.36	0.60
1:B:440:GLU:OE2	1:B:484:ARG:NH1	2.34	0.60
1:B:421:TYR:OH	1:B:454:LEU:HD21	2.00	0.60
1:B:16:ALA:HA	1:B:31:MSE:HE2	1.82	0.60
1:B:59:TYR:CE2	2:B:800:BOG:C5'	2.84	0.60
1:B:323:GLU:O	1:B:324:SER:CB	2.48	0.59
1:B:316:VAL:H	5:B:813:EDO:H11	1.66	0.59
1:B:370:THR:HG23	1:B:376:ILE:HG21	1.84	0.59
1:A:297:ASN:ND2	1:A:304:LEU:H	1.89	0.59
1:B:262:MSE:HE2	5:B:807:EDO:C1	2.33	0.59
1:A:391:ILE:O	1:A:393:GLY:N	2.30	0.59
1:A:239:VAL:HG23	1:A:240:HIS:CD2	2.38	0.59
1:A:394:ASP:HB3	1:A:397:ASP:HB2	1.84	0.58
1:A:478:ASN:C	1:A:478:ASN:HD22	2.06	0.58
1:A:148:ASP:OD1	1:A:149:ALA:N	2.35	0.58
1:A:290:ASN:CA	5:A:1956:EDO:H12	2.34	0.58
1:A:250:ASN:OD1	1:A:291:TYR:CZ	2.56	0.58
1:A:137:ARG:HH22	2:A:700:BOG:H5	1.68	0.57
1:A:406:TYR:CE1	10:A:2045:HOH:O	2.52	0.57
1:A:141:TYR:CZ	1:A:247:ILE:HD11	2.40	0.57
1:B:316:VAL:N	5:B:813:EDO:H11	2.20	0.57
1:A:341:GLU:CG	1:A:342:ASN:N	2.36	0.57
1:B:378:PRO:O	1:B:379:ALA:C	2.43	0.56
1:B:254:ARG:HH21	8:B:816:13P:H12	1.70	0.56
1:B:73:VAL:CG1	1:B:77:MSE:CE	2.77	0.56
5:A:1958:EDO:H21	10:A:2097:HOH:O	2.04	0.56
1:B:50:HIS:HE1	1:B:354:LYS:HZ1	1.52	0.56
1:B:62:ARG:HG3	1:B:63:LEU:N	2.20	0.56
1:B:405:ARG:NH2	10:B:947:HOH:O	2.37	0.56
1:A:211:LYS:NZ	1:A:215:ASP:OD2	2.37	0.56
1:A:370:THR:HG23	1:A:376:ILE:CG2	2.36	0.55
1:A:454:LEU:HB3	1:A:460:VAL:HG21	1.87	0.55
5:B:804:EDO:H21	10:B:924:HOH:O	2.04	0.55
1:B:262:MSE:HE1	5:B:807:EDO:O2	2.07	0.55
1:B:103:ILE:CD1	2:B:700:BOG:H6'2	2.37	0.55
1:A:101:ILE:HG22	1:A:105:LEU:HD22	1.88	0.55
1:A:473:GLN:NE2	5:A:1957:EDO:H21	2.22	0.55
1:B:262:MSE:CE	5:B:807:EDO:H12	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:811:EDO:H11	7:B:812:TAM:H62	1.88	0.54
1:A:72:GLU:OE2	1:A:114:ARG:HB2	2.07	0.54
1:B:373:TYR:CB	1:B:376:ILE:HD13	2.36	0.54
1:A:57:GLU:HB2	2:A:800:BOG:O6	2.08	0.54
1:A:97:PRO:HG2	1:A:100:MET:HB2	1.90	0.54
1:A:469:ARG:NH1	5:A:1953:EDO:O2	2.40	0.54
1:A:286:GLU:HA	1:A:286:GLU:OE1	2.07	0.54
1:A:230:LYS:HD3	1:A:282:VAL:HG23	1.87	0.54
1:A:494:GLN:HA	1:A:494:GLN:OE1	2.06	0.54
1:B:25:ARG:HD3	1:B:377:GLY:O	2.08	0.54
1:B:157:GLN:HG2	7:B:812:TAM:HN2	1.70	0.54
1:A:193:LYS:HD2	1:A:195:TYR:CZ	2.43	0.53
1:A:155:ASN:O	1:A:159:VAL:HG23	2.09	0.53
1:B:376:ILE:O	1:B:377:GLY:O	2.28	0.52
1:A:374:GLN:HB2	1:A:375:GLY:CA	2.19	0.52
1:B:101:ILE:HG23	2:B:800:BOG:H61	1.92	0.52
1:A:229:ILE:HD12	1:A:327:PRO:HB3	1.92	0.52
1:B:97:PRO:HD2	1:B:100:MET:SD	2.50	0.52
1:B:232:SER:O	1:B:270:THR:HG22	2.10	0.52
1:B:120:SER:HA	1:B:140:GLU:O	2.10	0.52
1:A:97:PRO:HB2	1:A:99:TRP:CD1	2.45	0.51
1:A:50:HIS:NE2	1:A:354:LYS:CE	2.74	0.51
1:A:391:ILE:C	1:A:393:GLY:H	2.13	0.51
1:B:27:LEU:CD1	1:B:376:ILE:HD11	2.38	0.51
1:A:54:ARG:HG2	10:A:2109:HOH:O	2.11	0.51
1:A:64:VAL:HG12	1:A:68:LEU:HD22	1.91	0.51
1:B:58:HIS:O	1:B:59:TYR:O	2.27	0.51
1:A:340:ASP:HB2	1:A:344:LYS:O	2.11	0.50
1:A:129:SER:O	1:A:301:LYS:HE2	2.12	0.50
1:A:114:ARG:HG2	1:A:114:ARG:O	2.09	0.50
1:A:40:ALA:O	5:A:1965:EDO:O1	2.28	0.50
1:B:97:PRO:HG2	1:B:100:MET:HB2	1.92	0.50
5:A:1958:EDO:H22	10:A:2097:HOH:O	2.07	0.50
1:B:272:ASP:HB2	5:B:802:EDO:H21	1.94	0.50
5:A:1953:EDO:H12	5:A:1965:EDO:O2	2.12	0.50
1:B:490:VAL:O	1:B:494:GLN:HB2	2.10	0.50
1:B:324:SER:O	1:B:325:ASP:CB	2.58	0.50
1:A:478:ASN:HD21	1:A:481:GLN:H	1.55	0.49
1:B:27:LEU:HD21	1:B:376:ILE:HD13	1.77	0.49
1:A:478:ASN:HD22	1:A:481:GLN:H	1.57	0.49
1:B:227:ARG:HG2	1:B:321:ASP:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ARG:O	1:A:346:PRO:HD2	2.12	0.49
5:A:1959:EDO:H11	6:A:1961:IMD:H2	1.94	0.49
1:B:376:ILE:O	1:B:377:GLY:C	2.49	0.49
1:B:49:ILE:HB	1:B:144:CYS:HB2	1.94	0.49
1:B:252:ASP:OD1	1:B:254:ARG:HB2	2.12	0.49
1:A:294:ASN:ND2	5:A:1955:EDO:O2	2.46	0.49
1:A:193:LYS:HE3	1:A:195:TYR:OH	2.12	0.49
1:A:424:ASN:HD21	6:A:1961:IMD:H4	1.75	0.49
1:A:237:PRO:CG	6:A:1966:IMD:N3	2.43	0.49
1:B:212:GLN:CG	5:B:810:EDO:H22	2.37	0.49
1:B:391:ILE:C	1:B:392:GLU:HG2	2.32	0.49
1:A:96:ARG:HE	2:A:800:BOG:H5	1.78	0.49
1:A:316:VAL:HG22	5:A:1958:EDO:H11	1.95	0.49
1:B:287:SER:HB3	9:B:821:BCN:H62	1.95	0.49
1:B:39:CYS:HA	1:B:469:ARG:HD3	1.95	0.49
1:B:2:GLU:O	1:B:4:LYS:HD2	2.13	0.48
1:B:336:LEU:CD2	1:B:350:VAL:HG22	2.43	0.48
1:B:311:TRP:O	1:B:312:THR:HG22	2.12	0.48
1:B:67:ALA:HB1	1:B:356:THR:HG21	1.94	0.48
1:A:416:HIS:ND1	5:A:1957:EDO:H11	2.27	0.48
1:B:59:TYR:HE2	2:B:800:BOG:C5'	2.25	0.48
1:B:459:TRP:CE2	5:B:811:EDO:H12	2.49	0.48
1:A:457:HIS:CA	6:A:1963:IMD:H4	2.44	0.48
1:B:457:HIS:C	5:B:811:EDO:H21	2.34	0.48
1:A:16:ALA:HA	1:A:31:MSE:HE2	1.95	0.48
1:B:336:LEU:HD22	1:B:350:VAL:HG22	1.95	0.47
1:B:54:ARG:HA	2:B:800:BOG:O2	2.14	0.47
1:A:421:TYR:OH	1:A:454:LEU:HD21	2.14	0.47
1:A:469:ARG:HG3	1:A:469:ARG:NH1	2.28	0.47
1:A:254:ARG:NH1	1:A:254:ARG:HB3	2.30	0.47
1:B:3:THR:HA	1:B:4:LYS:HB2	1.97	0.47
1:A:106:PHE:HE2	5:A:1964:EDO:HO1	1.63	0.47
1:A:114:ARG:NH2	1:A:118:PRO:O	2.47	0.47
1:A:158:MSE:HE3	1:A:161:ARG:HB3	1.97	0.47
1:A:241:THR:O	1:A:241:THR:CG2	2.63	0.47
8:B:816:13P:O3P	8:B:816:13P:H31	2.15	0.47
1:B:193:LYS:HD3	1:B:195:TYR:CZ	2.49	0.47
1:B:478:ASN:C	1:B:478:ASN:OD1	2.52	0.47
1:A:88:ARG:NE	1:A:244:GLN:HG3	2.30	0.47
1:A:255:ILE:HG13	1:A:255:ILE:H	1.58	0.46
1:A:67:ALA:HB1	1:A:356:THR:HG21	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:457:HIS:HD2	7:B:812:TAM:O6	1.98	0.46
1:B:59:TYR:HE2	2:B:800:BOG:H5'2	1.73	0.46
1:A:458:GLU:N	6:A:1963:IMD:H4	2.29	0.46
5:A:1957:EDO:H12	6:A:1960:IMD:H5	1.93	0.46
9:A:1969:BCN:H62	9:A:1969:BCN:H11	1.55	0.46
1:B:415:ARG:HH11	1:B:415:ARG:HG2	1.80	0.46
1:A:298:THR:HG22	5:A:1955:EDO:O1	2.15	0.46
1:A:293:LEU:HB2	5:A:1956:EDO:H21	1.98	0.46
1:B:311:TRP:C	1:B:312:THR:CG2	2.84	0.46
1:B:296:TYR:C	1:B:296:TYR:CD2	2.89	0.46
1:B:415:ARG:NH1	1:B:415:ARG:HG2	2.31	0.45
1:A:296:TYR:CD1	1:A:296:TYR:C	2.89	0.45
1:B:96:ARG:HH11	1:B:249:GLN:HE21	1.65	0.45
1:A:416:HIS:ND1	5:A:1957:EDO:C1	2.80	0.45
1:A:106:PHE:O	1:A:110:HIS:CD2	2.70	0.45
1:B:497:LEU:HA	1:B:497:LEU:HD23	1.85	0.45
1:B:200:ARG:O	1:B:346:PRO:HD2	2.16	0.45
4:A:600:FAD:H4B	4:A:600:FAD:O2A	2.17	0.45
9:B:821:BCN:O4	9:B:821:BCN:H12	2.17	0.45
1:A:469:ARG:HH11	1:A:469:ARG:HG3	1.82	0.45
1:B:370:THR:O	1:B:372:TYR:N	2.50	0.45
5:A:1959:EDO:C1	6:A:1961:IMD:H2	2.47	0.45
1:B:364:HIS:NE2	1:B:368:LYS:NZ	2.65	0.45
1:B:73:VAL:O	1:B:77:MSE:HE3	2.16	0.45
1:A:106:PHE:O	1:A:110:HIS:HD2	2.00	0.45
1:B:244:GLN:HE21	1:B:244:GLN:HB2	1.61	0.45
1:B:113:LYS:HE3	1:B:113:LYS:H	1.82	0.44
1:A:254:ARG:HD2	1:A:328:GLN:CB	2.42	0.44
1:B:232:SER:O	1:B:270:THR:CG2	2.66	0.44
1:B:21:ASP:O	1:B:22:ALA:C	2.56	0.44
1:A:359:ARG:NH1	1:A:381:THR:OG1	2.45	0.44
1:B:336:LEU:HD21	1:B:361:LEU:CD1	2.47	0.44
1:B:103:ILE:HD13	2:B:700:BOG:H6'2	1.99	0.44
1:B:77:MSE:HG2	1:B:386:LEU:HG	1.98	0.44
1:B:89:LEU:HD12	1:B:247:ILE:O	2.17	0.44
1:B:262:MSE:CE	5:B:807:EDO:C1	2.93	0.44
1:B:59:TYR:HE2	2:B:800:BOG:C6'	2.31	0.44
1:B:227:ARG:HG2	1:B:321:ASP:CB	2.48	0.44
1:B:250:ASN:ND2	1:B:291:TYR:CE1	2.86	0.44
1:B:261:TRP:CZ2	1:B:472:LYS:HD2	2.53	0.44
1:B:294:ASN:ND2	5:B:803:EDO:O1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:ARG:HH21	8:B:816:13P:C1	2.30	0.43
1:A:77:MSE:HE2	1:A:386:LEU:HG	2.00	0.43
1:B:233:HIS:CE1	1:B:270:THR:HG23	2.53	0.43
1:A:117:LEU:HD22	1:A:142:SER:HB3	2.00	0.43
1:B:3:THR:HA	1:B:4:LYS:CB	2.49	0.43
5:B:803:EDO:H21	5:B:817:EDO:H11	2.01	0.43
1:B:323:GLU:CB	10:B:912:HOH:O	2.67	0.42
1:A:366:LEU:HA	1:A:366:LEU:HD13	1.92	0.42
1:A:91:HIS:CE1	1:A:98:ALA:HB2	2.54	0.42
1:A:247:ILE:HG23	1:A:257:PHE:CE1	2.54	0.42
1:B:295:VAL:O	1:B:299:HIS:HD2	2.02	0.42
9:B:820:BCN:H62	9:B:820:BCN:H31	1.64	0.42
1:B:55:TYR:OH	8:B:816:13P:O1P	2.24	0.42
1:A:44:ALA:HB2	5:A:1965:EDO:C2	2.49	0.42
1:A:158:MSE:CA	1:A:158:MSE:HE3	2.41	0.42
1:B:232:SER:N	1:B:270:THR:HG22	2.34	0.42
1:A:248:LEU:O	1:A:255:ILE:HA	2.19	0.42
1:A:139:PHE:N	1:A:139:PHE:CD2	2.87	0.42
1:B:259:ILE:HD13	1:B:259:ILE:HG21	1.83	0.42
1:B:370:THR:O	1:B:371:PRO:C	2.57	0.42
1:A:228:LEU:HD23	1:A:228:LEU:HA	1.79	0.42
1:A:457:HIS:HA	6:A:1963:IMD:C4	2.50	0.42
1:A:374:GLN:HB3	1:A:375:GLY:CA	2.39	0.42
1:A:415:ARG:HD3	10:A:2077:HOH:O	2.18	0.42
1:A:358:TYR:C	1:A:358:TYR:CD2	2.93	0.42
5:A:1959:EDO:O1	6:A:1961:IMD:N1	2.53	0.42
1:B:440:GLU:CD	1:B:484:ARG:NH1	2.73	0.42
1:A:61:PHE:O	1:A:62:ARG:C	2.57	0.42
1:A:212:GLN:HB3	1:A:212:GLN:HE21	1.71	0.42
1:B:80:HIS:CD2	1:B:81:ILE:HG23	2.54	0.42
1:B:157:GLN:NE2	7:B:812:TAM:H41	2.35	0.42
1:B:91:HIS:NE2	1:B:98:ALA:HB2	2.35	0.42
1:A:241:THR:HG22	1:A:241:THR:O	2.20	0.42
1:A:68:LEU:HD11	1:A:108:TYR:CE2	2.55	0.41
1:B:495:GLN:C	1:B:497:LEU:H	2.22	0.41
1:B:270:THR:HB	1:B:271:THR:H	1.40	0.41
1:A:292:LEU:HA	1:A:292:LEU:HD23	1.77	0.41
5:A:1959:EDO:H21	6:A:1963:IMD:C4	2.46	0.41
1:B:77:MSE:HE3	1:B:77:MSE:HB2	1.96	0.41
1:B:257:PHE:HB3	1:B:259:ILE:HG13	2.03	0.41
1:A:66:GLU:HG3	1:A:360:LYS:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:ARG:HD3	5:A:1962:EDO:O2	2.20	0.41
1:A:254:ARG:HB3	1:A:254:ARG:CZ	2.51	0.41
1:A:158:MSE:O	1:A:162:LYS:HG3	2.20	0.41
1:B:171:ARG:HD2	5:B:815:EDO:O2	2.21	0.41
1:B:58:HIS:O	1:B:59:TYR:C	2.59	0.41
1:B:378:PRO:C	1:B:379:ALA:O	2.59	0.41
1:B:40:ALA:O	1:B:41:THR:C	2.58	0.41
1:B:326:SER:HA	1:B:327:PRO:HD3	1.89	0.41
1:B:416:HIS:CE1	1:B:420:THR:HG21	2.56	0.41
1:B:299:HIS:CE1	10:B:882:HOH:O	2.61	0.41
1:A:73:VAL:O	1:A:77:MSE:HG3	2.21	0.41
1:B:230:LYS:HD3	1:B:282:VAL:HG23	2.03	0.41
1:B:327:PRO:HA	1:B:330:ILE:HD12	2.02	0.41
1:B:318:PRO:O	1:B:352:GLY:HA2	2.21	0.41
1:A:176:ARG:CG	1:A:176:ARG:NH1	2.61	0.40
1:A:60:GLU:OE1	1:A:331:THR:OG1	2.31	0.40
1:A:49:ILE:HB	1:A:144:CYS:HB2	2.03	0.40
1:B:78:ALA:N	1:B:79:PRO:CD	2.85	0.40
1:A:182:TRP:O	1:A:198:GLN:HA	2.21	0.40

There are no symmetry-related clashes.

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	492/501 (98%)	456 (93%)	30 (6%)	6 (1%)	16	5
1	B	495/501 (99%)	454 (92%)	26 (5%)	15 (3%)	5	1
All	All	987/1002 (98%)	910 (92%)	56 (6%)	21 (2%)	9	2

All (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
1	B	325	ASP
1	B	379	ALA
1	B	59	TYR
1	B	495	GLN
1	B	496	ARG
1	A	374	GLN
1	B	380	TRP
1	A	2	GLU
1	A	380	TRP
1	B	4	LYS
1	B	115	THR
1	B	374	GLN
1	A	354	LYS
1	B	371	PRO
1	B	377	GLY
1	B	376	ILE

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	413/412 (100%)	377 (91%)	36 (9%)	13	3
1	B	416/412 (101%)	366 (88%)	50 (12%)	6	1
All	All	829/824 (101%)	743 (90%)	86 (10%)	9	2

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	32	LEU
1	A	50	HIS

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Mol	Chain	Res	Type
1	A	57	GLU
1	A	60	GLU
1	A	65	SER
1	A	68	LEU
1	A	102	ARG
1	A	105	LEU
1	A	113	LYS
1	A	114	ARG
1	A	121	THR
1	A	136	LYS
1	A	162	LYS
1	A	176	ARG
1	A	194	LYS
1	A	196	SER
1	A	212	GLN
1	A	244	GLN
1	A	247	ILE
1	A	250	ASN
1	A	255	ILE
1	A	298	THR
1	A	326	SER
1	A	348	LEU
1	A	349	SER
1	A	392	GLU
1	A	395	ARG
1	A	402	LEU
1	A	403	ARG
1	A	404	ARG
1	A	405	ARG
1	A	427	LEU
1	A	478	ASN
1	A	489	LEU
1	A	494	GLN
1	B	2	GLU
1	B	3	THR
1	B	4	LYS
1	B	35	GLN
1	B	53	LEU
1	B	56	LEU
1	B	62	ARG
1	B	103	ILE
1	B	105	LEU

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Mol	Chain	Res	Type
1	B	111	LEU
1	B	113	LYS
1	B	114	ARG
1	B	116	SER
1	B	121	THR
1	B	123	LEU
1	B	124	ARG
1	B	137	ARG
1	B	161	ARG
1	B	162	LYS
1	B	219	HIS
1	B	238	ARG
1	B	244	GLN
1	B	247	ILE
1	B	255	ILE
1	B	270	THR
1	B	272	ASP
1	B	276	LYS
1	B	280	LYS
1	B	306	ARG
1	B	312	THR
1	B	325	ASP
1	B	332	ARG
1	B	341	GLU
1	B	355	LEU
1	B	360	LYS
1	B	361	LEU
1	B	392	GLU
1	B	394	ASP
1	B	395	ARG
1	B	404	ARG
1	B	405	ARG
1	B	413	LEU
1	B	415	ARG
1	B	420	THR
1	B	428	LEU
1	B	429	LEU
1	B	484	ARG
1	B	494	GLN
1	B	495	GLN
1	B	496	ARG

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	110	HIS
1	A	128	ASN
1	A	212	GLN
1	A	242	GLN
1	A	244	GLN
1	A	250	ASN
1	A	290	ASN
1	A	297	ASN
1	A	364	HIS
1	A	424	ASN
1	A	444	HIS
1	A	473	GLN
1	A	478	ASN
1	A	482	GLN
1	B	50	HIS
1	B	244	GLN
1	B	249	GLN
1	B	294	ASN
1	B	299	HIS
1	B	424	ASN
1	B	457	HIS
1	B	494	GLN
1	B	495	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 ⓘ

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	0.94	1 (5%)	25,25,25	0.99	1 (4%)
2	BOG	A	1950	-	20,20,20	0.93	1 (5%)	25,25,25	1.74	5 (20%)
3	PO4	A	1951	-	4,4,4	0.20	0	6,6,6	0.29	0
5	EDO	A	1952	-	3,3,3	0.73	0	2,2,2	0.20	0
5	EDO	A	1953	-	3,3,3	0.63	0	2,2,2	0.98	0
5	EDO	A	1954	-	3,3,3	0.58	0	2,2,2	0.33	0
5	EDO	A	1955	-	3,3,3	0.70	0	2,2,2	0.44	0
5	EDO	A	1956	-	3,3,3	0.51	0	2,2,2	0.28	0
5	EDO	A	1957	-	3,3,3	1.10	0	2,2,2	0.80	0
5	EDO	A	1958	-	3,3,3	0.50	0	2,2,2	0.28	0
5	EDO	A	1959	-	3,3,3	0.69	0	2,2,2	0.56	0
6	IMD	A	1960	-	3,5,5	0.52	0	4,5,5	1.45	0
6	IMD	A	1961	-	3,5,5	0.54	0	4,5,5	0.75	0
5	EDO	A	1962	-	3,3,3	0.56	0	2,2,2	0.41	0
6	IMD	A	1963	-	3,5,5	0.71	0	4,5,5	0.63	0
5	EDO	A	1964	-	3,3,3	0.57	0	2,2,2	0.51	0
5	EDO	A	1965	-	3,3,3	0.64	0	2,2,2	0.70	0
6	IMD	A	1966	-	3,5,5	0.58	0	4,5,5	1.38	0
6	IMD	A	1967	-	3,5,5	0.72	0	4,5,5	0.79	0
8	13P	A	1968	-	9,9,9	5.31	6 (66%)	9,12,12	4.13	4 (44%)
9	BCN	A	1969	-	7,10,10	0.76	0	8,11,11	2.63	3 (37%)
4	FAD	A	600	-	48,58,58	1.79	15 (31%)	54,89,89	2.32	14 (25%)
2	BOG	A	700	-	20,20,20	0.74	1 (5%)	25,25,25	1.19	4 (16%)
2	BOG	A	800	-	20,20,20	0.62	1 (5%)	25,25,25	1.57	5 (20%)
4	FAD	B	600	-	48,58,58	2.05	14 (29%)	54,89,89	2.76	15 (27%)
2	BOG	B	700	-	20,20,20	0.78	1 (5%)	25,25,25	1.10	2 (8%)
2	BOG	B	800	-	20,20,20	0.55	0	25,25,25	1.27	3 (12%)
3	PO4	B	801	-	4,4,4	0.32	0	6,6,6	0.31	0
5	EDO	B	802	-	3,3,3	0.97	0	2,2,2	0.87	0
5	EDO	B	803	-	3,3,3	0.83	0	2,2,2	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	B	804	-	3,3,3	0.53	0	2,2,2	0.94	0
5	EDO	B	805	-	3,3,3	0.55	0	2,2,2	0.71	0
5	EDO	B	806	-	3,3,3	1.09	0	2,2,2	0.31	0
5	EDO	B	807	-	3,3,3	1.00	0	2,2,2	0.56	0
5	EDO	B	808	-	3,3,3	0.84	0	2,2,2	0.40	0
5	EDO	B	809	-	3,3,3	0.60	0	2,2,2	0.44	0
5	EDO	B	810	-	3,3,3	0.60	0	2,2,2	0.49	0
5	EDO	B	811	-	3,3,3	0.34	0	2,2,2	0.83	0
7	TAM	B	812	-	7,10,10	0.68	0	9,12,12	2.99	6 (66%)
5	EDO	B	813	-	3,3,3	0.26	0	2,2,2	0.90	0
5	EDO	B	814	-	3,3,3	0.73	0	2,2,2	0.24	0
5	EDO	B	815	-	3,3,3	0.39	0	2,2,2	0.95	0
8	13P	B	816	-	9,9,9	5.31	6 (66%)	9,12,12	3.80	4 (44%)
5	EDO	B	817	-	3,3,3	0.66	0	2,2,2	0.37	0
5	EDO	B	818	-	3,3,3	0.57	0	2,2,2	0.35	0
6	IMD	B	819	-	3,5,5	0.59	0	4,5,5	0.46	0
9	BCN	B	820	-	7,10,10	0.81	0	8,11,11	3.24	4 (50%)
9	BCN	B	821	-	7,10,10	0.65	0	8,11,11	3.80	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	IMD	A	1966	-	-	0/0/0/0	0/1/1/1
6	IMD	A	1967	-	-	0/0/0/0	0/1/1/1
8	13P	A	1968	-	-	0/7/8/8	0/0/0/0
9	BCN	A	1969	-	-	0/8/10/10	0/0/0/0
4	FAD	A	600	-	-	0/30/50/50	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	-	-	0/30/50/50	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
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
7	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
8	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
9	BCN	B	820	-	-	0/8/10/10	0/0/0/0
9	BCN	B	821	-	-	0/8/10/10	0/0/0/0

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	600	FAD	C4'-C3'	-3.61	1.46	1.53
4	A	600	FAD	C6-C5X	-3.55	1.36	1.41
4	A	600	FAD	PA-O2A	-3.20	1.41	1.54
4	B	600	FAD	C6-C5X	-3.10	1.37	1.41
4	A	600	FAD	P-O2P	-2.94	1.42	1.54
4	A	600	FAD	C9A-C5X	-2.84	1.36	1.42
4	A	600	FAD	C10-N10	-2.82	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	600	FAD	O4'-C4'	-2.77	1.37	1.43
4	B	600	FAD	O4B-C4B	-2.72	1.38	1.45
4	A	600	FAD	P-O1P	-2.71	1.41	1.51
4	B	600	FAD	C9A-C5X	-2.66	1.37	1.42
4	A	600	FAD	O2'-C2'	-2.58	1.37	1.43
4	A	600	FAD	O3'-C3'	-2.45	1.37	1.43
4	A	600	FAD	O4B-C4B	-2.39	1.39	1.45
4	A	600	FAD	C5A-N7A	-2.31	1.31	1.39
4	B	600	FAD	PA-O5B	-2.29	1.48	1.59
4	B	600	FAD	P-O2P	-2.25	1.45	1.54
4	B	600	FAD	C9-C9A	-2.18	1.36	1.40
4	A	600	FAD	O4B-C1B	-2.18	1.38	1.41
4	A	600	FAD	O3B-C3B	-2.10	1.37	1.43
4	B	600	FAD	PA-O2A	-2.09	1.46	1.54
4	A	600	FAD	C4X-C10	-2.03	1.37	1.41
4	A	600	FAD	C8M-C8	-2.03	1.46	1.51
4	B	600	FAD	C5'-C4'	2.01	1.54	1.51
2	A	800	BOG	O1-C1	2.02	1.43	1.40
4	B	600	FAD	C2A-N3A	2.07	1.35	1.32
4	B	600	FAD	PA-O1A	2.11	1.58	1.51
2	A	700	BOG	O1-C1	2.21	1.44	1.40
8	A	1968	13P	P-O1	2.36	1.68	1.60
8	B	816	13P	P-O1	2.55	1.68	1.60
2	B	700	BOG	O1-C1	2.70	1.45	1.40
2	A	1950	BOG	O1-C1	2.89	1.45	1.40
2	A	1949	BOG	O1-C1	2.93	1.45	1.40
8	B	816	13P	O3-C3	3.09	1.51	1.41
8	B	816	13P	C3-C2	3.47	1.59	1.50
8	A	1968	13P	O3-C3	3.67	1.53	1.41
8	A	1968	13P	C3-C2	3.90	1.61	1.50
4	B	600	FAD	C10-N1	4.02	1.42	1.35
4	B	600	FAD	C4X-N5	4.66	1.40	1.33
8	A	1968	13P	C1-C2	5.43	1.61	1.50
8	B	816	13P	O2-C2	5.43	1.31	1.21
8	B	816	13P	C1-C2	5.69	1.61	1.50
8	A	1968	13P	O2-C2	6.12	1.33	1.21
4	B	600	FAD	C1'-N10	7.05	1.55	1.48
8	A	1968	13P	O1-C1	12.07	1.51	1.43
8	B	816	13P	O1-C1	12.68	1.51	1.43

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	600	FAD	N3A-C2A-N1A	-9.99	121.25	128.89
4	A	600	FAD	N3A-C2A-N1A	-9.06	121.96	128.89
8	A	1968	13P	O3P-P-O1	-8.02	83.48	106.56
8	B	816	13P	O3P-P-O1	-7.22	85.77	106.56
8	A	1968	13P	O1-P-O1P	-5.10	94.16	107.14
7	B	812	TAM	C3-C-N	-4.89	98.18	108.28
7	B	812	TAM	C3-C-C2	-4.68	103.02	110.50
4	A	600	FAD	O2A-PA-O5B	-4.25	87.04	108.46
4	B	600	FAD	C4X-C10-N10	-4.07	118.12	120.52
4	B	600	FAD	O2'-C2'-C3'	-3.78	99.51	109.02
4	B	600	FAD	C4X-C4-N3	-3.26	119.12	123.59
2	A	800	BOG	O3-C3-C4	-2.98	103.63	110.34
4	B	600	FAD	C9A-C5X-N5	-2.96	117.97	122.36
8	B	816	13P	O1-P-O1P	-2.95	99.64	107.14
4	A	600	FAD	C4X-C4-N3	-2.82	119.73	123.59
4	B	600	FAD	O3'-C3'-C2'	-2.72	101.91	108.75
4	B	600	FAD	C1'-C2'-C3'	-2.68	102.16	109.82
4	B	600	FAD	O5'-P-O1P	-2.64	99.38	109.62
2	A	1950	BOG	O4-C4-C3	-2.40	104.93	110.34
7	B	812	TAM	O6-C6-C3	-2.31	105.86	111.14
2	A	800	BOG	O5-C1-C2	-2.30	105.55	110.28
4	B	600	FAD	C4B-O4B-C1B	-2.28	107.21	109.72
4	A	600	FAD	P-O3P-PA	-2.22	126.50	132.73
4	A	600	FAD	C4A-C5A-N7A	-2.18	107.47	109.48
2	B	800	BOG	O3-C3-C4	-2.02	105.79	110.34
2	A	700	BOG	C3-C4-C5	2.02	113.71	110.20
2	B	700	BOG	O5-C1-O1	2.02	114.93	110.05
4	B	600	FAD	C2B-C3B-C4B	2.06	106.84	102.61
2	A	700	BOG	O1-C1-C2	2.10	110.70	108.04
4	A	600	FAD	O4'-C4'-C3'	2.11	114.31	109.02
4	A	600	FAD	C2B-C1B-N9A	2.13	117.55	114.29
2	B	800	BOG	C4-C3-C2	2.21	114.92	110.79
9	B	821	BCN	C5-N1-C3	2.27	116.90	111.45
4	A	600	FAD	O5B-PA-O1A	2.31	118.60	109.62
7	B	812	TAM	C3-C-C1	2.41	114.36	110.50
2	A	700	BOG	C1-O5-C5	2.42	118.44	113.75
4	B	600	FAD	O3P-PA-O5B	2.43	109.38	102.94
2	A	700	BOG	O2-C2-C1	2.46	115.42	110.02
4	A	600	FAD	C5X-C9A-N10	2.53	119.54	117.62
9	B	820	BCN	C1-N1-C5	2.55	116.60	111.28
4	A	600	FAD	O5B-C5B-C4B	2.62	118.77	109.12
7	B	812	TAM	C2-C-C1	2.66	114.75	110.50
2	A	1950	BOG	O5-C5-C4	2.88	115.08	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	700	BOG	O5-C5-C6	2.91	113.72	106.36
4	B	600	FAD	O2'-C2'-C1'	2.93	117.16	109.94
4	A	600	FAD	C4B-O4B-C1B	2.94	112.95	109.72
2	A	800	BOG	C4-C3-C2	2.95	116.29	110.79
2	A	1950	BOG	C4-C3-C2	2.97	116.33	110.79
2	A	1949	BOG	O1-C1-C2	3.04	111.88	108.04
4	A	600	FAD	C4X-N5-C5X	3.22	120.46	116.76
2	A	800	BOG	O5-C5-C4	3.24	115.76	109.68
2	A	1950	BOG	O1-C1-C2	3.26	112.16	108.04
9	A	1969	BCN	C1-N1-C3	3.43	118.44	111.28
9	B	820	BCN	C5-N1-C3	3.46	119.77	111.45
2	A	800	BOG	C3-C4-C5	3.52	116.33	110.20
9	A	1969	BCN	C1-N1-C5	3.61	118.83	111.28
2	B	800	BOG	C1-C2-C3	3.71	117.28	109.97
9	B	821	BCN	C1-N1-C3	3.80	119.22	111.28
7	B	812	TAM	C2-C-N	4.02	116.59	108.28
4	B	600	FAD	C4-C4X-N5	4.04	123.62	118.72
9	A	1969	BCN	C5-N1-C3	4.70	122.72	111.45
4	A	600	FAD	O3P-PA-O5B	5.10	116.47	102.94
8	A	1968	13P	O3P-P-O1P	5.17	127.21	110.58
2	A	1950	BOG	C3-C4-C5	5.31	119.44	110.20
9	B	820	BCN	C2-C1-N1	5.39	121.52	113.53
8	B	816	13P	O3P-P-O1P	5.49	128.24	110.58
8	A	1968	13P	O2P-P-O1	5.73	123.05	106.56
8	B	816	13P	O2P-P-O1	5.86	123.44	106.56
9	B	820	BCN	C1-N1-C3	5.91	123.63	111.28
9	B	821	BCN	C1-N1-C5	6.02	123.85	111.28
4	B	600	FAD	C4X-N5-C5X	6.96	124.77	116.76
9	B	821	BCN	C2-C1-N1	7.55	124.73	113.53
4	A	600	FAD	C4-N3-C2	7.80	121.99	115.25
4	B	600	FAD	C4-N3-C2	10.02	123.91	115.25

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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
9	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
7	B	812	TAM	7	0
5	B	813	EDO	6	0
5	B	815	EDO	1	0
8	B	816	13P	4	0
5	B	817	EDO	1	0
6	B	819	IMD	1	0
9	B	820	BCN	2	0
9	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	487/501 (97%)	1.45	120 (24%) ⓘ ⓘ	20, 41, 65, 84	0
1	B	490/501 (97%)	1.50	117 (23%) ⓘ ⓘ	19, 41, 66, 98	0
All	All	977/1002 (97%)	1.47	237 (24%) ⓘ ⓘ	19, 41, 66, 98	0

All (237) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	113	LYS	11.4
1	B	494	GLN	9.5
1	B	59	TYR	8.4
1	A	1	MET	8.1
1	B	106	PHE	6.9
1	B	1	MET	6.5
1	A	115	THR	6.2
1	A	325	ASP	5.8
1	B	376	ILE	5.6
1	B	141	TYR	4.8
1	B	135	ILE	4.7
1	A	197	TRP	4.7
1	A	23	ALA	4.6
1	B	497	LEU	4.6
1	B	111	LEU	4.6
1	A	369	LEU	4.4
1	A	320	CYS	4.3
1	B	391	ILE	4.1
1	A	58	HIS	4.1
1	B	110	HIS	4.1
1	B	100	MET	4.1
1	B	374	GLN	4.0
1	B	26	GLY	4.0
1	B	49	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	163	GLY	3.9
1	A	98	ALA	3.8
1	A	318	PRO	3.8
1	B	389	GLY	3.8
1	A	111	LEU	3.7
1	A	113	LYS	3.6
1	A	345	ALA	3.6
1	B	402	LEU	3.6
1	A	453	TYR	3.6
1	B	117	LEU	3.6
1	A	117	LEU	3.5
1	B	435	VAL	3.5
1	A	19	ALA	3.5
1	A	319	LEU	3.5
1	A	81	ILE	3.4
1	B	139	PHE	3.4
1	B	72	GLU	3.3
1	A	106	PHE	3.3
1	A	122	GLY	3.3
1	B	375	GLY	3.3
1	B	247	ILE	3.2
1	B	181	LEU	3.2
1	A	64	VAL	3.2
1	A	59	TYR	3.2
1	A	8	VAL	3.1
1	A	121	THR	3.1
1	A	272	ASP	3.1
1	B	346	PRO	3.1
1	B	124	ARG	3.1
1	A	380	TRP	3.1
1	B	131	LEU	3.0
1	A	107	MET	3.0
1	A	123	LEU	3.0
1	A	427	LEU	3.0
1	A	437	ASP	3.0
1	B	273	VAL	3.0
1	B	133	PRO	3.0
1	B	66	GLU	2.9
1	B	83	PHE	2.9
1	B	367	GLU	2.9
1	B	142	SER	2.9
1	A	367	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	330	ILE	2.9
1	B	291	TYR	2.9
1	A	355	LEU	2.9
1	A	402	LEU	2.9
1	B	365	ALA	2.9
1	A	304	LEU	2.9
1	B	361	LEU	2.9
1	A	337	ASP	2.9
1	A	160	VAL	2.9
1	A	195	TYR	2.9
1	B	309	ILE	2.8
1	A	12	GLY	2.8
1	A	6	LEU	2.8
1	A	51	GLY	2.8
1	A	243	LYS	2.8
1	A	329	ALA	2.8
1	A	29	VAL	2.8
1	A	393	GLY	2.8
1	B	198	GLN	2.8
1	B	210	VAL	2.8
1	A	74	LEU	2.7
1	B	355	LEU	2.7
1	B	98	ALA	2.7
1	A	37	LEU	2.7
1	A	144	CYS	2.7
1	B	183	ILE	2.7
1	A	204	ASN	2.7
1	B	108	TYR	2.7
1	A	61	PHE	2.7
1	B	67	ALA	2.7
1	B	312	THR	2.7
1	A	443	GLY	2.7
1	A	11	GLY	2.7
1	A	432	ALA	2.7
1	B	228	LEU	2.7
1	A	488	TRP	2.7
1	B	259	ILE	2.7
1	A	429	LEU	2.7
1	B	145	TRP	2.7
1	B	27	LEU	2.6
1	B	107	MET	2.6
1	A	436	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	184	VAL	2.6
1	B	226	ILE	2.6
1	B	282	VAL	2.6
1	A	143	ASP	2.6
1	B	127	ALA	2.6
1	A	399	ALA	2.6
1	B	180	GLY	2.6
1	A	159	VAL	2.6
1	A	247	ILE	2.6
1	B	252	ASP	2.6
1	B	341	GLU	2.5
1	A	291	TYR	2.5
1	B	257	PHE	2.5
1	A	13	ILE	2.5
1	B	255	ILE	2.5
1	A	418	ALA	2.5
1	A	347	LEU	2.5
1	B	392	GLU	2.5
1	B	342	ASN	2.5
1	A	9	ILE	2.4
1	A	44	ALA	2.4
1	A	375	GLY	2.4
1	B	60	GLU	2.4
1	B	314	SER	2.4
1	A	49	ILE	2.4
1	B	101	ILE	2.4
1	A	118	PRO	2.4
1	B	195	TYR	2.4
1	A	32	LEU	2.4
1	B	459	TRP	2.4
1	A	226	ILE	2.4
1	A	277	GLY	2.4
1	A	166	VAL	2.4
1	A	261	TRP	2.4
1	B	373	TYR	2.4
1	B	34	ALA	2.4
1	B	462	ARG	2.4
1	A	135	ILE	2.3
1	A	18	ILE	2.3
1	A	338	ILE	2.3
1	B	246	TYR	2.3
1	B	248	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	384	SER	2.3
1	B	496	ARG	2.3
1	B	272	ASP	2.3
1	A	339	HIS	2.3
1	A	67	ALA	2.3
1	A	336	LEU	2.3
1	A	213	PHE	2.3
1	A	105	LEU	2.3
1	A	348	LEU	2.3
1	A	276	LYS	2.3
1	A	101	ILE	2.3
1	A	183	ILE	2.3
1	B	334	TYR	2.3
1	B	48	LEU	2.2
1	B	114	ARG	2.2
1	B	427	LEU	2.2
1	B	468	TRP	2.2
1	B	188	ASP	2.2
1	A	346	PRO	2.2
1	B	295	VAL	2.2
1	B	304	LEU	2.2
1	A	258	VAL	2.2
1	B	121	THR	2.2
1	B	420	THR	2.2
1	A	479	ALA	2.2
1	B	284	ILE	2.2
1	B	372	TYR	2.2
1	A	385	VAL	2.2
1	A	206	THR	2.2
1	A	202	LEU	2.2
1	A	57	GLU	2.2
1	A	176	ARG	2.2
1	B	112	GLY	2.2
1	B	109	ASP	2.2
1	B	495	GLN	2.2
1	A	56	LEU	2.2
1	A	366	LEU	2.2
1	B	3	THR	2.2
1	A	435	VAL	2.2
1	B	160	VAL	2.2
1	A	422	GLY	2.1
1	B	394	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	257	PHE	2.1
1	B	351	PHE	2.1
1	B	172	ALA	2.1
1	A	332	ARG	2.1
1	A	4	LYS	2.1
1	B	234	ILE	2.1
1	B	313	TYR	2.1
1	A	75	LEU	2.1
1	B	32	LEU	2.1
1	A	457	HIS	2.1
1	B	418	ALA	2.1
1	A	130	VAL	2.1
1	B	485	VAL	2.1
1	A	216	ASP	2.1
1	B	298	THR	2.1
1	B	97	PRO	2.1
1	A	30	LEU	2.1
1	B	151	LEU	2.1
1	A	311	TRP	2.1
1	A	409	LEU	2.1
1	A	413	LEU	2.1
1	B	68	LEU	2.1
1	B	243	LYS	2.1
1	B	50	HIS	2.1
1	A	494	GLN	2.1
1	B	9	ILE	2.0
1	A	293	LEU	2.0
1	B	28	SER	2.0
1	B	489	LEU	2.0
1	B	350	VAL	2.0
1	A	364	HIS	2.0
1	A	2	GLU	2.0
1	B	396	ASP	2.0
1	B	199	ALA	2.0
1	A	7	ILE	2.0
1	A	361	LEU	2.0
1	A	398	TYR	2.0
1	A	451	LEU	2.0
1	B	75	LEU	2.0
1	B	95	LEU	2.0
1	B	366	LEU	2.0
1	A	397	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	325	ASP	2.0
1	A	350	VAL	2.0
1	A	109	ASP	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	BOG	A	800	20/20	0.02	1.70	31.75	131,136,138,138	0
5	EDO	B	806	4/4	0.35	0.63	21.00	34,45,50,55	0
6	IMD	A	1960	5/5	0.53	0.37	9.86	58,58,60,60	0
5	EDO	A	1956	4/4	0.71	0.49	9.39	41,44,50,54	0
3	PO4	B	801	5/5	0.76	0.51	8.99	68,68,70,71	0
5	EDO	A	1958	4/4	0.92	0.37	7.95	32,34,40,46	0
5	EDO	A	1955	4/4	0.84	0.31	7.88	38,50,50,52	0
7	TAM	B	812	11/11	0.45	0.49	7.66	56,63,66,70	0
9	BCN	A	1969	11/11	0.20	0.59	6.62	63,76,79,79	0
9	BCN	B	820	11/11	0.63	0.47	6.12	64,69,72,74	0
2	BOG	B	800	20/20	0.42	0.66	5.81	133,136,139,140	0
9	BCN	B	821	11/11	0.52	0.45	5.23	58,64,70,70	0
5	EDO	A	1953	4/4	0.85	0.22	4.63	32,45,46,47	0
5	EDO	B	802	4/4	0.56	0.37	3.81	38,44,48,50	0
2	BOG	B	700	20/20	0.83	0.30	3.07	63,71,77,79	0
5	EDO	B	811	4/4	0.91	0.28	3.03	36,43,44,49	0
5	EDO	B	808	4/4	0.63	0.30	2.84	52,56,57,60	0
5	EDO	A	1952	4/4	0.81	0.23	2.73	63,63,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	EDO	A	1965	4/4	0.80	0.24	2.64	37,37,42,42	0
5	EDO	A	1957	4/4	0.77	0.17	2.27	43,48,48,49	0
5	EDO	B	810	4/4	0.71	0.25	2.17	53,53,54,58	0
5	EDO	B	813	4/4	0.83	0.25	1.68	36,39,41,43	0
5	EDO	B	807	4/4	0.52	0.22	1.35	46,47,50,52	0
6	IMD	A	1961	5/5	0.67	0.25	1.35	73,73,74,74	0
8	13P	B	816	10/10	0.81	0.24	1.11	28,40,45,45	0
8	13P	A	1968	10/10	0.83	0.23	0.82	28,38,43,44	0
2	BOG	A	700	20/20	0.51	0.31	0.73	86,91,94,94	0
6	IMD	A	1967	5/5	0.85	0.19	0.49	63,64,65,67	0
6	IMD	A	1963	5/5	0.76	0.20	0.38	42,47,49,50	0
5	EDO	B	815	4/4	0.88	0.17	-0.25	54,57,59,62	0
4	FAD	A	600	53/53	0.92	0.16	-0.37	18,26,29,36	0
4	FAD	B	600	53/53	0.90	0.15	-0.41	19,25,29,32	0
5	EDO	A	1962	4/4	0.85	0.16	-1.10	70,71,72,74	0
5	EDO	A	1959	4/4	0.90	0.14	-1.71	43,48,49,52	0
5	EDO	B	809	4/4	0.47	0.19	-	65,66,67,68	0
6	IMD	A	1966	5/5	0.68	0.24	-	70,70,72,72	0
6	IMD	B	819	5/5	0.66	0.18	-	78,78,79,81	0
5	EDO	B	803	4/4	0.81	0.23	-	47,49,52,53	0
5	EDO	B	814	4/4	0.76	0.23	-	54,56,56,56	0
2	BOG	A	1949	20/20	0.10	0.55	-	92,95,97,97	0
2	BOG	A	1950	20/20	0.12	0.67	-	90,93,94,95	0
5	EDO	A	1954	4/4	0.77	0.16	-	64,65,65,66	0
5	EDO	A	1964	4/4	0.52	0.20	-	64,66,66,67	0
5	EDO	B	805	4/4	0.70	0.20	-	63,64,64,68	0
3	PO4	A	1951	5/5	0.89	0.15	-	84,84,84,85	0
5	EDO	B	817	4/4	0.76	0.73	-	55,62,65,66	0
5	EDO	B	818	4/4	0.70	0.21	-	72,75,75,75	0
5	EDO	B	804	4/4	0.76	0.22	-	49,49,51,52	0

6.5 Other polymers ⓘ

There are no such residues in this entry.