



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:31 am GMT

PDB ID : 4A0R  
Title : Structure of bifunctional DAPA aminotransferase-DTB synthetase from *Arabidopsis 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

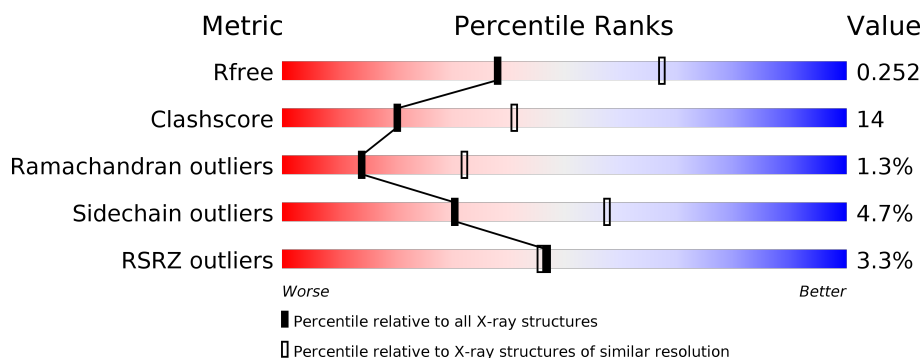
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.68 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))
$R_{free}$	100719	3050 (2.70-2.66)
Clashscore	112137	3418 (2.70-2.66)
Ramachandran outliers	110173	3367 (2.70-2.66)
Sidechain outliers	110143	3367 (2.70-2.66)
RSRZ outliers	101464	3069 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	831	
1	B	831	

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	B	1809	-	-	X	-
4	DTB	A	1811	-	-	-	X
4	DTB	B	1808	-	-	-	X

## 2 Entry composition

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-OXONONANOATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	755	Total	C	N	O	S	0	2	0
			5788	3703	974	1079	32			
1	B	748	Total	C	N	O	S	0	2	0
			5704	3652	961	1059	32			

There are 40 discrepancies between the modelled and reference sequences:

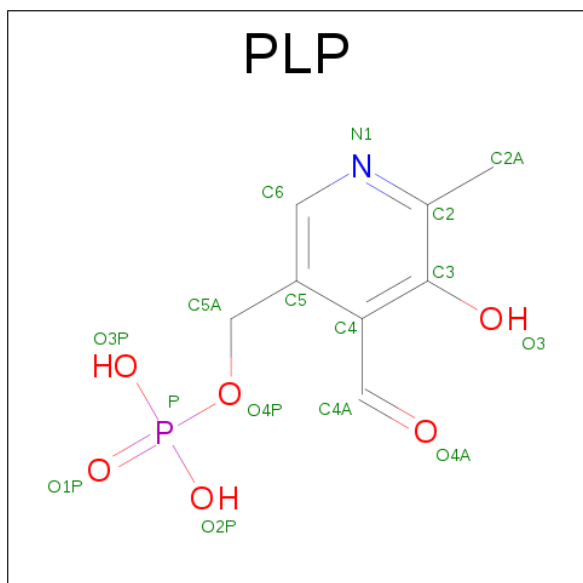
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	GLY	-	EXPRESSION TAG	UNP B0F481
A	-18	SER	-	EXPRESSION TAG	UNP B0F481
A	-17	SER	-	EXPRESSION TAG	UNP B0F481
A	-16	HIS	-	EXPRESSION TAG	UNP B0F481
A	-15	HIS	-	EXPRESSION TAG	UNP B0F481
A	-14	HIS	-	EXPRESSION TAG	UNP B0F481
A	-13	HIS	-	EXPRESSION TAG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

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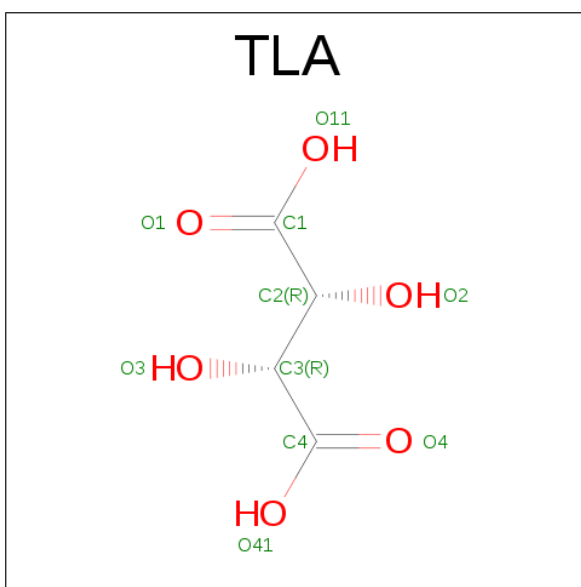
Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	HIS	-	EXPRESSION TAG	UNP B0F481
B	-14	HIS	-	EXPRESSION TAG	UNP B0F481
B	-13	HIS	-	EXPRESSION TAG	UNP B0F481
B	-12	HIS	-	EXPRESSION TAG	UNP B0F481
B	-11	HIS	-	EXPRESSION TAG	UNP B0F481
B	-10	SER	-	EXPRESSION TAG	UNP B0F481
B	-9	SER	-	EXPRESSION TAG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

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



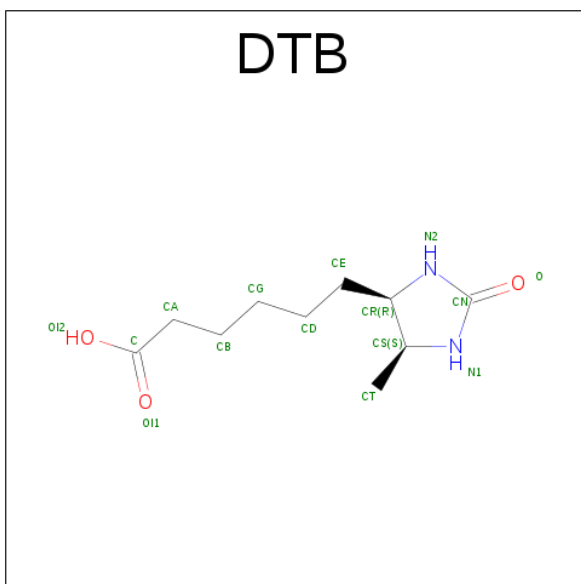
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	4	6		
3	B	1	Total	C	O	0	0
			10	4	6		

- 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	A	1	Total	C	N	O	0	0
			15	10	2	3		

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	70	Total	O	0	0
			70	70		
5	B	51	Total	O	0	0
			51	51		





ASP	K644	E540	D449	V321	L168	L74
ALA	L645	I541	F542	H329	M172	R80
SER	L646	T647	CYS	V332	GLU	
ASN	G648	G649	ALA	V340	CYS	I85
GLY	M650	S556	THR	I350	GLY	S86
TYR	V651	A557	GLU	I350	VAL	I87
SER	P652	Y558	GLU	I350	LYS	S88
ALA	L653	L559	GLU	I350	SER	N89
L758	A654	S560	LYS	S354	GLU	S90
Y759	V655	K561	HIS	D355	LYS	V91
A760	T656	H562	LYS	K356	SER	L92
S762	L657	L563	V462	S357	D182	H93
L763	A658	Q564	V464	S358	L183	S94
L764	T659	GLU	K465	L359	L184	S95
I765	D660	HIS	V466		C185	L96
M766	V661	SER		Q362	L186	P97
L767	V662	GLY	L478		V187	A98
R768	F663	VAL		A365		A99
	D664	ARG	E482		G191	K100
F773	S665	GLN		W370	G192	S101
T774	F666	SER	S487	T371	V193	L102
R775	S667	A573	P488	Q372	A194	GLY
P776	G668	H574	Y489	G373		LEU
L777	D669	V575	T490	P374	L206	ASN
			G491		Y207	VAL
P787	H677		F492	L382	R208	GLU
			L493		P209	VAL
Y802	K699	V593	Q494	V396		SER
L803	D700	D594	Q495	M397	L222	GLU
R804	G710	P595	P496	F398		SER
L805	T703	L596	W497	P399	I225	G112
G806		F597			S226	M113
E807	T708	Q598	R501	L407		
PHE	S709	R599	G502	K408	D241	L116
ASN	Q710		V510		I242	
ARG	G711			L414	V256	D120
THR	K712		N514	V417	P257	A127
	T713		G515	W421	L269	L130
	L714		S516			
			V517		D281	T134
	D719		P522		L282	L135
E720	F617		F525		I283	Y136
L721	L624		S526		E284	
L722	GLU		GLU	T433	F293	E139
Q723	G625		ILE	I437	L296	L146
Q724	V626		ALA		K297	
Q725	E627		PRO	K440		E151
S728	T628		GLU	M441		N152
H729			TYR	A442	R307	A153
S730			GLY	F443	L308	T154
	V737		T534	R444	V155	
			F535	V445	E156	
L744				F446	D157	
K747	A748		R538	V448		M163
			D539		E322	

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	246.67Å 76.63Å 79.84Å 90.00° 108.02° 90.00°	Depositor
Resolution (Å)	40.44 – 2.68 40.72 – 2.68	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.44-2.68) 99.5 (40.72-2.68)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 2.69Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.184 , 0.259 0.178 , 0.252	Depositor DCC
$R_{free}$ test set	2000 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.6	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 65.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.027 for -h+k-l,-l,-k 0.005 for -h-k-l,l,k 0.023 for -h-2*l,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11693	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DTB, TLA, PLP

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	0.48	1/5922 (0.0%)	0.64	3/8050 (0.0%)
1	B	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	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	307	ARG	CZ-NH1	-11.03	1.18	1.33
1	A	307	ARG	CZ-NH1	-9.79	1.20	1.33
1	B	307	ARG	CZ-NH2	-5.56	1.25	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	307	ARG	NE-CZ-NH2	17.58	129.09	120.30
1	B	307	ARG	NE-CZ-NH2	16.14	128.37	120.30
1	B	307	ARG	NH1-CZ-NH2	-8.37	110.19	119.40
1	A	44	PRO	N-CA-CB	6.33	110.90	103.30
1	A	307	ARG	NH1-CZ-NH2	-5.93	112.87	119.40
1	B	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	B	45	SER	Peptide

## 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	5788	0	5697	161	0
1	B	5704	0	5585	181	0
2	A	15	0	6	1	0
2	B	15	0	6	1	0
3	A	10	0	3	3	0
3	B	10	0	4	4	0
4	A	15	0	17	2	0
4	B	15	0	17	5	0
5	A	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:O	1:A:490:THR:HG23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:HIS:HB2	1:B:172:MET:HE3	1.55	0.86
1:B:42:GLN:HA	1:B:42:GLN:OE1	1.75	0.84
1:A:659:THR:HG22	1:A:661:ALA:N	1.95	0.81
1:A:317:LEU:HD23	1:B:407:LEU:HD11	1.62	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:428:SER:HB2	1:A:433:THR:OG1	1.99	0.62
1:A:96:LEU:HB3	1:A:97:PRO:HD3	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:766:MET:CB	1:A:804:ARG:HD2	2.31	0.60
1:A:414:LEU:CD1	1:B:321:VAL:HG22	2.32	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:706:ASN:O	1:A:714:LEU:HA	2.04	0.57
1:A:96:LEU:HD22	1:A:108:VAL:HG21	1.86	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:104:LEU:O	1:A:105:ASN:C	2.43	0.57
1:A:87:ILE:HG22	1:A:130:LEU:HB3	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:194:ALA:HB3	1:B:226:SER:HA	1.92	0.51
1:A:28:LYS:NZ	3:A:1810:TLA:H3	2.26	0.51
1:B:370:TRP:N	1:B:370:TRP:CD1	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:CG2	1:A:660:ASP:N	2.73	0.51
1:A:659:THR:HG22	1:A:660:ASP:N	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:N	1:A:370:TRP:CD1	2.80	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:B:97:PRO:HA	1:B:100:LYS:HE2	1.95	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: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:325:PRO:HG2	1:B:399:PRO:HG3	1.95	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:441:MET:HE3	1:B:639:ILE:HG12	1.96	0.47
1:B:85:ILE:HA	1:B:127:ALA:HB1	1.95	0.47
1:A:97:PRO:HA	1:A:100:LYS:HE2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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: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:B:91:VAL:HG22	1:B:134:THR:HB	1.97	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: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:A:482:GLU:HB2	1:B:497:TRP:CZ3	2.50	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
4:B:1808:DTB:HCS	3:B:1809:TLA:C1	2.46	0.45
1:B:93:HIS:CB	1:B:113:MET:HE1	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:B:157:ASP:HB3	1:B:206:LEU:HD13	1.99	0.44
1:A:321:VAL:HG22	1:B:414:LEU:HD12	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:HA	1:B:146:LEU:HD23	1.82	0.44
1:B:183:LEU:HD23	1:B:184:LEU:N	2.33	0.44
1:A:297:LYS:HE2	1:A:297:LYS:HB3	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:627:GLU:CD	1:A:699:LYS:HE3	2.39	0.43
1:A:88:SER:HA	1:A:120:ASP:O	2.17	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:617:VAL:HG11	2:A:1644:PLP:C5	2.48	0.43
1:B:113:MET:HB3	1:B:113:MET:HE2	1.77	0.43
1:A:497:TRP:CD1	1:B:501:ARG:CD	3.02	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:C	1:B:744:LEU:HD12	2.39	0.43
1:A:541:ILE:HG22	1:A:595:PRO:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:C	1:A:700:ASP:OD1	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: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:A:66:ASP:O	1:A:70:VAL:HG23	2.19	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:B:208:ARG:N	1:B:209:PRO:CD	2.84	0.41
1:B:34:GLY:HA3	1:B:293:PHE:CD1	2.55	0.41
1:A:58:GLN:O	1:A:137:ALA:HA	2.21	0.41
1:A:744:LEU:O	1:A:744:LEU:HD12	2.20	0.41
1:B:639:ILE:HA	1:B:657:LEU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:94:SER:HB3	1:B:116:LEU:HD11	2.03	0.40
1:B:11:PRO:HG2	1:B:172:MET:HG3	2.03	0.40
1:A:146:LEU:HA	1:A:146:LEU:HD23	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:O	1:A:155:VAL:HG13	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	Percentiles	
1	A	745/831 (90%)	687 (92%)	46 (6%)	12 (2%)	11	26
1	B	736/831 (89%)	696 (95%)	33 (4%)	7 (1%)	18	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1481/1662 (89%)	1383 (93%)	79 (5%)	19 (1%)	14	32

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	490	THR
1	B	355	ASP
1	B	490	THR
1	A	373	GLY
1	A	561	LYS
1	B	45	SER
1	B	373	GLY
1	A	105	ASN
1	A	355	ASP
1	A	500	GLY
1	A	643	ALA
1	A	644	LYS
1	B	643	ALA
1	B	644	LYS
1	A	421	TRP
1	A	725	GLN
1	B	421	TRP
1	A	708	THR
1	A	103	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	622/704 (88%)	592 (95%)	30 (5%)	30	56
1	B	605/704 (86%)	575 (95%)	30 (5%)	28	54
All	All	1227/1408 (87%)	1167 (95%)	60 (5%)	30	55

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

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

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

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

Mol	Chain	Res	Type
1	A	13	ASN
1	A	14	HIS
1	A	362	GLN
1	B	14	HIS
1	B	329	HIS
1	B	362	GLN
1	B	514	ASN

### 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

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	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PLP	A	1644	1	15,15,16	1.84	3 (20%)	20,22,23	1.64	2 (10%)
3	TLA	A	1810	-	3,9,9	1.94	1 (33%)	6,12,12	3.07	3 (50%)
4	DTB	A	1811	-	12,15,15	0.82	1 (8%)	12,19,19	1.07	1 (8%)
2	PLP	B	1644	1	15,15,16	1.86	3 (20%)	20,22,23	1.70	1 (5%)
4	DTB	B	1808	-	12,15,15	0.82	0	12,19,19	1.73	2 (16%)
3	TLA	B	1809	-	3,9,9	1.70	1 (33%)	6,12,12	2.93	2 (33%)

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	PLP	A	1644	1	-	0/6/6/8	0/1/1/1
3	TLA	A	1810	-	-	0/4/12/12	0/0/0/0
4	DTB	A	1811	-	-	0/6/20/20	0/1/1/1
2	PLP	B	1644	1	-	0/6/6/8	0/1/1/1
4	DTB	B	1808	-	-	0/6/20/20	0/1/1/1
3	TLA	B	1809	-	-	0/4/12/12	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1644	PLP	O3-C3	-5.86	1.23	1.37
2	A	1644	PLP	O3-C3	-5.75	1.23	1.37
3	A	1810	TLA	O3-C3	-3.28	1.36	1.42
3	B	1809	TLA	O2-C2	-2.53	1.37	1.42
4	A	1811	DTB	CN-N1	-2.14	1.32	1.35
2	B	1644	PLP	C3-C2	-2.08	1.39	1.40
2	B	1644	PLP	C2-N1	2.03	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1644	PLP	C2-N1	2.32	1.38	1.33
2	A	1644	PLP	C6-N1	2.40	1.39	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1810	TLA	C1-C2-C3	-5.84	100.54	113.11
3	B	1809	TLA	C4-C3-C2	-4.90	102.56	113.11
3	B	1809	TLA	C1-C2-C3	-4.80	102.78	113.11
3	A	1810	TLA	C4-C3-C2	-3.91	104.70	113.11
4	B	1808	DTB	CD-CE-CR	-3.71	106.26	114.01
4	B	1808	DTB	CR-N2-CN	-2.88	109.31	112.45
2	A	1644	PLP	O3P-P-O4P	-2.53	100.01	106.73
4	A	1811	DTB	CS-CR-N2	-2.06	99.63	102.09
3	A	1810	TLA	O2-C2-C1	2.11	116.27	111.13
2	A	1644	PLP	O4P-C5A-C5	5.24	119.86	109.32
2	B	1644	PLP	O4P-C5A-C5	5.94	121.27	109.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1644	PLP	1	0
3	A	1810	TLA	3	0
4	A	1811	DTB	2	0
2	B	1644	PLP	1	0
4	B	1808	DTB	5	0
3	B	1809	TLA	4	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	755/831 (90%)	-0.02	24 (3%)	48 47	15, 31, 68, 94	0
1	B	748/831 (90%)	-0.03	25 (3%)	47 46	14, 30, 68, 94	0
All	All	1503/1662 (90%)	-0.03	49 (3%)	47 46	14, 31, 68, 94	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	488	PRO	5.2
1	A	709	SER	3.9
1	B	563	LEU	3.8
1	A	492	PHE	3.7
1	A	451	ASN	3.7
1	B	99	ALA	3.6
1	B	806	GLY	3.6
1	A	333	HIS	3.6
1	B	446	PHE	3.2
1	A	708	THR	3.1
1	A	710	GLN	3.1
1	B	559	LEU	3.0
1	B	661	ALA	2.9
1	A	493	LEU	2.9
1	A	758	LEU	2.8
1	B	463	VAL	2.7
1	B	575	VAL	2.7
1	A	759	TYR	2.7
1	B	668	GLY	2.7
1	A	117	ASN	2.7
1	A	450	HIS	2.6
1	B	607	ASN	2.5
1	B	730	SER	2.5
1	B	669	ASP	2.5

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

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	DTB	A	1811	15/15	0.97	0.18	2.78	5,33,64,71	0
4	DTB	B	1808	15/15	0.95	0.21	2.25	2,23,45,51	0
3	TLA	A	1810	10/10	0.94	0.16	0.70	7,28,39,45	0
3	TLA	B	1809	10/10	0.94	0.16	0.21	22,37,47,56	0
2	PLP	A	1644	15/16	0.97	0.21	0.14	16,31,39,40	0
2	PLP	B	1644	15/16	0.97	0.18	-0.32	15,31,36,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.