

Full wwPDB X-ray Structure Validation Report (i)

Apr 21, 2024 - 09:28 am BST

PDB ID	:	4A0R
Title	:	Structure of bifunctional DAPA aminotransferase-DTB synthetase from Ara-
		bidopsis thaliana bound to dethiobiotin (DTB).
Authors	:	Cobessi, D.; Dumas, R.; Pautre, V.; Meinguet, C.; Ferrer, J.L.; Alban, C.
Deposited on	:	2011-09-12
Resolution	:	2.68 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 https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.68 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}	130704	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	
1	А	831	3% 67%	22%	• 9%
1	В	831	3% 64%	23%	• 10%

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



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	TLA	В	1809	-	Х	Х	-



4A0R

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11693 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 ADENOSYLMETHIONINE-8-AMINO-7-OXONONANOAT E AMINOTRANSFERASE.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms			ZeroOcc	AltConf	Trace
1	А	755	Total 5788	C 3703	N 974	O 1079	S 32	0	2	0
1	В	748	Total 5704	C 3652	N 961	O 1059	S 32	0	2	0

Chain	Residue	Modelled	Actual	Comment	Reference
А	-19	GLY	-	expression tag	UNP B0F481
А	-18	SER	-	expression tag	UNP B0F481
А	-17	SER	-	expression tag	UNP B0F481
А	-16	HIS	-	expression tag	UNP B0F481
А	-15	HIS	-	expression tag	UNP B0F481
А	-14	HIS	-	expression tag	UNP B0F481
А	-13	HIS	-	expression tag	UNP B0F481
А	-12	HIS	-	expression tag	UNP B0F481
А	-11	HIS	-	expression tag	UNP B0F481
А	-10	SER	-	expression tag	UNP B0F481
A	-9	SER	-	expression tag	UNP B0F481
A	-8	GLY	-	expression tag	UNP B0F481
А	-7	LEU	-	expression tag	UNP B0F481
А	-6	VAL	-	expression tag	UNP B0F481
А	-5	PRO	-	expression tag	UNP B0F481
А	-4	ARG	-	expression tag	UNP B0F481
А	-3	GLY	-	expression tag	UNP B0F481
А	-2	SER	-	expression tag	UNP B0F481
А	-1	HIS	-	expression tag	UNP B0F481
А	0	MET	-	expression tag	UNP B0F481
В	-19	GLY	-	expression tag	UNP B0F481
B	-18	SER	-	expression tag	UNP B0F481
В	-17	SER	-	expression tag	UNP B0F481
B	-16	HIS	-	expression tag	UNP B0F481

There are 40 discrepancies between the modelled and reference sequences:



4/	40	\mathbf{R}

Chain	Residue	Modelled	Actual	Comment	Reference
В	-15	HIS	_	expression tag	UNP B0F481
В	-14	HIS	-	expression tag	UNP B0F481
В	-13	HIS	-	expression tag	UNP B0F481
В	-12	HIS	-	expression tag	UNP B0F481
В	-11	HIS	-	expression tag	UNP B0F481
В	-10	SER	-	expression tag	UNP B0F481
В	-9	SER	-	expression tag	UNP B0F481
В	-8	GLY	-	expression tag	UNP B0F481
В	-7	LEU	-	expression tag	UNP B0F481
В	-6	VAL	-	expression tag	UNP B0F481
В	-5	PRO	-	expression tag	UNP B0F481
В	-4	ARG	-	expression tag	UNP B0F481
В	-3	GLY	-	expression tag	UNP B0F481
В	-2	SER	-	expression tag	UNP B0F481
B	-1	HIS	-	expression tag	UNP B0F481
В	0	MET	-	expression tag	UNP B0F481

• Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	Λ	1	Total	С	Ν	0	Р	0	0
	Л	I	15	8	1	5	1	0	0
0	Р	1	Total	С	Ν	Ο	Р	0	0
	D	L	15	8	1	5	1	0	U

• Molecule 3 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: $C_4H_6O_6$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total C O 10 4 6	0	0
3	В	1	Total C O 10 4 6	0	0

• Molecule 4 is 6-(5-METHYL-2-OXO-IMIDAZOLIDIN-4-YL)-HEXANOIC ACID (three-letter code: DTB) (formula: $C_{10}H_{18}N_2O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	А	1	Total 15	C 10	N 2	O 3	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	В	1	Total	С	Ν	Ο	0	0
4	D	L	15	10	2	3	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	70	Total O 70 70	0	0
5	В	51	$\begin{array}{cc} \text{Total} & \text{O} \\ 51 & 51 \end{array}$	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: ADENOSYLMETHIONINE-8-AMINO-7-OXONONANOATE AMINOTRANS-FERASE



• Molecule 1: ADENOSYLMETHIONINE-8-AMINO-7-OXONONANOATE AMINOTRANS-FERASE











4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	246.67Å 76.63Å 79.84Å	Deperitor
a, b, c, α , β , γ	90.00° 108.02° 90.00°	Depositor
$\mathbf{P}_{\text{oscolution}}(\hat{\mathbf{A}})$	40.44 - 2.68	Depositor
Resolution (A)	40.72 - 2.68	EDS
% Data completeness	99.8 (40.44-2.68)	Depositor
(in resolution range)	99.5(40.72 - 2.68)	EDS
R _{merge}	0.15	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.90 (at 2.69 \text{\AA})$	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
B B.	0.184 , 0.259	Depositor
It, It _{free}	0.179 , 0.253	DCC
R_{free} test set	2000 reflections $(5.01%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	34.6	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.38 , 65.7	EDS
L-test for $twinning^2$	$< L >=0.48, < L^2>=0.31$	Xtriage
	0.027 for -h+k-l,-l,-k	
Estimated twinning fraction	0.005 for -h-k-l,l,k	Xtriage
	0.023 for -h-2*l,-k,l	
F_o, F_c correlation	0.94	EDS
Total number of atoms	11693	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 3.73% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: PLP, DTB, TLA

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).

Mal	Chain	Bo	nd lengths	Bond angles		
1VIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.48	1/5922~(0.0%)	0.64	3/8050~(0.0%)	
1	В	0.48	2/5836~(0.0%)	0.65	3/7938~(0.0%)	
All	All	0.48	3/11758~(0.0%)	0.64	6/15988~(0.0%)	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	В	0	1

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
1	В	307	ARG	CZ-NH1	-11.03	1.18	1.33
1	А	307	ARG	CZ-NH1	-9.79	1.20	1.33
1	В	307	ARG	CZ-NH2	-5.56	1.25	1.33

All (3) bond length outliers are listed below:

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$\mathbf{Ideal}(^{o})$
1	А	307	ARG	NE-CZ-NH2	17.58	129.09	120.30
1	В	307	ARG	NE-CZ-NH2	16.14	128.37	120.30
1	В	307	ARG	NH1-CZ-NH2	-8.37	110.19	119.40
1	А	44	PRO	N-CA-CB	6.33	110.90	103.30
1	А	307	ARG	NH1-CZ-NH2	-5.93	112.87	119.40
1	В	44	PRO	N-CA-CB	5.83	110.29	103.30

There are no chirality outliers.



All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	В	45	SER	Peptide

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	А	5788	0	5697	161	0
1	В	5704	0	5585	181	0
2	А	15	0	6	1	0
2	В	15	0	6	1	0
3	А	10	0	3	3	0
3	В	10	0	4	4	0
4	А	15	0	17	2	0
4	В	15	0	17	5	0
5	А	70	0	0	1	0
5	B	51	0	0	2	0
All	All	11693	0	11335	321	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 14.

All (321) 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:522:PRO:HG2	1:B:525:PHE:HD2	1.07	1.13
1:A:12:LEU:HD11	1:A:359:LEU:HG	1.41	1.02
1:B:522:PRO:HG2	1:B:525:PHE:CD2	1.97	1.00
1:A:659:THR:HG22	1:A:661:ALA:H	1.22	1.00
1:B:659:THR:HG22	1:B:661:ALA:H	1.24	0.99
1:B:12:LEU:HD11	1:B:359:LEU:HG	1.45	0.96
1:A:396:VAL:HG11	1:B:340:ILE:HG21	1.49	0.91
1:A:490:THR:HG23	1:A:490:THR:O	1.72	0.87
1:A:223:GLY:HA2	4:B:1808:DTB:HCA1	1.56	0.87
1:B:490:THR:HG23	1:B:490:THR:O	1.71	0.86
1:B:465:LYS:HG2	1:B:502:GLY:HA2	1.56	0.86



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:14:HIS:HB2	1:B:172:MET:HE3	1.55	0.86
1:B:42:GLN:OE1	1:B:42:GLN:HA	1.75	0.84
1:A:317:LEU:HD23	1:B:407:LEU:HD11	1.62	0.81
1:A:659:THR:HG22	1:A:661:ALA:N	1.95	0.81
1:A:340:ILE:HG21	1:B:396:VAL:HG11	1.61	0.80
1:B:522:PRO:CG	1:B:525:PHE:HD2	1.93	0.80
1:A:14:HIS:HB2	1:A:172:MET:HE3	1.61	0.80
1:B:659:THR:HG22	1:B:661:ALA:N	1.96	0.79
1:B:710:GLN:HB3	1:B:712:LYS:HG2	1.65	0.76
1:B:625:GLY:HA2	1:B:714:LEU:HD12	1.67	0.76
1:B:510:VAL:HG11	1:B:541:ILE:HD13	1.67	0.75
1:B:766:MET:HE2	1:B:804:ARG:HH11	1.52	0.74
1:A:668:GLY:HA3	1:A:673:LYS:HD2	1.68	0.74
1:B:766:MET:HB3	1:B:804:ARG:HD2	1.70	0.74
1:A:223:GLY:CA	4:B:1808:DTB:HCA1	2.17	0.73
1:A:766:MET:HB3	1:A:804:ARG:HD2	1.70	0.73
1:A:223:GLY:HA2	4:B:1808:DTB:CA	2.19	0.73
1:A:316:LYS:HE2	1:A:320:GLU:OE2	1.88	0.72
1:B:28:LYS:HZ3	3:B:1809:TLA:H2	1.54	0.72
1:A:766:MET:HE2	1:A:804:ARG:HH11	1.55	0.72
1:B:316:LYS:HE2	1:B:320:GLU:OE2	1.89	0.72
1:B:465:LYS:HE2	1:B:502:GLY:C	2.10	0.71
1:A:104:LEU:HD12	1:A:116:LEU:HD22	1.70	0.71
1:B:168:LEU:O	1:B:172:MET:HG2	1.92	0.70
1:A:373:GLY:H	1:A:374:PRO:HD2	1.58	0.69
1:B:708:THR:HG23	1:B:710:GLN:N	2.08	0.68
1:A:708:THR:HG23	1:A:711:GLY:H	1.59	0.68
1:B:373:GLY:H	1:B:374:PRO:HD2	1.59	0.67
1:B:28:LYS:NZ	3:B:1809:TLA:H2	2.09	0.66
1:A:407:LEU:HD11	1:B:317:LEU:HD23	1.77	0.65
1:B:428:SER:HB2	1:B:433:THR:OG1	1.95	0.65
1:B:547:ASP:OD1	1:B:599:ARG:NH1	2.29	0.65
1:A:708:THR:HG23	1:A:710:GLN:H	1.61	0.65
1:A:36:ALA:HA	1:A:51:LEU:HD13	1.80	0.64
1:B:515:GLY:HA2	1:B:724:GLN:OE1	1.97	0.63
1:A:96:LEU:HB3	1:A:97:PRO:HD3	1.81	0.62
1:A:428:SER:HB2	1:A:433:THR:OG1	1.99	0.62
1:B:708:THR:HG23	1:B:710:GLN:H	1.64	0.62
1:A:223:GLY:N	4:B:1808:DTB:HCA1	2.15	0.62
1:A:168:LEU:O	1:A:172:MET:HG2	2.00	0.61
1:A:396:VAL:CG1	1:B:340:ILE:HD13	2.30	0.61



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:490:THR:O	1:B:490:THR:CG2	2.45	0.61
1:A:12:LEU:CD1	1:A:359:LEU:HG	2.24	0.61
1:B:768:ARG:NH2	1:B:773:PHE:CE2	2.59	0.61
1:B:12:LEU:CD1	1:B:359:LEU:HG	2.27	0.60
1:A:18:LEU:HD23	1:A:187:VAL:HB	1.83	0.60
1:B:93:HIS:HB3	1:B:113:MET:CE	2.30	0.60
1:B:36:ALA:HA	1:B:51:LEU:HD13	1.83	0.60
1:A:414:LEU:CD1	1:B:321:VAL:HG22	2.32	0.60
1:A:766:MET:CB	1:A:804:ARG:HD2	2.31	0.60
1:B:478:LEU:HD13	1:B:495:GLN:HG2	1.83	0.58
1:A:437:ILE:HD11	1:A:677:HIS:CD2	2.39	0.58
1:A:766:MET:CE	1:A:807:GLU:HG3	2.34	0.58
1:A:96:LEU:HD22	1:A:108:VAL:HG21	1.86	0.57
1:A:706:ASN:O	1:A:714:LEU:HA	2.04	0.57
1:B:96:LEU:HB3	1:B:97:PRO:HD3	1.85	0.57
1:A:707:ILE:CG2	1:A:711:GLY:HA2	2.35	0.57
1:A:87:ILE:HG22	1:A:130:LEU:HB3	1.87	0.57
1:A:104:LEU:O	1:A:105:ASN:C	2.43	0.57
1:B:18:LEU:HD23	1:B:187:VAL:HB	1.87	0.56
1:A:547:ASP:OD1	1:A:599:ARG:NH1	2.38	0.56
1:B:766:MET:CE	1:B:804:ARG:HH11	2.15	0.56
1:B:766:MET:CE	1:B:807:GLU:HG3	2.35	0.56
1:A:762:SER:O	1:A:766:MET:HG3	2.05	0.56
1:B:510:VAL:CG1	1:B:541:ILE:HD13	2.34	0.56
1:B:517:TRP:CZ2	1:B:538:ARG:HG3	2.41	0.56
1:A:444:ARG:HG3	1:A:666:PHE:CZ	2.40	0.56
1:B:593:VAL:HG12	1:B:594:ASP:N	2.20	0.55
1:B:617:VAL:HG12	1:B:644:LYS:NZ	2.21	0.55
1:A:142:ILE:HD12	1:A:146:LEU:HB3	1.88	0.55
1:A:766:MET:HE3	1:A:807:GLU:HG3	1.87	0.55
1:B:804:ARG:O	1:B:807:GLU:HG2	2.06	0.55
1:A:719:ASP:O	1:A:723:VAL:HG23	2.07	0.55
1:B:762:SER:O	1:B:766:MET:HG3	2.07	0.55
1:A:443:PHE:CD1	1:A:464:VAL:HG11	2.42	0.55
1:A:61:PHE:O	1:A:139:GLU:HA	2.07	0.55
1:B:87:ILE:HG22	1:B:130:LEU:HB3	1.88	0.55
1:A:329:HIS:HA	1:A:332:VAL:HG12	1.89	0.55
1:A:766:MET:CE	1:A:804:ARG:HH11	2.18	0.55
1:A:497:TRP:CD1	1:B:501:ARG:HD2	2.42	0.54
1:B:443:PHE:CD1	1:B:464:VAL:HG11	2.42	0.54
1:A:497:TRP:CE2	1:B:501:ARG:HD2	2.43	0.54



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:617:VAL:HG12	1:A:644:LYS:NZ	2.23	0.54
1:B:444:ARG:HG3	1:B:666:PHE:CZ	2.43	0.54
1:B:766:MET:CB	1:B:804:ARG:HD2	2.37	0.54
1:A:766:MET:HB3	1:A:804:ARG:NH1	2.23	0.54
1:B:61:PHE:CG	1:B:62:PRO:HA	2.42	0.54
1:B:256:VAL:HB	1:B:257:PRO:HD3	1.90	0.53
1:A:768:ARG:NH2	1:A:773:PHE:CE2	2.75	0.53
1:A:16:THR:HG23	1:A:185:CYS:SG	2.48	0.53
1:A:708:THR:HG23	1:A:711:GLY:N	2.22	0.53
1:B:241:ASP:O	1:B:242:ILE:HD13	2.09	0.53
1:A:365:ALA:HB3	1:A:774:THR:HB	1.89	0.53
1:B:365:ALA:HB3	1:B:774:THR:HB	1.91	0.52
1:A:501:ARG:HH21	1:B:501:ARG:HH22	1.57	0.52
1:B:94:SER:N	1:B:113:MET:HE1	2.25	0.52
1:B:478:LEU:HD13	1:B:495:GLN:CG	2.40	0.52
1:A:559:LEU:HD21	1:A:597:PHE:CZ	2.45	0.52
1:B:80:ARG:HH21	1:B:284:GLU:CD	2.13	0.52
1:A:373:GLY:H	1:A:374:PRO:CD	2.23	0.52
1:A:676:LEU:N	1:B:494:GLN:OE1	2.40	0.52
1:A:208:ARG:HD2	1:A:208:ARG:O	2.10	0.52
1:B:766:MET:HE2	1:B:804:ARG:NH1	2.22	0.52
1:A:256:VAL:HB	1:A:257:PRO:HD3	1.91	0.51
1:B:730:SER:O	1:B:747:LYS:NZ	2.36	0.51
1:B:708:THR:HG22	1:B:711:GLY:H	1.75	0.51
1:A:28:LYS:NZ	3:A:1810:TLA:H3	2.26	0.51
1:A:194:ALA:HB3	1:B:226:SER:HA	1.92	0.51
1:B:370:TRP:CD1	1:B:370:TRP:N	2.78	0.51
1:B:329:HIS:HA	1:B:332:VAL:HG12	1.91	0.51
1:B:417:VAL:CG1	1:B:642:PHE:CZ	2.94	0.51
1:A:659:THR:HG22	1:A:660:ASP:N	2.25	0.51
1:A:659:THR:CG2	1:A:660:ASP:N	2.73	0.51
1:A:281[A]:ASP:O	1:A:282:LEU:HB2	2.10	0.51
1:A:10:LEU:O	1:A:358:SER:HB2	2.11	0.51
1:A:706:ASN:O	1:A:715:ARG:N	2.43	0.51
1:B:113:MET:HG2	1:B:153:ALA:HB1	1.93	0.51
1:B:559:LEU:HD21	1:B:597:PHE:CZ	2.46	0.50
1:B:700:ASP:HB3	1:B:703:THR:OG1	2.11	0.50
1:A:708:THR:HG23	1:A:710:GLN:N	2.26	0.50
1:A:414:LEU:HD12	1:B:321:VAL:HG22	1.93	0.50
1:B:651:VAL:HG22	1:B:652:PRO:HD2	1.94	0.50
1:A:622:TRP:CE3	1:A:714:LEU:HD13	2.47	0.50



Atom 1 Atom 2		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:725:GLN:HB3	1:B:802:TYR:CE1	2.46	0.50
1:A:744:LEU:C	1:A:744:LEU:HD12	2.33	0.50
1:B:517:TRP:CE2	1:B:538:ARG:HB2	2.47	0.50
1:B:659:THR:HG22	1:B:660:ASP:N	2.27	0.50
1:B:281[A]:ASP:O	1:B:282:LEU:HB2	2.12	0.49
1:B:766:MET:HE3	1:B:807:GLU:HG3	1.93	0.49
1:A:805:LEU:O	1:A:808:PHE:N	2.45	0.49
1:A:195:SER:HB3	4:A:1811:DTB:HCA1	1.94	0.49
1:B:534:THR:HG22	1:B:534:THR:O	2.10	0.49
1:B:623:ARG:HG3	1:B:624:LEU:HD13	1.92	0.49
1:B:659:THR:CG2	1:B:660:ASP:N	2.75	0.49
1:B:88:SER:HA	1:B:120:ASP:O	2.13	0.49
1:A:593:VAL:HG12	1:A:594:ASP:N	2.27	0.49
1:A:93:HIS:HB2	1:A:136:TYR:CD1	2.48	0.49
1:B:93:HIS:HB2	1:B:136:TYR:CD1	2.48	0.49
1:B:763:LEU:HD23	1:B:763:LEU:HA	1.66	0.49
1:B:542:PHE:CE1	1:B:595:PRO:HG3	2.48	0.48
1:A:370:TRP:CD1	1:A:370:TRP:N	2.80	0.48
1:B:97:PRO:HA	1:B:100:LYS:HE2	1.95	0.48
1:B:437:ILE:O	1:B:441:MET:HG3	2.13	0.48
1:B:522:PRO:CG	1:B:525:PHE:CD2	2.80	0.48
1:A:497:TRP:O	1:A:499:THR:HG23	2.14	0.48
1:B:759:TYR:O	1:B:762:SER:HB2	2.13	0.48
1:A:623:ARG:HG3	1:A:624:LEU:HD13	1.95	0.48
1:A:804:ARG:O	1:A:807:GLU:HG2	2.12	0.48
1:B:308:LEU:HD11	1:B:357:SER:HB3	1.95	0.48
1:A:417:VAL:CG1	1:A:642:PHE:CZ	2.97	0.48
1:A:718:TRP:CE3	1:A:794:CYS:HB3	2.48	0.48
1:B:350:ILE:HG12	1:B:362:GLN:HE21	1.79	0.48
1:A:325:PRO:HG2	1:B:399:PRO:HG3	1.95	0.48
1:A:510:VAL:HG11	1:A:541:ILE:HD13	1.95	0.48
1:A:766:MET:HE2	1:A:804:ARG:NH1	2.25	0.48
1:A:589:GLY:HA2	1:A:777:LEU:HD22	1.95	0.48
1:B:478:LEU:O	1:B:482:GLU:HG2	2.14	0.48
1:B:720:GLU:O	1:B:724:GLN:HG2	2.14	0.48
1:B:373:GLY:H	1:B:374:PRO:CD	2.25	0.48
1:B:417:VAL:HG11	1:B:642:PHE:CZ	2.49	0.48
1:B:155:VAL:HA	5:B:2013:HOH:O	2.14	0.47
1:B:85:ILE:HA	1:B:127:ALA:HB1	1.95	0.47
1:B:441:MET:HE3	1:B:639:ILE:HG12	1.96	0.47
1:A:97:PRO:HA	1:A:100:LYS:HE2	1.95	0.47



	At any 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:100:LYS:C	1:A:103:GLY:H	2.18	0.47
1:B:97:PRO:HG2	1:B:151:GLU:HB3	1.96	0.47
1:B:91:VAL:HG22	1:B:134:THR:HB	1.97	0.47
1:B:297:LYS:HB3	1:B:297:LYS:HE2	1.72	0.47
1:B:374:PRO:HD3	1:B:648:GLY:O	2.15	0.47
1:A:627:GLU:OE2	1:A:699:LYS:HE3	2.15	0.47
1:B:93:HIS:HB3	1:B:113:MET:HE1	1.96	0.47
1:A:60:GLY:O	1:A:64:ASP:N	2.40	0.47
1:A:490:THR:O	1:A:490:THR:CG2	2.46	0.47
1:A:495:GLN:HE21	1:B:440:LYS:HE2	1.80	0.46
1:A:805:LEU:O	1:A:808:PHE:HD1	1.98	0.46
1:A:85:ILE:HA	1:A:127:ALA:HB1	1.97	0.46
1:A:373:GLY:HA2	1:A:787:PRO:HD2	1.96	0.46
1:A:482:GLU:HB2	1:B:497:TRP:CZ3	2.50	0.46
1:A:651:VAL:HG22	1:A:652:PRO:HD2	1.97	0.46
1:A:700:ASP:HB3	1:A:703:THR:OG1	2.16	0.46
1:B:517:TRP:NE1	1:B:538:ARG:HB2	2.30	0.46
1:A:708:THR:HB	1:A:713:THR:HG23	1.98	0.46
1:B:44:PRO:O	1:B:45:SER:CB	2.63	0.46
1:A:367:ALA:HB1	1:A:372:GLN:HB2	1.97	0.46
1:A:478:LEU:HD13	1:A:495:GLN:HG2	1.96	0.46
1:B:710:GLN:CB	1:B:712:LYS:HG2	2.41	0.46
1:B:21:SER:HB3	1:B:28:LYS:HG3	1.97	0.46
1:A:396:VAL:HG11	1:B:340:ILE:HD13	1.98	0.45
1:A:61:PHE:CG	1:A:62:PRO:HA	2.52	0.45
1:B:514:ASN:ND2	1:B:728:SER:HA	2.31	0.45
1:A:340:ILE:HD13	1:B:396:VAL:CG1	2.45	0.45
1:A:478:LEU:O	1:A:482:GLU:HG2	2.16	0.45
1:B:61:PHE:O	1:B:139:GLU:HA	2.17	0.45
1:A:269:LEU:HD13	1:A:296:LEU:HD13	1.99	0.45
1:B:93:HIS:CB	1:B:113:MET:HE1	2.47	0.45
4:B:1808:DTB:HCS	3:B:1809:TLA:C1	2.46	0.45
1:A:269:LEU:CD1	1:A:296:LEU:HD13	2.46	0.45
1:B:37:ALA:HA	1:B:74:LEU:HD21	1.98	0.45
1:A:226:SER:HA	1:B:194:ALA:HB3	1.98	0.45
1:B:208:ARG:HD2	1:B:208:ARG:O	2.17	0.45
1:B:398:PHE:HB3	1:B:399:PRO:HD3	1.99	0.45
1:A:353:ALA:C	1:A:355:ASP:H	2.19	0.45
1:B:441:MET:CE	1:B:639:ILE:HG23	2.47	0.45
1:B:708:THR:CG2	1:B:711:GLY:H	2.29	0.45
1:A:28:LYS:HZ3	3:A:1810:TLA:H3	1.81	0.45



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:708:THR:CG2	1:A:711:GLY:H	2.29	0.45
1:A:281[A]:ASP:HB3	1:A:283:ILE:HG12	1.99	0.44
1:A:497:TRP:NE1	1:B:501:ARG:HD2	2.33	0.44
1:A:763:LEU:HA	1:A:763:LEU:HD23	1.65	0.44
1:A:241:ASP:O	1:A:242:ILE:HD13	2.17	0.44
1:A:281[A]:ASP:HB3	1:A:283:ILE:H	1.82	0.44
1:A:478:LEU:HD13	1:A:495:GLN:CG	2.47	0.44
1:B:558:TYR:O	1:B:562:HIS:ND1	2.50	0.44
1:A:98:ALA:O	1:A:101:SER:HB2	2.17	0.44
1:A:321:VAL:HG22	1:B:414:LEU:HD12	1.99	0.44
1:B:157:ASP:HB3	1:B:206:LEU:HD13	1.99	0.44
1:A:220:GLY:O	1:A:250:HIS:HB2	2.18	0.44
1:A:321:VAL:HG22	1:B:414:LEU:CD1	2.46	0.44
1:B:146:LEU:HD23	1:B:146:LEU:HA	1.82	0.44
1:B:183:LEU:HD23	1:B:184:LEU:N	2.33	0.44
1:A:297:LYS:HB3	1:A:297:LYS:HE2	1.72	0.44
1:B:354:SER:O	1:B:355:ASP:O	2.36	0.44
1:A:111:SER:HB2	1:A:154:THR:HG22	1.99	0.44
1:A:440:LYS:HE2	1:B:495:GLN:HB2	2.00	0.44
1:B:382:LEU:HD13	1:B:650:MET:HG3	2.00	0.44
1:B:136:TYR:OH	1:B:163:MET:HG3	2.18	0.44
1:B:708:THR:CG2	1:B:710:GLN:HB2	2.48	0.44
1:A:88:SER:HA	1:A:120:ASP:O	2.17	0.43
1:A:627:GLU:CD	1:A:699:LYS:HE3	2.39	0.43
1:B:21:SER:HB3	1:B:28:LYS:CG	2.48	0.43
1:B:417:VAL:HG22	1:B:628:THR:HB	2.00	0.43
1:B:538:ARG:NH1	1:B:737:VAL:O	2.52	0.43
1:B:589:GLY:HA2	1:B:777:LEU:HD22	1.98	0.43
1:A:707:ILE:HG23	1:A:711:GLY:HA2	1.99	0.43
1:B:269:LEU:HD13	1:B:296:LEU:HD13	1.99	0.43
1:A:417:VAL:HG11	1:A:642:PHE:CZ	2.54	0.43
1:A:497:TRP:CD1	1:B:501:ARG:CD	3.02	0.43
1:A:617:VAL:HG11	2:A:1644:PLP:C5	2.48	0.43
1:B:113:MET:HE2	1:B:113:MET:HB3	1.77	0.43
1:A:353:ALA:C	1:A:355:ASP:N	2.71	0.43
1:B:556:SER:O	1:B:560:SER:HB2	2.18	0.43
1:B:617:VAL:HG11	2:B:1644:PLP:C5	2.49	0.43
1:A:91:VAL:HG22	1:A:134:THR:HB	2.00	0.43
1:A:417:VAL:HG22	1:A:628:THR:HB	2.01	0.43
1:B:744:LEU:HD12	1:B:744:LEU:C	2.39	0.43
1:A:541:ILE:HG22	1:A:595:PRO:HG2	2.00	0.43



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:808:PHE:N	1:A:808:PHE:CD1	2.86	0.43
1:B:725:GLN:HB3	1:B:802:TYR:CZ	2.54	0.43
1:A:59:THR:HB	1:A:140:ALA:O	2.19	0.42
1:A:700:ASP:OD1	1:A:700:ASP:C	2.57	0.42
1:B:281[A]:ASP:HB3	1:B:283:ILE:H	1.83	0.42
1:B:619:THR:HG22	1:B:624:LEU:HD22	2.01	0.42
1:A:66:ASP:O	1:A:70:VAL:HG23	2.19	0.42
1:A:166:LYS:O	1:A:170:GLU:HB2	2.19	0.42
1:A:325:PRO:HD3	5:A:2033:HOH:O	2.18	0.42
1:A:487:SER:H	1:A:490:THR:CG2	2.32	0.42
1:B:155:VAL:HG13	1:B:155:VAL:O	2.20	0.42
1:A:350:ILE:HG12	1:A:362:GLN:HE21	1.83	0.42
1:B:627:GLU:CD	1:B:699:LYS:HE3	2.40	0.42
1:B:647:THR:CG2	1:B:653:LEU:HB3	2.49	0.42
1:B:373:GLY:HA2	1:B:787:PRO:HD2	2.02	0.42
1:A:37:ALA:HA	1:A:74:LEU:HD21	2.01	0.42
1:A:708:THR:CG2	1:A:711:GLY:N	2.83	0.42
1:B:16:THR:HG23	1:B:185:CYS:SG	2.60	0.42
1:B:805:LEU:O	1:B:807:GLU:N	2.53	0.42
1:A:157:ASP:HB3	1:A:206:LEU:HD13	2.02	0.41
1:B:307:ARG:NH2	5:B:2018:HOH:O	2.45	0.41
1:B:372:GLN:O	1:B:645:LEU:HD21	2.20	0.41
1:B:424:ARG:HG3	1:B:663:PHE:CG	2.55	0.41
3:A:1810:TLA:O41	3:A:1810:TLA:O2	2.38	0.41
1:B:225:ILE:HD13	1:B:257:PRO:HG2	2.01	0.41
1:B:766:MET:HB3	1:B:804:ARG:NH1	2.35	0.41
1:B:10:LEU:O	1:B:358:SER:HB2	2.20	0.41
1:B:67:SER:HB3	1:B:89:ASN:OD1	2.20	0.41
1:A:281[A]:ASP:O	1:A:282:LEU:CB	2.68	0.41
1:B:764:LEU:HD21	1:B:776:PRO:HD3	2.03	0.41
1:B:437:ILE:HD11	1:B:677:HIS:CD2	2.55	0.41
1:A:12:LEU:HB2	1:A:357:SER:O	2.20	0.41
1:B:12:LEU:HB2	1:B:357:SER:O	2.20	0.41
1:B:495:GLN:OE1	1:B:496:PRO:HD2	2.20	0.41
1:A:807:GLU:HB2	1:A:808:PHE:CE1	2.55	0.41
1:B:487:SER:H	1:B:490:THR:CG2	2.33	0.41
1:A:58:GLN:O	1:A:137:ALA:HA	2.21	0.41
1:A:744:LEU:HD12	1:A:744:LEU:O	2.20	0.41
1:B:34:GLY:HA3	1:B:293:PHE:CD1	2.55	0.41
1:B:208:ARG:N	1:B:209:PRO:CD	2.84	0.41
1:B:639:ILE:HA	1:B:657:LEU:O	2.21	0.41



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:766:MET:HE1	1:B:807:GLU:HG3	2.03	0.41
1:A:93:HIS:HA	1:A:114:CYS:O	2.19	0.41
4:A:1811:DTB:HCB1	1:B:222:LEU:CD1	2.50	0.41
1:B:514:ASN:HD22	1:B:728:SER:HA	1.85	0.41
1:B:593:VAL:CG1	1:B:594:ASP:N	2.84	0.41
1:B:11:PRO:HG2	1:B:172:MET:HG3	2.03	0.40
1:B:94:SER:HB3	1:B:116:LEU:HD11	2.03	0.40
1:A:146:LEU:HD23	1:A:146:LEU:HA	1.86	0.40
1:A:129:GLU:HG2	1:A:131:LEU:CD1	2.51	0.40
1:A:638:ASP:C	1:A:639:ILE:HG13	2.41	0.40
1:B:135:LEU:HD22	1:B:163:MET:HE2	2.04	0.40
1:B:626:VAL:HG12	1:B:713:THR:HG22	2.03	0.40
1:B:191:GLY:N	3:B:1809:TLA:O11	2.46	0.40
1:A:13:ASN:H	1:A:13:ASN:ND2	2.20	0.40
1:A:155:VAL:HG13	1:A:155:VAL:O	2.22	0.40
1:A:182:ASP:HB3	1:A:183:LEU:H	1.81	0.40
1:A:237:LEU:HD12	1:A:237:LEU:HA	1.93	0.40
1:A:445:LYS:CE	1:A:449:ASP:OD2	2.69	0.40
1:A:535:PHE:CG	1:A:541:ILE:HG12	2.57	0.40
1:A:615:ASP:OD1	1:A:615:ASP:C	2.58	0.40
1:B:535:PHE:CD1	1:B:535:PHE:N	2.66	0.40
1:B:614:PHE:CG	1:B:637:PRO:HB3	2.56	0.40
1:B:719:ASP:HB3	1:B:722:LEU:HB2	2.04	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	\mathbf{P}	erce	entile	\mathbf{es}
1	А	745/831~(90%)	687 (92%)	46 (6%)	12 (2%)		9	22	
1	В	736/831~(89%)	696 (95%)	33 (4%)	7 (1%)		15	34	



Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1481/1662~(89%)	1383~(93%)	79~(5%)	19 (1%)	12 27

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	490	THR
1	В	355	ASP
1	В	490	THR
1	А	373	GLY
1	А	561	LYS
1	В	45	SER
1	В	373	GLY
1	А	105	ASN
1	А	355	ASP
1	А	500	GLY
1	А	643	ALA
1	А	644	LYS
1	В	643	ALA
1	В	644	LYS
1	А	421	TRP
1	А	725	GLN
1	В	421	TRP
1	А	708	THR
1	А	103	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
1	А	622/704~(88%)	592~(95%)	30~(5%)	25	49
1	В	605/704~(86%)	575~(95%)	30~(5%)	24	47
All	All	1227/1408~(87%)	1167 (95%)	60~(5%)	26	49

All (60) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	А	10	LEU
1	А	13	ASN
1	А	63	SER
1	А	67	SER
1	А	74	LEU
1	А	109	SER
1	А	110	GLU
1	А	117	ASN
1	А	120	ASP
1	А	146	LEU
1	А	154	THR
1	А	193	VAL
1	А	253	VAL
1	А	281[A]	ASP
1	А	281[B]	ASP
1	А	308	LEU
1	А	317	LEU
1	А	321	VAL
1	А	370	TRP
1	А	384	ARG
1	А	417	VAL
1	А	428	SER
1	А	466	VAL
1	А	562	HIS
1	А	628	THR
1	А	655	VAL
1	А	664	ASP
1	А	713	THR
1	А	727	SER
1	А	764	LEU
1	В	10	LEU
1	В	63	SER
1	В	67	SER
1	В	74	LEU
1	В	120	ASP
1	В	146	LEU
1	В	154	THR
1	В	193	VAL
1	В	281[A]	ASP
1	В	281[B]	ASP
1	В	307	ARG
1	В	317	LEU
1	В	321	VAL



Mol	Chain	Res	Type
1	В	370	TRP
1	В	408	LYS
1	В	417	VAL
1	В	428	SER
1	В	466	VAL
1	В	501	ARG
1	В	535	PHE
1	В	539	ASP
1	В	562	HIS
1	В	624	LEU
1	В	628	THR
1	В	655	VAL
1	В	664	ASP
1	В	708	THR
1	В	709	SER
1	В	723	VAL
1	В	763	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	13	ASN
1	А	14	HIS
1	А	362	GLN
1	В	14	HIS
1	В	329	HIS
1	В	362	GLN
1	В	514	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.



5.6 Ligand geometry (i)

6 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		Pog Link		Bo	ond leng	ths	Bond angles			
1VIOI	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
4	DTB	А	1811	-	$15,\!15,\!15$	0.96	0	16, 19, 19	1.01	1 (6%)
2	PLP	А	1644	1	$15,\!15,\!16$	1.86	3 (20%)	$20,\!22,\!23$	1.70	2 (10%)
3	TLA	А	1810	-	9,9,9	2.04	2 (22%)	12,12,12	2.40	7 (58%)
4	DTB	В	1808	-	15,15,15	0.95	1 (6%)	16,19,19	1.46	2 (12%)
3	TLA	В	1809	-	9,9,9	2.08	5 (55%)	12,12,12	2.32	7 (58%)
2	PLP	В	1644	1	15,15,16	1.85	2 (13%)	20,22,23	1.76	1 (5%)

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
4	DTB	А	1811	-	-	7/8/20/20	0/1/1/1
2	PLP	А	1644	1	-	1/6/6/8	0/1/1/1
3	TLA	А	1810	-	-	4/12/12/12	-
4	DTB	В	1808	-	-	5/8/20/20	0/1/1/1
3	TLA	В	1809	-	-	4/12/12/12	-
2	PLP	В	1644	1	-	1/6/6/8	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
2	В	1644	PLP	O3-C3	-5.81	1.23	1.37
2	А	1644	PLP	O3-C3	-5.71	1.23	1.37
3	А	1810	TLA	C3-C4	-3.82	1.47	1.52
3	В	1809	TLA	C2-C1	-3.46	1.47	1.52
3	А	1810	TLA	O3-C3	-2.96	1.36	1.42
2	А	1644	PLP	C2-N1	2.57	1.38	1.33



Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
2	А	1644	PLP	C6-N1	2.44	1.39	1.34
2	В	1644	PLP	C2-N1	2.25	1.38	1.33
3	В	1809	TLA	O2-C2	-2.22	1.37	1.42
4	В	1808	DTB	OI2-C	-2.20	1.23	1.30
3	В	1809	TLA	O11-C1	-2.17	1.23	1.30
3	В	1809	TLA	O41-C4	-2.13	1.23	1.30
3	В	1809	TLA	O1-C1	2.04	1.28	1.22

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
2	В	1644	PLP	O4P-C5A-C5	6.26	121.27	109.35
2	А	1644	PLP	O4P-C5A-C5	5.51	119.86	109.35
3	А	1810	TLA	C3-C2-C1	-4.18	100.54	109.87
4	В	1808	DTB	CD-CE-CR	-3.75	106.26	113.93
3	В	1809	TLA	O1-C1-C2	-3.31	112.94	121.63
3	В	1809	TLA	C2-C3-C4	-3.27	102.56	109.87
3	А	1810	TLA	O4-C4-C3	-3.19	113.25	121.63
3	В	1809	TLA	C3-C2-C1	-3.18	102.78	109.87
3	В	1809	TLA	O4-C4-C3	-3.11	113.44	121.63
3	А	1810	TLA	O1-C1-C2	-3.06	113.58	121.63
3	А	1810	TLA	O11-C1-C2	2.88	121.06	113.27
3	В	1809	TLA	O41-C4-C3	2.81	120.86	113.27
3	А	1810	TLA	O2-C2-C1	2.68	116.27	110.66
3	В	1809	TLA	O11-C1-C2	2.67	120.50	113.27
3	А	1810	TLA	O41-C4-C3	2.60	120.31	113.27
2	А	1644	PLP	O3P-P-O4P	-2.53	100.01	106.73
4	В	1808	DTB	CR-N2-CN	-2.41	109.31	112.46
3	А	1810	TLA	C2-C3-C4	-2.32	104.70	109.87
3	В	1809	TLA	O3-C3-C4	2.06	114.98	110.66
4	А	1811	DTB	CS-CR-N2	-2.03	99.63	102.17

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms
3	А	1810	TLA	O3-C3-C4-O4
3	А	1810	TLA	O3-C3-C4-O41
3	В	1809	TLA	O1-C1-C2-O2
3	В	1809	TLA	O11-C1-C2-O2
4	А	1811	DTB	C-CA-CB-CG
4	А	1811	DTB	CE-CD-CG-CB



Mol

4

4

4

3

3

4

2

 $\overline{2}$

3

4

4

3

4

4

4

4

Atoms
CG-CD-CE-CR
CA-CB-CG-CD
CE-CD-CG-CB
O1-C1-C2-C3
O11-C1-C2-C3
CG-CD-CE-CR
C5A-O4P-P-O1P

C5A-O4P-P-O1P

01-C1-C2-C3

OI1-C-CA-CB

OI2-C-CA-CB

O11-C1-C2-C3

OI2-C-CA-CB

OI1-C-CA-CB CD-CE-CR-CS

CD-CE-CR-CS

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 \mathbf{Res}

1808

1811

1808

1809

1809

1811

1644

1644

1810

1808

1808

1810

1811

1811

1811

1808

Type DTB

DTB

DTB

TLA

TLA DTB

PLP

PLP

TLA

DTB

DTB

TLA

DTB

DTB

DTB

DTB

Chain

В

А

В

В

В

А

А

В

А

В

В

А

А

А

A B

There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	А	1811	DTB	2	0
2	А	1644	PLP	1	0
3	А	1810	TLA	3	0
4	В	1808	DTB	5	0
3	В	1809	TLA	4	0
2	В	1644	PLP	1	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, 95^{th} 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 $>$	#RS	$\mathbf{RZ}>$	-2	$OWAB(Å^2)$	Q<0.9
1	А	755/831~(90%)	-0.02	24 (3%)	47	47	15, 31, 68, 94	0
1	В	748/831~(90%)	-0.03	25 (3%)	46	45	14, 30, 68, 94	0
All	All	1503/1662~(90%)	-0.03	49 (3%)	46	45	14, 31, 68, 94	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	488	PRO	5.1
1	А	709	SER	3.9
1	В	563	LEU	3.8
1	А	492	PHE	3.7
1	А	451	ASN	3.7
1	В	99	ALA	3.6
1	В	806	GLY	3.6
1	А	333	HIS	3.6
1	В	446	PHE	3.1
1	А	708	THR	3.1
1	А	710	GLN	3.0
1	В	559	LEU	3.0
1	В	661	ALA	2.9
1	А	493	LEU	2.9
1	А	758	LEU	2.8
1	В	463	VAL	2.7
1	В	575	VAL	2.7
1	А	759	TYR	2.7
1	В	668	GLY	2.7
1	А	117	ASN	2.7
1	А	450	HIS	2.6
1	В	607	ASN	2.6
1	В	730	SER	2.6
1	В	669	ASP	2.5



Mol	Chain	Res	Type	RSRZ
1	В	489	TYR	2.5
1	А	334	GLN	2.5
1	А	332	VAL	2.4
1	А	354	SER	2.4
1	В	449	ASP	2.4
1	А	330	LYS	2.4
1	В	807	GLU	2.4
1	В	759	TYR	2.3
1	В	492	PHE	2.3
1	А	806	GLY	2.2
1	В	96	LEU	2.2
1	В	761	LYS	2.2
1	А	45	SER	2.2
1	А	431	GLY	2.2
1	В	448	VAL	2.1
1	В	608	ARG	2.1
1	В	802	TYR	2.1
1	А	574	HIS	2.1
1	А	335	GLU	2.1
1	В	609	LYS	2.1
1	В	760	ALA	2.1
1	А	668	GLY	2.1
1	А	608	ARG	2.1
1	А	428	SER	2.1
1	А	609	LYS	2.0

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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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
3	TLA	А	1810	10/10	0.94	0.16	7,28,39,45	0
3	TLA	В	1809	10/10	0.94	0.16	22,37,47,56	0
4	DTB	В	1808	15/15	0.95	0.20	2,23,45,51	0
2	PLP	В	1644	15/16	0.97	0.18	15,31,36,40	0
4	DTB	А	1811	15/15	0.97	0.18	5,33,64,71	0
2	PLP	А	1644	15/16	0.97	0.21	16,31,39,40	0

6.5 Other polymers (i)

There are no such residues in this entry.

