



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:31 AM GMT

PDB ID : 2R46
Title : Crystal structure of Escherichia coli Glycerol-3-phosphate Dehydrogenase in complex with 2-phosphopyruvic acid.
Authors : Yeh, J.I.; Du, S.; Chinte, U.
Deposited on : 2007-08-30
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
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

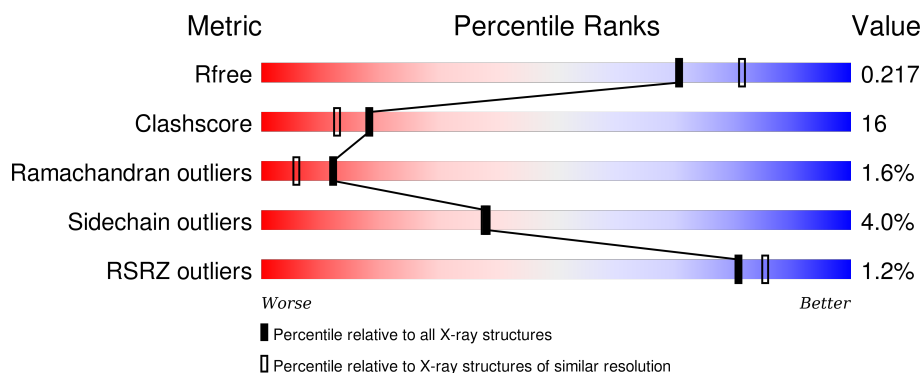
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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 ≥ 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 style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 22%, green 74%, grey 3%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> % 74% 22% .. </div> </div>
1	B	501	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 23%, green 72%, grey 3%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> % 72% 23% .. </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	-	-	X
2	BOG	A	800	X	-	X	X
2	BOG	A	900	-	-	-	X
2	BOG	B	900	-	-	-	X
3	EDO	A	1950	-	-	-	X
3	EDO	A	1951	-	-	-	X
3	EDO	A	1954	-	-	-	X
3	EDO	A	7068	-	-	-	X
3	EDO	B	901	-	-	-	X
3	EDO	B	902	-	-	-	X
3	EDO	B	904	-	-	-	X
3	EDO	B	908	-	-	-	X
6	PEP	A	700	-	-	X	X
6	PEP	B	700	-	-	-	X

2 Entry composition [i](#)

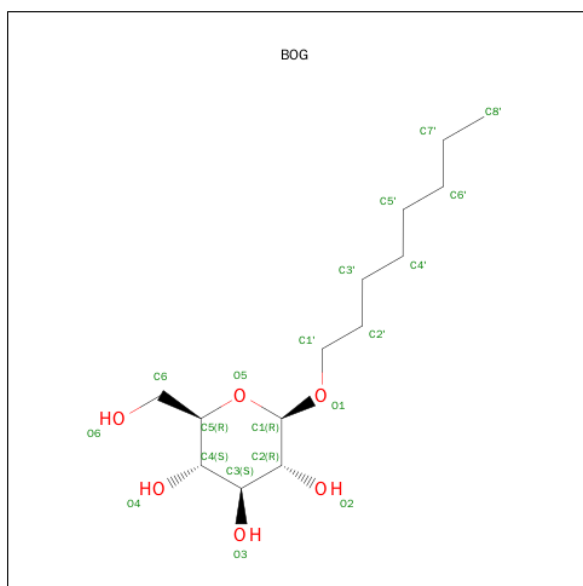
There are 8 unique types of molecules in this entry. The entry contains 8658 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	495	Total	C	N	O	S	0	0	0
			3962	2515	705	729	13			
1	B	495	Total	C	N	O	S	0	0	0
			3962	2515	705	729	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	A	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	B	1	Total	C	O	0	0
			20	14	6		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



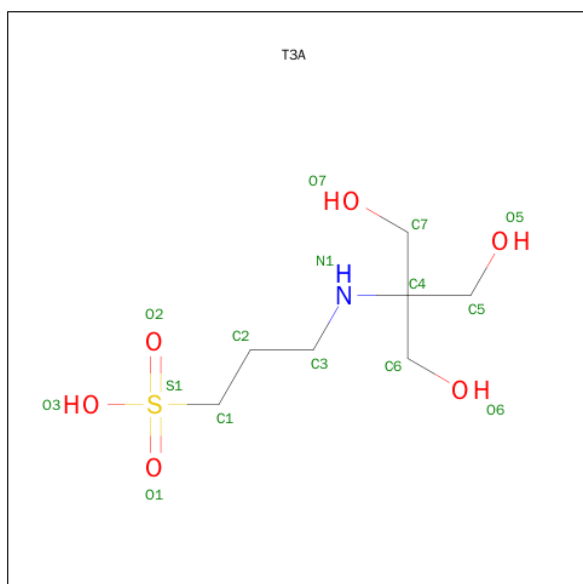
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

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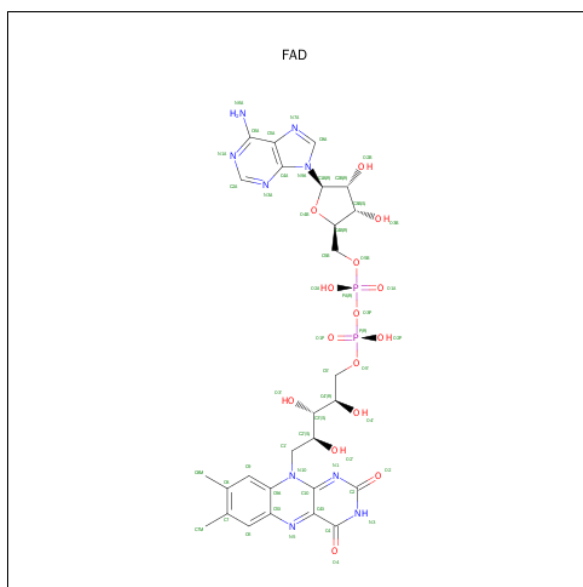
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total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

- Molecule 4 is N-(TRIS(HYDROXYMETHYL)METHYL)-3-AMINOPROPANESULFONIC ACID (three-letter code: T3A) (formula: $C_7H_{17}NO_6S$).



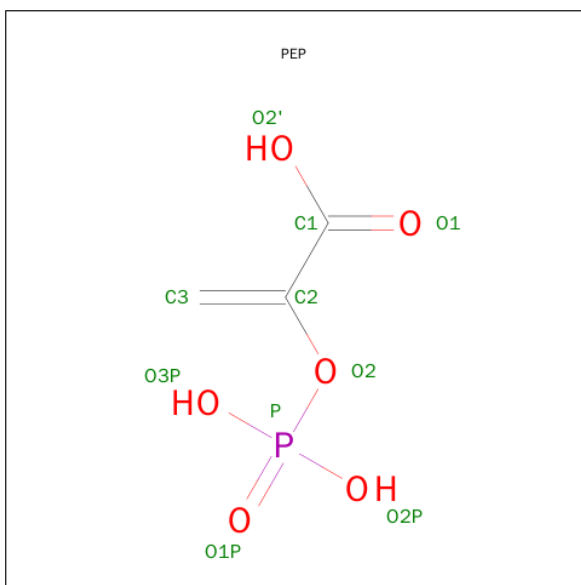
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			15	7	1	6	1		
4	B	1	Total	C	N	O	S	0	0
			15	7	1	6	1		

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



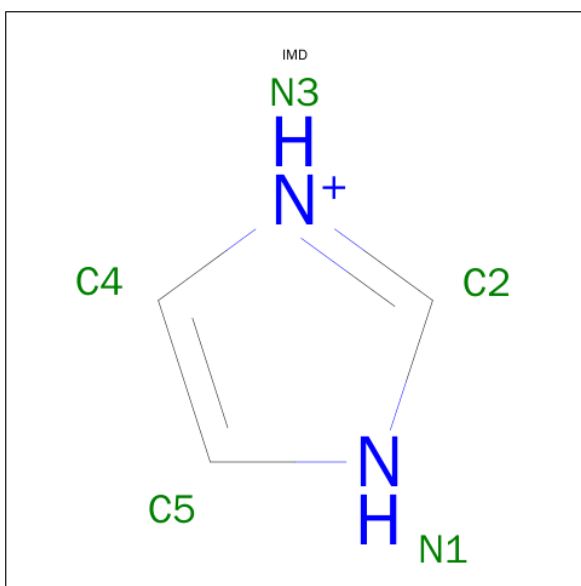
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 6 is PHOSPHOENOLPYRUVATE (three-letter code: PEP) (formula: $C_3H_5O_6P$).



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

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



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

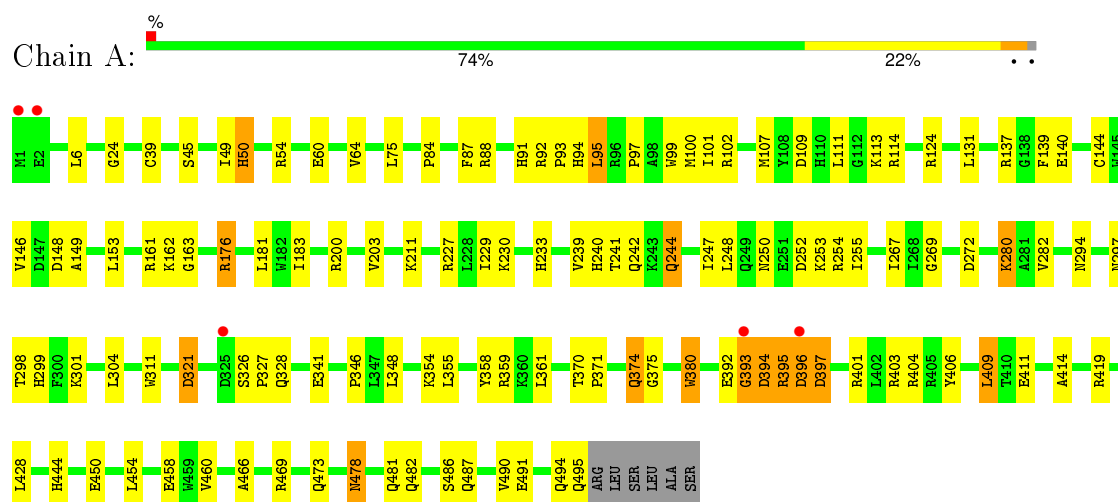
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	196	Total 196	O 196	0	0
8	B	189	Total 189	O 189	0	0

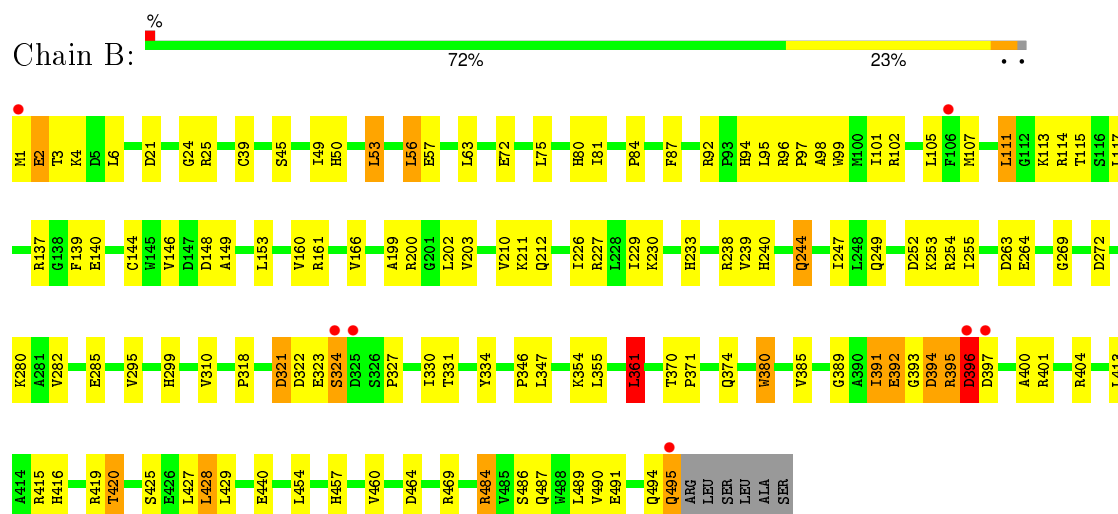
3 Residue-property plots

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, α , β , γ	113.82Å 113.94Å 192.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.10 28.84 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (10.00-2.10) 99.8 (28.84-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.43 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.191 , 0.230 0.217 , 0.217	Depositor DCC
R_{free} test set	3693 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	39.6	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.480 for k,h,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 73532 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8658	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IMD, PEP, EDO, T3A, 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	0.34	0/4057	0.59	0/5494
1	B	0.32	0/4057	0.60	2/5494 (0.0%)
All	All	0.33	0/8114	0.60	2/10988 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	395	ARG	N-CA-C	-5.64	95.76	111.00
1	B	361	LEU	CA-CB-CG	5.17	127.18	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3962	0	3911	128	0
1	B	3962	0	3911	128	0
2	A	60	0	81	22	0
2	B	40	0	56	11	0
3	A	48	0	72	5	0
3	B	40	0	60	4	0
4	A	15	0	17	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	15	0	17	1	0
5	A	53	0	31	1	0
5	B	53	0	31	1	0
6	A	10	0	3	4	0
6	B	10	0	3	3	0
7	B	5	0	5	2	0
8	A	196	0	0	6	0
8	B	189	0	0	4	0
All	All	8658	0	8198	257	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 16.

All (257) 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:137:ARG:HH22	2:A:800:BOG:C5	1.62	1.10
1:A:137:ARG:HH22	2:A:800:BOG:H5	0.93	1.04
1:A:137:ARG:NH2	2:A:800:BOG:H5	1.77	0.99
1:A:254:ARG:HH11	6:A:700:PEP:H31	1.27	0.96
1:B:254:ARG:HH21	6:B:700:PEP:H31	1.32	0.94
1:B:105:LEU:HD13	2:B:900:BOG:O6	1.71	0.91
1:A:102:ARG:HD2	2:A:800:BOG:H3'1	1.53	0.90
1:A:254:ARG:NH1	6:A:700:PEP:H31	1.85	0.90
1:B:254:ARG:NH2	6:B:700:PEP:H31	1.86	0.90
1:A:297:ASN:HD21	1:A:304:LEU:H	1.20	0.89
1:B:391:ILE:HG13	1:B:392:GLU:H	1.38	0.87
1:B:395:ARG:HG2	1:B:419:ARG:HH12	1.42	0.85
1:B:415:ARG:HG2	1:B:419:ARG:HD2	1.58	0.84
1:A:102:ARG:HE	2:A:800:BOG:H1'1	1.43	0.83
1:A:395:ARG:NH1	1:A:419:ARG:HE	1.77	0.82
1:B:272:ASP:H	3:B:901:EDO:H21	1.45	0.80
1:A:395:ARG:HB2	1:A:395:ARG:NH1	1.96	0.80
1:A:478:ASN:ND2	1:A:481:GLN:H	1.79	0.80
2:A:1949:BOG:H2'1	2:A:1949:BOG:H8'3	1.63	0.80
1:B:324:SER:OG	1:B:330:ILE:HG12	1.80	0.80
1:A:272:ASP:H	3:A:1954:EDO:H12	1.48	0.79
1:A:254:ARG:HH11	6:A:700:PEP:C3	1.96	0.78
1:B:464:ASP:H	7:B:7068:IMD:HN3	1.28	0.78
1:B:105:LEU:CD1	2:B:900:BOG:O6	2.31	0.78
1:B:395:ARG:CG	1:B:419:ARG:HH12	1.98	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:LEU:HD22	2:B:900:BOG:H5	1.65	0.76
1:B:395:ARG:HD3	1:B:419:ARG:HH22	1.49	0.76
1:A:478:ASN:C	1:A:478:ASN:HD22	1.89	0.76
1:A:102:ARG:NE	2:A:800:BOG:H1'1	2.01	0.76
1:A:102:ARG:NH2	1:A:137:ARG:HH21	1.84	0.76
1:B:397:ASP:HA	1:B:400:ALA:HB3	1.68	0.76
1:B:416:HIS:O	1:B:420:THR:HG23	1.86	0.75
1:B:1:MET:HE3	1:B:2:GLU:HG2	1.67	0.75
1:B:254:ARG:HH21	6:B:700:PEP:C3	2.00	0.74
1:A:93:PRO:HB3	2:A:1949:BOG:H5	1.69	0.74
1:B:96:ARG:HH11	1:B:249:GLN:HE21	1.36	0.73
1:B:393:GLY:CA	1:B:396:ASP:HB2	2.18	0.73
1:B:495:GLN:HE21	1:B:495:GLN:N	1.86	0.72
1:B:391:ILE:HG13	1:B:392:GLU:N	2.04	0.72
1:A:395:ARG:HB2	1:A:395:ARG:HH11	1.53	0.72
1:A:137:ARG:HH22	2:A:800:BOG:C6	2.03	0.72
1:B:322:ASP:OD2	1:B:331:THR:HG22	1.89	0.71
1:A:137:ARG:NH2	2:A:800:BOG:H62	2.06	0.71
1:B:393:GLY:HA3	1:B:396:ASP:HB2	1.73	0.71
1:B:6:LEU:HD11	1:B:203:VAL:HG23	1.74	0.69
1:A:137:ARG:NH2	2:A:800:BOG:C6	2.56	0.69
1:B:395:ARG:O	1:B:397:ASP:N	2.26	0.68
1:A:102:ARG:NH2	1:A:137:ARG:NH2	2.41	0.68
1:A:137:ARG:NH2	2:A:800:BOG:C5	2.46	0.67
1:A:49:ILE:HB	1:A:144:CYS:HB2	1.77	0.66
1:B:49:ILE:HB	1:B:144:CYS:HB2	1.75	0.66
1:A:397:ASP:HB3	1:A:401:ARG:HD3	1.78	0.66
1:A:403:ARG:HD2	1:A:411:GLU:HA	1.79	0.65
1:B:374:GLN:CD	1:B:374:GLN:H	1.99	0.65
1:A:54:ARG:HA	2:A:900:BOG:H61	1.79	0.65
1:B:102:ARG:HD2	2:B:800:BOG:H62	1.78	0.64
1:B:393:GLY:O	1:B:394:ASP:HB2	1.99	0.63
1:B:202:LEU:HD13	1:B:203:VAL:N	2.14	0.62
1:B:72:GLU:OE1	1:B:115:THR:HG22	1.99	0.62
1:A:94:HIS:CE1	1:A:95:LEU:HD13	2.35	0.62
1:B:50:HIS:CE1	1:B:354:LYS:HZ3	2.17	0.62
1:A:107:MET:O	1:A:111:LEU:HB2	2.00	0.62
1:B:395:ARG:HG2	1:B:419:ARG:NH1	2.15	0.61
1:B:393:GLY:O	1:B:394:ASP:CB	2.47	0.61
1:A:478:ASN:HD21	1:A:481:GLN:H	1.47	0.61
1:A:294:ASN:O	1:A:298:THR:HG23	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:GLN:H	1:B:244:GLN:NE2	1.99	0.61
1:A:93:PRO:CB	2:A:1949:BOG:H5	2.30	0.61
1:B:57:GLU:HB2	2:B:900:BOG:O2	2.01	0.61
1:A:102:ARG:CD	2:A:800:BOG:H1'1	2.31	0.60
1:B:105:LEU:HD13	2:B:900:BOG:HO6	1.63	0.60
1:A:49:ILE:HD11	1:A:146:VAL:HB	1.82	0.60
1:A:393:GLY:O	1:A:394:ASP:CB	2.49	0.60
1:B:334:TYR:CD2	1:B:361:LEU:HD22	2.36	0.60
1:B:395:ARG:CD	1:B:419:ARG:HH22	2.15	0.60
1:B:428:LEU:HD12	1:B:428:LEU:O	2.01	0.60
1:A:490:VAL:O	1:A:494:GLN:HG2	2.01	0.60
1:A:6:LEU:HD11	1:A:203:VAL:HG23	1.83	0.60
1:B:392:GLU:HG2	1:B:401:ARG:HH12	1.68	0.59
1:B:50:HIS:CE1	1:B:354:LYS:NZ	2.71	0.58
1:A:487:GLN:O	1:A:491:GLU:HG3	2.03	0.58
1:A:24:GLY:HA2	1:A:162:LYS:HD3	1.85	0.58
1:A:395:ARG:CZ	1:A:419:ARG:HE	2.17	0.58
1:B:24:GLY:HA3	1:B:380:TRP:CZ2	2.39	0.58
1:A:241:THR:HG22	1:A:241:THR:O	2.03	0.57
1:A:102:ARG:HD2	2:A:800:BOG:C1'	2.34	0.57
1:B:487:GLN:O	1:B:491:GLU:HG3	2.04	0.57
1:A:54:ARG:HA	2:A:900:BOG:C6	2.35	0.56
1:B:397:ASP:O	1:B:401:ARG:N	2.23	0.56
1:B:324:SER:CB	1:B:330:ILE:HG12	2.35	0.56
1:B:229:ILE:HD12	1:B:327:PRO:HB3	1.88	0.56
1:A:102:ARG:HD2	2:A:800:BOG:H1'1	1.87	0.56
1:A:428:LEU:C	1:A:428:LEU:HD23	2.27	0.55
1:B:247:ILE:HG13	1:B:255:ILE:HG23	1.87	0.55
1:A:200:ARG:O	1:A:346:PRO:HD2	2.07	0.55
1:A:444:HIS:HE1	8:A:7156:HOH:O	1.88	0.55
1:A:102:ARG:HH22	1:A:137:ARG:HH21	1.52	0.55
1:A:374:GLN:CG	1:A:375:GLY:H	2.19	0.55
1:B:113:LYS:HB2	8:B:7227:HOH:O	2.05	0.55
1:B:252:ASP:O	1:B:253:LYS:HB2	2.08	0.54
1:A:403:ARG:HD3	8:A:7254:HOH:O	2.08	0.54
1:B:238:ARG:HG3	1:B:264:GLU:C	2.27	0.54
1:A:406:TYR:HB2	1:A:409:LEU:HD22	1.90	0.54
1:B:113:LYS:HB2	1:B:113:LYS:NZ	2.24	0.53
1:B:107:MET:O	1:B:111:LEU:HB2	2.07	0.53
1:A:102:ARG:HD2	2:A:800:BOG:C3'	2.34	0.53
1:B:428:LEU:HD12	1:B:428:LEU:C	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:ASN:ND2	1:A:481:GLN:HG3	2.24	0.53
1:B:99:TRP:HB3	2:B:800:BOG:H1'2	1.91	0.52
1:A:428:LEU:HD11	1:A:450:GLU:HG3	1.91	0.52
3:A:1956:EDO:O1	1:B:161:ARG:HB2	2.09	0.52
1:A:478:ASN:HD21	1:A:481:GLN:HG3	1.74	0.51
1:B:230:LYS:NZ	1:B:285:GLU:HG3	2.25	0.51
1:B:272:ASP:N	3:B:901:EDO:H21	2.21	0.51
1:B:440:GLU:OE1	1:B:484:ARG:HD3	2.11	0.51
1:A:99:TRP:HA	2:A:800:BOG:H1'2	1.92	0.51
1:B:391:ILE:O	1:B:392:GLU:CB	2.59	0.51
1:A:88:ARG:NE	1:A:244:GLN:HG3	2.25	0.51
1:B:49:ILE:HD11	1:B:146:VAL:HB	1.91	0.51
1:A:24:GLY:HA3	1:A:380:TRP:CZ2	2.46	0.51
1:A:240:HIS:CE1	1:A:242:GLN:HB2	2.46	0.51
1:A:137:ARG:NH1	2:A:1949:BOG:O2	2.44	0.50
1:A:252:ASP:O	1:A:253:LYS:HB2	2.10	0.50
1:A:247:ILE:HG23	1:A:247:ILE:O	2.12	0.50
1:A:227:ARG:HG2	1:A:321:ASP:HB2	1.94	0.50
1:A:478:ASN:C	1:A:478:ASN:ND2	2.62	0.50
1:A:444:HIS:HD2	1:A:473:GLN:OE1	1.95	0.50
1:B:200:ARG:O	1:B:346:PRO:HD2	2.12	0.50
1:A:403:ARG:NH1	1:A:409:LEU:O	2.46	0.49
1:A:454:LEU:HB3	1:A:460:VAL:HG21	1.94	0.49
1:A:494:GLN:HB3	1:A:495:GLN:OE1	2.12	0.49
1:B:370:THR:HB	1:B:371:PRO:HD3	1.94	0.49
1:B:92:ARG:HD2	1:B:299:HIS:HE1	1.77	0.49
1:B:98:ALA:HB3	2:B:800:BOG:H3	1.94	0.49
1:A:326:SER:OG	1:A:328:GLN:HG2	2.13	0.48
1:A:392:GLU:HB2	1:A:401:ARG:NH1	2.28	0.48
1:A:229:ILE:HD12	1:A:327:PRO:HB3	1.94	0.48
1:A:176:ARG:HD2	1:A:183:ILE:HB	1.94	0.48
1:B:212:GLN:NE2	8:B:7127:HOH:O	2.46	0.48
1:B:21:ASP:O	1:B:25:ARG:HG3	2.12	0.48
1:B:391:ILE:CG1	1:B:392:GLU:H	2.09	0.48
1:A:395:ARG:HH22	1:A:419:ARG:HG3	1.78	0.48
1:B:396:ASP:N	1:B:396:ASP:OD2	2.47	0.48
1:A:102:ARG:HH12	1:A:139:PHE:HE1	1.61	0.48
1:B:94:HIS:CE1	1:B:95:LEU:HG	2.48	0.48
1:A:148:ASP:OD1	1:A:149:ALA:N	2.46	0.48
8:A:7174:HOH:O	1:B:457:HIS:HE1	1.95	0.48
1:B:101:ILE:HA	2:B:900:BOG:H61	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:CE	1:B:2:GLU:HG2	2.39	0.47
1:B:454:LEU:HB3	1:B:460:VAL:HG21	1.94	0.47
1:A:395:ARG:HH12	1:A:419:ARG:HE	1.58	0.47
1:B:153:LEU:HD13	1:B:153:LEU:C	2.35	0.47
1:B:202:LEU:HD12	1:B:347:LEU:CD1	2.44	0.47
1:B:295:VAL:O	1:B:299:HIS:HD2	1.97	0.47
1:B:92:ARG:HD2	1:B:299:HIS:CE1	2.49	0.47
1:A:397:ASP:HB3	1:A:401:ARG:HH11	1.79	0.47
1:A:374:GLN:CG	1:A:375:GLY:N	2.78	0.46
1:A:97:PRO:HG2	1:A:100:MET:HB2	1.97	0.46
1:B:1:MET:HE3	1:B:2:GLU:H	1.80	0.46
1:B:72:GLU:OE2	1:B:114:ARG:HA	2.15	0.46
1:A:102:ARG:HG2	1:A:102:ARG:HH11	1.81	0.46
1:A:94:HIS:NE2	1:A:95:LEU:HD13	2.31	0.46
1:A:75:LEU:HD21	1:A:84:PRO:HG3	1.98	0.46
1:A:255:ILE:HD12	1:A:255:ILE:O	2.16	0.46
1:A:272:ASP:H	3:A:1954:EDO:C1	2.23	0.46
1:A:181:LEU:HD23	8:A:7239:HOH:O	2.16	0.46
1:A:60:GLU:O	1:A:64:VAL:HG23	2.15	0.46
1:B:227:ARG:HG2	1:B:321:ASP:CB	2.45	0.46
1:B:101:ILE:HG21	1:B:139:PHE:CD2	2.51	0.46
1:A:478:ASN:O	1:A:482:GLN:HG3	2.16	0.46
1:B:427:LEU:HD12	8:B:7217:HOH:O	2.16	0.46
1:B:102:ARG:NH2	1:B:137:ARG:HH12	2.13	0.46
1:B:233:HIS:CD2	1:B:269:GLY:HA3	2.51	0.46
1:B:391:ILE:O	1:B:392:GLU:HB3	2.15	0.45
1:B:210:VAL:HG13	1:B:211:LYS:N	2.31	0.45
1:B:226:ILE:HD11	1:B:318:PRO:C	2.37	0.45
1:B:97:PRO:HB2	1:B:99:TRP:CD1	2.51	0.45
1:A:176:ARG:HH11	1:A:176:ARG:HG3	1.82	0.45
1:B:395:ARG:HG3	1:B:395:ARG:HH11	1.81	0.45
1:A:406:TYR:O	1:A:409:LEU:HB2	2.16	0.45
1:A:241:THR:O	1:A:241:THR:CG2	2.64	0.45
1:B:39:CYS:HA	1:B:469:ARG:HD3	1.97	0.45
1:A:248:LEU:O	1:A:255:ILE:HA	2.17	0.45
1:A:102:ARG:NH1	1:A:139:PHE:HE1	2.14	0.45
1:B:227:ARG:HG2	1:B:321:ASP:HB2	1.98	0.45
1:B:87:PHE:O	1:B:140:GLU:HA	2.17	0.45
1:A:161:ARG:HH21	3:A:1953:EDO:H11	1.80	0.45
1:A:50:HIS:NE2	1:A:354:LYS:NZ	2.47	0.45
1:B:96:ARG:HD2	1:B:249:GLN:NE2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:ARG:HG3	1:A:414:ALA:HB2	1.98	0.45
1:A:87:PHE:O	1:A:140:GLU:HA	2.16	0.44
1:B:490:VAL:HG13	1:B:494:GLN:NE2	2.32	0.44
1:B:419:ARG:HH11	1:B:419:ARG:CG	2.30	0.44
1:B:419:ARG:HH11	1:B:419:ARG:HG3	1.82	0.44
1:B:45:SER:HB2	5:B:600:FAD:C4X	2.47	0.44
1:A:45:SER:HB2	5:A:600:FAD:C4X	2.47	0.44
1:A:163:GLY:HA3	1:B:404:ARG:HG2	1.98	0.44
1:A:233:HIS:CD2	1:A:269:GLY:HA3	2.52	0.44
1:B:202:LEU:HD13	1:B:202:LEU:C	2.38	0.44
1:B:148:ASP:OD1	1:B:149:ALA:N	2.50	0.44
1:B:50:HIS:HE1	1:B:354:LYS:NZ	2.16	0.44
1:A:91:HIS:CD2	1:A:93:PRO:HD3	2.52	0.44
1:B:495:GLN:N	1:B:495:GLN:NE2	2.60	0.44
1:A:162:LYS:HE3	1:A:380:TRP:CH2	2.53	0.44
1:A:267:ILE:HD12	8:A:7242:HOH:O	2.18	0.44
1:B:72:GLU:OE2	1:B:117:LEU:HD23	2.18	0.44
1:B:202:LEU:HD12	1:B:347:LEU:HD13	2.00	0.43
1:A:102:ARG:CD	2:A:800:BOG:C1'	2.95	0.43
1:A:101:ILE:HG21	1:A:139:PHE:CD2	2.54	0.43
1:B:107:MET:HB3	1:B:111:LEU:HD22	2.00	0.43
1:B:486:SER:O	1:B:490:VAL:HG23	2.17	0.43
1:A:49:ILE:CD1	1:A:146:VAL:HB	2.48	0.43
1:A:255:ILE:C	1:A:255:ILE:HD12	2.38	0.43
1:B:230:LYS:HD3	1:B:282:VAL:HG23	2.00	0.43
1:A:280:LYS:HA	1:A:280:LYS:HE3	2.01	0.43
1:A:230:LYS:HD3	1:A:282:VAL:HG23	2.01	0.43
1:B:80:HIS:CD2	1:B:81:ILE:HG23	2.53	0.43
1:A:254:ARG:NH1	6:A:700:PEP:C3	2.66	0.43
1:B:457:HIS:HA	4:B:7066:T3A:H22	2.01	0.43
1:A:361:LEU:C	1:A:361:LEU:HD23	2.39	0.43
1:B:322:ASP:OD1	1:B:330:ILE:HG23	2.19	0.42
1:B:361:LEU:HD12	1:B:361:LEU:C	2.39	0.42
1:B:487:GLN:HE21	1:B:491:GLU:CG	2.33	0.42
1:A:131:LEU:O	1:A:301:LYS:HE3	2.19	0.42
1:A:460:VAL:HG11	1:A:466:ALA:HB2	2.00	0.42
1:B:385:VAL:CG2	1:B:385:VAL:O	2.66	0.42
1:B:247:ILE:HG13	1:B:255:ILE:CG2	2.48	0.42
1:A:348:LEU:HD23	1:A:348:LEU:C	2.40	0.42
1:B:75:LEU:HD21	1:B:84:PRO:HG3	2.02	0.42
1:A:109:ASP:HB3	1:A:114:ARG:HH21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:THR:HB	1:A:371:PRO:HD3	2.00	0.42
1:A:39:CYS:HA	1:A:469:ARG:HD3	2.02	0.42
1:B:56:LEU:HB3	2:B:900:BOG:H1'2	2.01	0.42
1:B:395:ARG:CG	1:B:419:ARG:HH22	2.32	0.42
1:B:53:LEU:CD2	2:B:900:BOG:H5	2.42	0.41
1:A:239:VAL:HG23	1:A:240:HIS:CD2	2.55	0.41
1:A:211:LYS:HD3	8:A:7218:HOH:O	2.21	0.41
1:B:484:ARG:HH21	1:B:487:GLN:HG3	1.85	0.41
1:A:97:PRO:HB2	1:A:99:TRP:CD1	2.54	0.41
1:A:374:GLN:HG2	1:A:375:GLY:N	2.36	0.41
1:B:425:SER:O	1:B:429:LEU:HD23	2.20	0.41
1:A:153:LEU:HD21	1:A:458:GLU:CD	2.40	0.41
1:A:311:TRP:HA	3:A:7069:EDO:H21	2.03	0.41
1:B:239:VAL:HG23	1:B:240:HIS:CD2	2.56	0.41
1:A:393:GLY:O	1:A:394:ASP:HB2	2.19	0.41
1:A:358:TYR:CG	1:A:359:ARG:N	2.88	0.41
1:A:393:GLY:O	1:A:394:ASP:HB3	2.21	0.41
1:A:486:SER:O	1:A:490:VAL:HG23	2.21	0.41
1:B:160:VAL:HG22	3:B:7067:EDO:H21	2.03	0.41
7:B:7068:IMD:H4	8:B:7195:HOH:O	2.19	0.41
1:B:4:LYS:O	1:B:199:ALA:HA	2.21	0.41
1:A:92:ARG:HD2	1:A:299:HIS:NE2	2.36	0.40
1:B:166:VAL:O	3:B:7067:EDO:H11	2.21	0.40
1:B:392:GLU:HG2	1:B:401:ARG:NH1	2.33	0.40
1:A:92:ARG:HA	1:A:93:PRO:HD2	1.84	0.40
1:B:322:ASP:O	1:B:323:GLU:HB2	2.22	0.40
1:B:361:LEU:C	1:B:361:LEU:CD1	2.90	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	493/501 (98%)	466 (94%)	21 (4%)	6 (1%)	16	10
1	B	493/501 (98%)	465 (94%)	18 (4%)	10 (2%)	9	4
All	All	986/1002 (98%)	931 (94%)	39 (4%)	16 (2%)	12	6

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	374	GLN
1	A	394	ASP
1	B	392	GLU
1	B	394	ASP
1	B	396	ASP
1	B	2	GLU
1	A	380	TRP
1	A	393	GLY
1	A	396	ASP
1	B	321	ASP
1	B	3	THR
1	B	380	TRP
1	A	321	ASP
1	B	263	ASP
1	B	391	ILE
1	B	389	GLY

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	414/419 (99%)	398 (96%)	16 (4%)	39	39
1	B	414/419 (99%)	397 (96%)	17 (4%)	37	36
All	All	828/838 (99%)	795 (96%)	33 (4%)	38	38

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	HIS
1	A	95	LEU
1	A	113	LYS
1	A	124	ARG
1	A	176	ARG
1	A	244	GLN
1	A	250	ASN
1	A	280	LYS
1	A	341	GLU
1	A	355	LEU
1	A	395	ARG
1	A	396	ASP
1	A	397	ASP
1	A	404	ARG
1	A	409	LEU
1	A	478	ASN
1	B	53	LEU
1	B	56	LEU
1	B	63	LEU
1	B	111	LEU
1	B	244	GLN
1	B	280	LYS
1	B	310	VAL
1	B	324	SER
1	B	355	LEU
1	B	361	LEU
1	B	396	ASP
1	B	413	LEU
1	B	420	THR
1	B	428	LEU
1	B	484	ARG
1	B	489	LEU
1	B	495	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	35	GLN
1	A	128	ASN
1	A	179	ASN
1	A	212	GLN
1	A	242	GLN

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Mol	Chain	Res	Type
1	A	250	ASN
1	A	290	ASN
1	A	294	ASN
1	A	297	ASN
1	A	424	ASN
1	A	444	HIS
1	A	473	GLN
1	A	478	ASN
1	A	482	GLN
1	A	494	GLN
1	B	50	HIS
1	B	91	HIS
1	B	212	GLN
1	B	244	GLN
1	B	249	GLN
1	B	290	ASN
1	B	299	HIS
1	B	339	HIS
1	B	364	HIS
1	B	424	ASN
1	B	457	HIS
1	B	473	GLN
1	B	487	GLN
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 ⓘ

34 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	0.53	0	25,25,25	2.66	7 (28%)
3	EDO	A	1950	-	3,3,3	0.50	0	2,2,2	0.38	0
3	EDO	A	1951	-	3,3,3	0.54	0	2,2,2	0.37	0
3	EDO	A	1952	-	3,3,3	0.46	0	2,2,2	0.41	0
3	EDO	A	1953	-	3,3,3	0.51	0	2,2,2	0.39	0
3	EDO	A	1954	-	3,3,3	0.48	0	2,2,2	0.40	0
3	EDO	A	1955	-	3,3,3	0.46	0	2,2,2	0.41	0
3	EDO	A	1956	-	3,3,3	0.49	0	2,2,2	0.39	0
3	EDO	A	1957	-	3,3,3	0.48	0	2,2,2	0.41	0
5	FAD	A	600	-	48,58,58	1.73	11 (22%)	54,89,89	2.84	9 (16%)
6	PEP	A	700	-	5,9,9	5.84	2 (40%)	8,13,13	3.71	3 (37%)
4	T3A	A	7066	-	13,14,14	1.05	1 (7%)	17,19,19	1.75	6 (35%)
3	EDO	A	7067	-	3,3,3	0.47	0	2,2,2	0.44	0
3	EDO	A	7068	-	3,3,3	0.51	0	2,2,2	0.40	0
3	EDO	A	7069	-	3,3,3	0.52	0	2,2,2	0.39	0
3	EDO	A	7070	-	3,3,3	0.32	0	2,2,2	0.71	0
2	BOG	A	800	-	20,20,20	3.41	3 (15%)	25,25,25	4.51	8 (32%)
2	BOG	A	900	-	20,20,20	0.46	0	25,25,25	0.63	0
5	FAD	B	600	-	48,58,58	1.61	7 (14%)	54,89,89	2.57	13 (24%)
6	PEP	B	700	-	5,9,9	6.17	3 (60%)	8,13,13	3.43	4 (50%)
4	T3A	B	7066	-	13,14,14	1.07	1 (7%)	17,19,19	1.79	6 (35%)
3	EDO	B	7067	-	3,3,3	0.48	0	2,2,2	0.41	0
7	IMD	B	7068	-	3,5,5	0.45	0	4,5,5	0.57	0
3	EDO	B	7069	-	3,3,3	0.42	0	2,2,2	0.96	0
2	BOG	B	800	-	20,20,20	0.57	0	25,25,25	2.51	10 (40%)
2	BOG	B	900	-	20,20,20	0.45	0	25,25,25	0.62	0
3	EDO	B	901	-	3,3,3	0.49	0	2,2,2	0.41	0
3	EDO	B	902	-	3,3,3	0.49	0	2,2,2	0.39	0
3	EDO	B	903	-	3,3,3	0.46	0	2,2,2	0.42	0
3	EDO	B	904	-	3,3,3	0.53	0	2,2,2	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	B	905	-	3,3,3	0.52	0	2,2,2	0.37	0
3	EDO	B	906	-	3,3,3	0.51	0	2,2,2	0.41	0
3	EDO	B	907	-	3,3,3	0.48	0	2,2,2	0.40	0
3	EDO	B	908	-	3,3,3	0.44	0	2,2,2	0.44	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BOG	A	1949	-	2/2/5/5	0/11/31/31	0/1/1/1
3	EDO	A	1950	-	-	0/1/1/1	0/0/0/0
3	EDO	A	1951	-	-	0/1/1/1	0/0/0/0
3	EDO	A	1952	-	-	0/1/1/1	0/0/0/0
3	EDO	A	1953	-	-	0/1/1/1	0/0/0/0
3	EDO	A	1954	-	-	0/1/1/1	0/0/0/0
3	EDO	A	1955	-	-	0/1/1/1	0/0/0/0
3	EDO	A	1956	-	-	0/1/1/1	0/0/0/0
3	EDO	A	1957	-	-	0/1/1/1	0/0/0/0
5	FAD	A	600	-	-	0/30/50/50	0/6/6/6
6	PEP	A	700	-	-	0/5/9/9	0/0/0/0
4	T3A	A	7066	-	-	0/18/18/18	0/0/0/0
3	EDO	A	7067	-	-	0/1/1/1	0/0/0/0
3	EDO	A	7068	-	-	0/1/1/1	0/0/0/0
3	EDO	A	7069	-	-	0/1/1/1	0/0/0/0
3	EDO	A	7070	-	-	0/1/1/1	0/0/0/0
2	BOG	A	800	-	2/2/5/5	0/11/31/31	0/1/1/1
2	BOG	A	900	-	-	0/11/31/31	0/1/1/1
5	FAD	B	600	-	-	0/30/50/50	0/6/6/6
6	PEP	B	700	-	-	0/5/9/9	0/0/0/0
4	T3A	B	7066	-	-	0/18/18/18	0/0/0/0
3	EDO	B	7067	-	-	0/1/1/1	0/0/0/0
7	IMD	B	7068	-	-	0/0/0/0	0/1/1/1
3	EDO	B	7069	-	-	0/1/1/1	0/0/0/0
2	BOG	B	800	-	-	0/11/31/31	0/1/1/1
2	BOG	B	900	-	-	0/11/31/31	0/1/1/1
3	EDO	B	901	-	-	0/1/1/1	0/0/0/0
3	EDO	B	902	-	-	0/1/1/1	0/0/0/0
3	EDO	B	903	-	-	0/1/1/1	0/0/0/0
3	EDO	B	904	-	-	0/1/1/1	0/0/0/0
3	EDO	B	905	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	906	-	-	0/1/1/1	0/0/0/0
3	EDO	B	907	-	-	0/1/1/1	0/0/0/0
3	EDO	B	908	-	-	0/1/1/1	0/0/0/0

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	800	BOG	C4-C3	-11.24	1.22	1.52
2	A	800	BOG	C4-C5	-8.46	1.35	1.53
5	A	600	FAD	C6-C5X	-2.53	1.37	1.41
6	B	700	PEP	P-O3P	-2.52	1.45	1.54
5	A	600	FAD	C7M-C7	-2.36	1.46	1.51
5	B	600	FAD	C5A-N7A	-2.28	1.31	1.39
4	B	7066	T3A	C6-C4	2.00	1.55	1.53
4	A	7066	T3A	O3-S1	2.17	1.52	1.46
5	A	600	FAD	C5X-N5	2.47	1.39	1.35
5	A	600	FAD	C5'-C4'	2.61	1.55	1.51
5	B	600	FAD	C5X-N5	2.78	1.39	1.35
5	A	600	FAD	C4A-N3A	2.88	1.39	1.35
5	A	600	FAD	C2A-N1A	2.93	1.39	1.33
5	A	600	FAD	C10-N1	2.98	1.40	1.35
5	B	600	FAD	C10-N1	3.11	1.40	1.35
5	B	600	FAD	C4-N3	3.36	1.39	1.33
6	A	700	PEP	O2-C2	3.38	1.49	1.39
6	B	700	PEP	O2-C2	3.43	1.49	1.39
5	B	600	FAD	C1'-N10	3.51	1.52	1.48
5	A	600	FAD	C4-N3	3.74	1.40	1.33
5	A	600	FAD	C2A-N3A	3.80	1.38	1.32
5	B	600	FAD	C2A-N3A	3.90	1.39	1.32
5	A	600	FAD	C4X-N5	4.09	1.39	1.33
5	A	600	FAD	C1'-N10	5.04	1.53	1.48
2	A	800	BOG	O4-C4	5.27	1.55	1.43
5	B	600	FAD	C4X-N5	5.73	1.42	1.33
6	A	700	PEP	C3-C2	12.42	1.56	1.33
6	B	700	PEP	C3-C2	13.10	1.57	1.33

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	600	FAD	N3A-C2A-N1A	-15.16	117.29	128.89
5	B	600	FAD	N3A-C2A-N1A	-12.79	119.10	128.89
6	A	700	PEP	O2-C2-C3	-9.45	105.62	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	700	PEP	O2-C2-C3	-8.52	107.50	124.73
2	A	800	BOG	O5-C5-C4	-7.05	96.46	109.68
2	A	800	BOG	C6-C5-C4	-6.30	97.47	113.02
5	A	600	FAD	C4X-C4-N3	-5.59	115.94	123.59
2	B	800	BOG	O5-C1-C2	-4.52	101.00	110.28
2	B	800	BOG	C1'-O1-C1	-4.22	106.57	113.94
2	B	800	BOG	O5-C5-C4	-3.68	102.77	109.68
5	B	600	FAD	C4X-C4-N3	-3.61	118.66	123.59
2	B	800	BOG	O5-C1-O1	-2.90	103.06	110.05
6	A	700	PEP	O3P-P-O1P	-2.90	101.26	110.58
5	B	600	FAD	O4'-C4'-C5'	-2.88	103.91	110.19
4	A	7066	T3A	C3-N1-C4	-2.85	111.81	116.07
5	B	600	FAD	C4A-C5A-N7A	-2.81	106.90	109.48
4	B	7066	T3A	C3-N1-C4	-2.78	111.92	116.07
2	B	800	BOG	C1-O5-C5	-2.74	108.42	113.75
6	B	700	PEP	O2P-P-O1P	-2.65	102.04	110.58
5	A	600	FAD	C4B-O4B-C1B	-2.65	106.81	109.72
4	B	7066	T3A	O3-S1-O2	-2.57	105.63	111.61
4	A	7066	T3A	O3-S1-O2	-2.52	105.75	111.61
2	B	800	BOG	C1-C2-C3	-2.46	105.12	109.97
5	B	600	FAD	C4-C4X-C10	-2.31	118.46	119.94
5	B	600	FAD	C1B-N9A-C4A	-2.28	123.50	126.94
4	B	7066	T3A	O3-S1-O1	-2.24	106.41	111.61
4	A	7066	T3A	O3-S1-O1	-2.20	106.49	111.61
2	A	1949	BOG	O2-C2-C3	-2.15	105.50	110.34
5	A	600	FAD	O4'-C4'-C5'	-2.03	105.77	110.19
2	A	1949	BOG	O4-C4-C3	2.00	114.84	110.34
5	B	600	FAD	O3B-C3B-C2B	2.08	118.59	111.83
2	B	800	BOG	O3-C3-C4	2.09	115.04	110.34
6	B	700	PEP	O2P-P-O2	2.16	112.30	105.25
2	A	800	BOG	O6-C6-C5	2.17	118.51	111.33
4	B	7066	T3A	O2-S1-O1	2.20	121.50	113.48
4	A	7066	T3A	O2-S1-O1	2.22	121.56	113.48
5	A	600	FAD	O3B-C3B-C2B	2.22	119.05	111.83
6	A	700	PEP	C1-C2-C3	2.29	125.02	120.97
6	B	700	PEP	O3P-P-O2P	2.33	116.25	107.38
5	B	600	FAD	C4-C4X-N5	2.34	121.56	118.72
5	B	600	FAD	C1'-N10-C9A	2.43	121.59	118.86
5	A	600	FAD	C2A-N1A-C6A	2.44	123.13	118.77
5	B	600	FAD	C4X-N5-C5X	2.46	119.59	116.76
2	A	1949	BOG	C4-C3-C2	2.48	115.42	110.79
5	B	600	FAD	C2B-C1B-N9A	2.53	118.16	114.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	600	FAD	C4-C4X-C10	2.63	121.63	119.94
4	A	7066	T3A	O2-S1-C1	2.64	109.16	106.91
2	B	800	BOG	O2-C2-C1	2.70	115.93	110.02
4	B	7066	T3A	O2-S1-C1	2.78	109.28	106.91
2	A	1949	BOG	C1-C2-C3	2.78	115.46	109.97
2	A	800	BOG	C1'-O1-C1	2.93	119.07	113.94
2	A	1949	BOG	O5-C5-C6	3.00	113.94	106.36
2	A	800	BOG	O5-C5-C6	3.04	114.03	106.36
2	B	800	BOG	O2-C2-C3	3.09	117.29	110.34
2	A	800	BOG	O5-C1-O1	3.37	118.16	110.05
4	A	7066	T3A	O1-S1-C1	3.65	110.02	106.91
4	B	7066	T3A	O1-S1-C1	3.90	110.23	106.91
5	B	600	FAD	C5X-C9A-N10	3.95	120.62	117.62
5	A	600	FAD	C4X-N5-C5X	4.17	121.56	116.76
2	A	1949	BOG	O3-C3-C4	4.51	120.49	110.34
2	B	800	BOG	O1-C1-C2	6.25	115.93	108.04
2	A	800	BOG	O3-C3-C4	7.43	127.07	110.34
5	B	600	FAD	C4-N3-C2	8.56	122.64	115.25
5	A	600	FAD	C4-N3-C2	8.91	122.95	115.25
2	A	1949	BOG	O2-C2-C1	10.61	133.29	110.02
2	A	800	BOG	C3-C4-C5	17.97	141.52	110.20

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	800	BOG	C4
2	A	800	BOG	C3
2	A	1949	BOG	C2
2	A	1949	BOG	C3

There are no torsion outliers.

There are no ring outliers.

17 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1949	BOG	4	0
3	A	1953	EDO	1	0
3	A	1954	EDO	2	0
3	A	1956	EDO	1	0
5	A	600	FAD	1	0
6	A	700	PEP	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	7069	EDO	1	0
2	A	800	BOG	16	0
2	A	900	BOG	2	0
5	B	600	FAD	1	0
6	B	700	PEP	3	0
4	B	7066	T3A	1	0
3	B	7067	EDO	2	0
7	B	7068	IMD	2	0
2	B	800	BOG	3	0
2	B	900	BOG	8	0
3	B	901	EDO	2	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 [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, 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	495/501 (98%)	-0.04	5 (1%) 84 87	15, 32, 52, 81	0
1	B	495/501 (98%)	-0.02	7 (1%) 78 82	16, 32, 52, 80	0
All	All	990/1002 (98%)	-0.03	12 (1%) 81 85	15, 32, 52, 81	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	396	ASP	4.2
1	B	1	MET	4.0
1	B	325	ASP	3.7
1	B	397	ASP	3.4
1	A	325	ASP	3.1
1	B	396	ASP	2.9
1	A	393	GLY	2.7
1	A	2	GLU	2.6
1	A	1	MET	2.6
1	B	495	GLN	2.4
1	B	324	SER	2.3
1	B	106	PHE	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 ⓘ

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
3	EDO	B	908	4/4	0.77	0.45	18.68	44,44,46,47	0
2	BOG	A	900	20/20	0.40	0.56	17.45	95,98,102,102	0
2	BOG	B	900	20/20	0.36	0.58	12.12	95,97,100,101	0
3	EDO	A	7068	4/4	0.51	0.24	8.76	62,64,65,65	0
3	EDO	B	904	4/4	0.85	0.22	8.14	25,37,41,41	0
3	EDO	A	1954	4/4	0.68	0.27	7.73	35,39,40,40	0
3	EDO	B	901	4/4	0.80	0.27	6.74	38,41,44,46	0
3	EDO	A	1951	4/4	0.84	0.18	5.38	26,38,39,42	0
6	PEP	A	700	10/10	0.90	0.19	4.67	30,34,39,43	0
2	BOG	A	800	20/20	0.67	0.34	3.46	106,111,112,112	0
2	BOG	A	1949	20/20	0.71	0.31	3.40	80,86,90,91	0
3	EDO	A	1950	4/4	0.69	0.27	2.92	51,54,56,58	0
3	EDO	B	902	4/4	0.61	0.23	2.70	54,56,57,59	0
6	PEP	B	700	10/10	0.90	0.18	2.44	25,31,38,39	0
3	EDO	B	7067	4/4	0.86	0.19	1.72	48,52,52,55	0
3	EDO	B	907	4/4	0.88	0.17	1.47	60,61,62,62	0
4	T3A	A	7066	15/15	0.94	0.14	0.84	26,36,44,45	0
3	EDO	A	1953	4/4	0.77	0.16	0.59	50,50,51,52	0
3	EDO	B	7069	4/4	0.90	0.12	0.20	20,20,20,20	0
4	T3A	B	7066	15/15	0.94	0.12	0.12	25,37,44,46	0
3	EDO	A	1956	4/4	0.85	0.15	0.01	50,51,52,54	0
3	EDO	A	7070	4/4	0.95	0.11	-0.60	20,20,20,20	0
5	FAD	A	600	53/53	0.98	0.09	-1.06	14,18,21,22	0
5	FAD	B	600	53/53	0.98	0.09	-1.11	15,19,21,22	0
2	BOG	B	800	20/20	0.58	0.31	-	100,101,104,105	0
3	EDO	A	1957	4/4	0.77	0.17	-	57,60,61,63	0
3	EDO	B	903	4/4	0.87	0.15	-	51,51,52,55	0
3	EDO	B	905	4/4	0.77	0.20	-	56,58,58,58	0
7	IMD	B	7068	5/5	0.95	0.19	-	32,44,45,47	0
3	EDO	B	906	4/4	0.51	0.21	-	54,57,58,58	0
3	EDO	A	1955	4/4	0.80	0.20	-	64,66,68,69	0
3	EDO	A	7069	4/4	0.64	0.20	-	52,53,53,54	0
3	EDO	A	7067	4/4	0.68	0.27	-	60,63,64,65	0
3	EDO	A	1952	4/4	0.92	0.12	-	47,47,48,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.