Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:38 PM 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

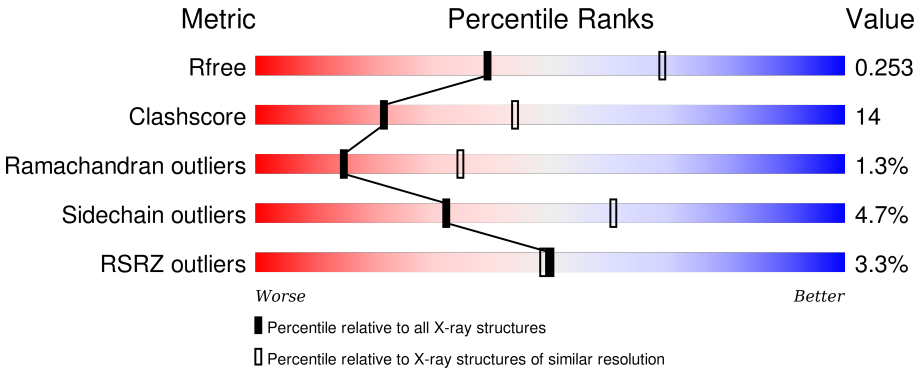
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	2780 (2.70-2.66)
Clashscore	102246	3138 (2.70-2.66)
Ramachandran outliers	100387	3089 (2.70-2.66)
Sidechain outliers	100360	3089 (2.70-2.66)
RSRZ outliers	91569	2789 (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 >=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 <=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	3% 67% 22% • 9%
1	B	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	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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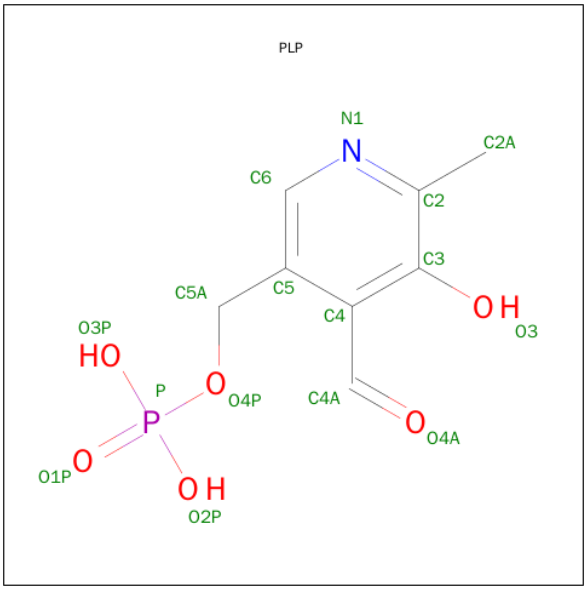
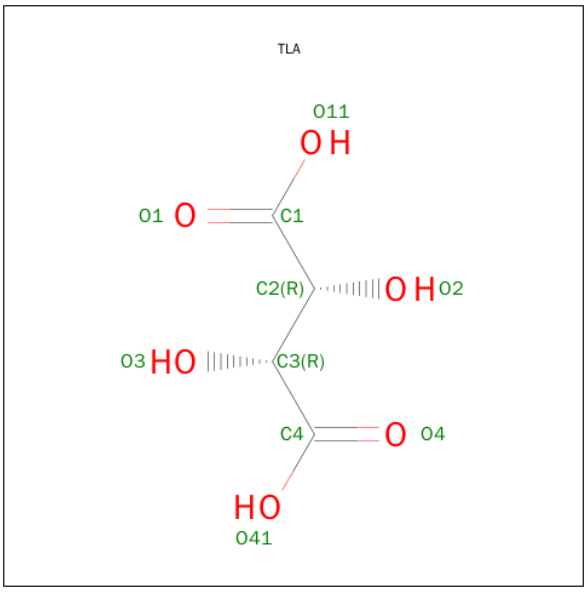
Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	HIS	-	EXPRESSION TAG	UNP B0F481
B	-14	HIS	-	EXPRESSION TAG	UNP B0F481
B	-13	HIS	-	EXPRESSION TAG	UNP B0F481
B	-12	HIS	-	EXPRESSION TAG	UNP B0F481
B	-11	HIS	-	EXPRESSION TAG	UNP B0F481
B	-10	SER	-	EXPRESSION TAG	UNP B0F481
B	-9	SER	-	EXPRESSION TAG	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: $C_8H_{10}NO_6P$).



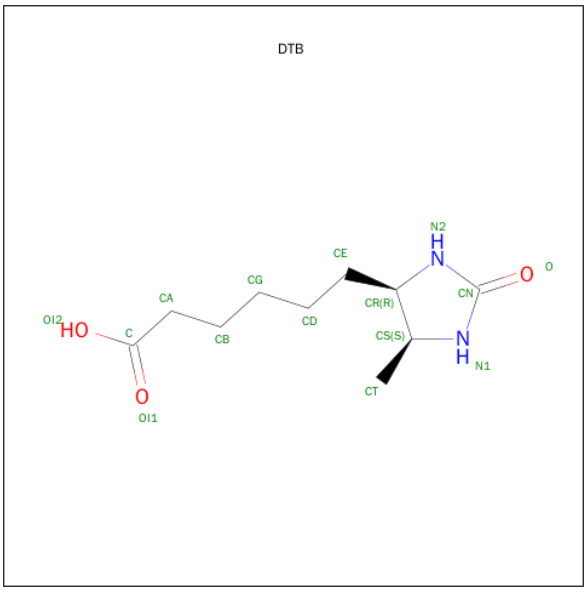
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- 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 10 4 6	0	0
3	B	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	A	1	Total C N O 15 10 2 3	0	0

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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.

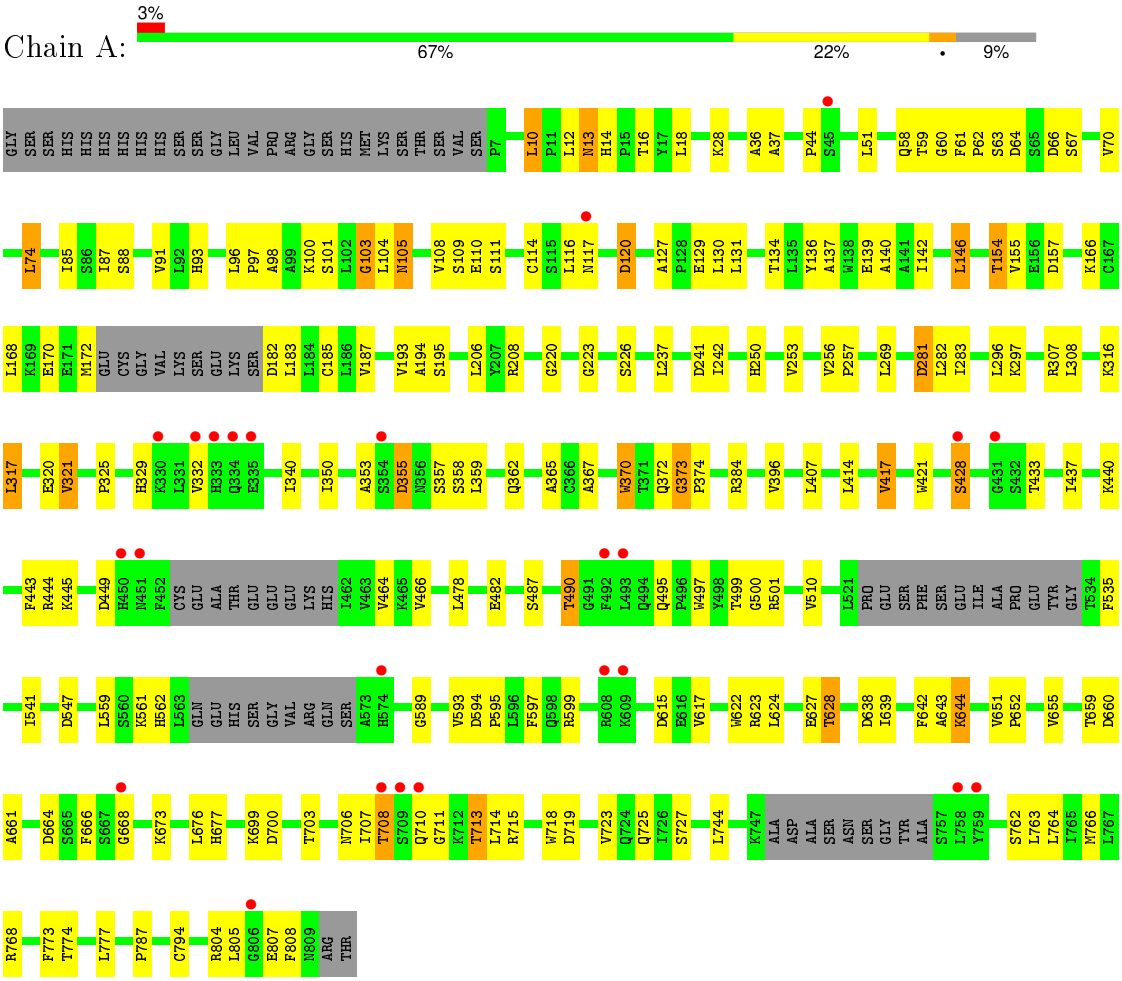
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	70	Total	O	0	0
			70	70		
5	B	51	Total	O	0	0
			51	51		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (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.

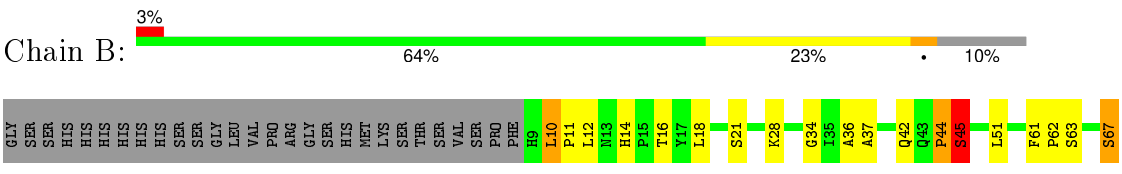
• Molecule 1: ADENOSYLMETHIONINE-8-AMINO-7-OXONONANOATE AMINOTRANSFERASE

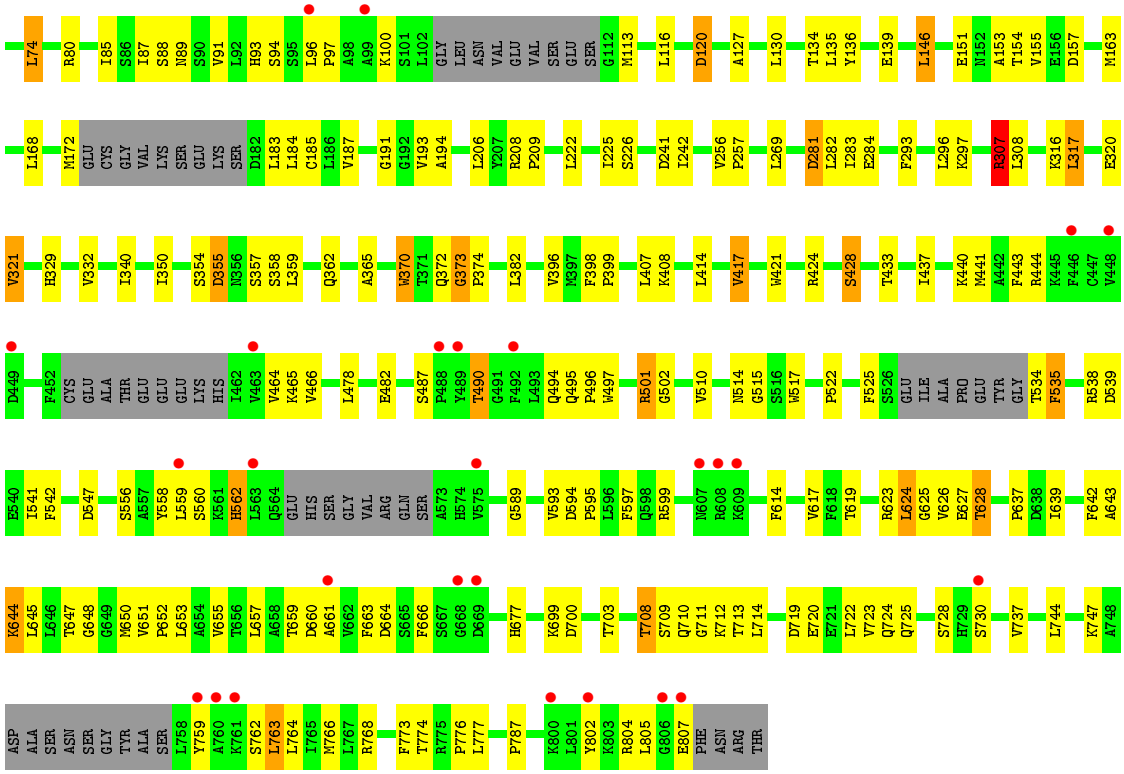
Chain A:



• Molecule 1: ADENOSYLMETHIONINE-8-AMINO-7-OXONONANOATE AMINOTRANSFERASE

Chain B:




L74 R80 I85 S86 I87 S88 N89 S90 V91 L92 H93 S94 S95 L96 P97 A98 A99 K100 S101 L102 G112 M113 L116 D120 A127 L130 T134 L135 Y136 E139 L146 E151 N152 A153 T154 V155 E156 D157 M163
L168 M172 E182 C185 L186 V187 G191 G192 V193 A194 L206 Y207 R208 P209 L222 I225 S226 D241 I242 V256 P257 L269 D281 L282 I283 E284 F293 L296 K297 R307 I308 K316 L317 E320
V321 H329 V332 I340 I350 S354 D355 N356 S357 S358 L359 Q362 A365 W370 T371 Q372 G373 P374 L382 V396 N397 F398 P399 L407 K408 L414 V417 W421 R424 S428 T433 I437 K440 M441 A442 F443 R444 K445 F446 C447 V448
D449 F452 R462 V463 V464 K465 V466 L478 E482 S487 P488 Y489 T490 G491 F492 L493 Q494 Q495 P496 W497 R501 G502 V510 N514 G515 S516 W517 P522 F525 S526 I534 F535 R538 D539
E540 I541 F542 D547 S556 A557 Y558 L559 S560 K561 H562 L563 Q564 A573 H574 V575 G589 V593 D594 P595 L596 F597 Q598 R599 M607 R608 K609 F614 V617 F618 T619 R623 L624 G625 V626 E627 T628 P637 D638 I639 F642 A643
K644 L645 L646 T647 G648 G649 M650 V651 P652 L653 A654 V655 T656 L657 A658 T659 D660 A661 V662 F663 D664 S665 F666 S667 G668 D669 H677 K699 D700 T703 T708 S709 Q710 G711 K712 T713 L714 D719 E720 E721 L722 V723 Q724 Q725 S728 H729 S730 V737 L744 K747 A748
ASP ALA SER ASN SER GLY TYR ALA SER L758 Y759 A760 K761 S762 L763 L764 I765 M766 L767 R768 F773 T774 R775 P776 L777 P787 K800 L801 Y802 K803 R804 L805 G806 E807 PHE ASN ARG THR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	1.90 (at 2.69Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.184 , 0.259 0.184 , 0.253	Depositor DCC
R_{free} test set	2000 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	34.6	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 65.7	EDS
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
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 39935 reflections	Xtriage
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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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(^{o})	Ideal(^{o})
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:B:522:PRO:CG	1:B:525:PHE:HD2	1.93	0.80
1:A:340:ILE:HG21	1:B:396:VAL:HG11	1.61	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:B:708:THR:HG23	1:B:710:GLN:H	1.64	0.62
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:A:223:GLY:N	4:B:1808:DTB:HCA1	2.15	0.62
1:A:396:VAL:CG1	1:B:340:ILE:HD13	2.30	0.61
1:A:168:LEU:O	1:A:172:MET:HG2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:490:THR:CG2	1:B:490:THR:O	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: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: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:B:804:ARG:O	1:B:807:GLU:HG2	2.06	0.55
1:A:766:MET:HE3	1:A:807:GLU:HG3	1.87	0.55
1:A:142:ILE:HD12	1:A:146:LEU:HB3	1.88	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:B:443:PHE:CD1	1:B:464:VAL:HG11	2.42	0.54
1:A:497:TRP:CD1	1:B:501:ARG:HD2	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:B:766:MET:CB	1:B:804:ARG:HD2	2.37	0.54
1:B:444:ARG:HG3	1:B:666:PHE:CZ	2.43	0.54
1:A:617:VAL:HG12	1:A:644:LYS:NZ	2.23	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:B:766:MET:HE2	1:B:804:ARG:NH1	2.22	0.52
1:A:208:ARG:HD2	1:A:208:ARG:O	2.10	0.52
1:B:730:SER:O	1:B:747:LYS:NZ	2.36	0.51
1:A:256:VAL:HB	1:A:257:PRO:HD3	1.91	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:B:370:TRP:N	1:B:370:TRP:CD1	2.78	0.51
1:A:28:LYS:NZ	3:A:1810:TLA:H3	2.26	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:B:113:MET:HG2	1:B:153:ALA:HB1	1.93	0.51
1:A:706:ASN:O	1:A:715:ARG:N	2.43	0.51
1:A:10:LEU:O	1:A:358:SER:HB2	2.11	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:B:517:TRP:CE2	1:B:538:ARG:HB2	2.47	0.50
1:A:744:LEU:C	1:A:744:LEU:HD12	2.33	0.50
1:B:659:THR:HG22	1:B:660:ASP:N	2.27	0.50
1:B:766:MET:HE3	1:B:807:GLU:HG3	1.93	0.49
1:B:281[A]:ASP:O	1:B:282:LEU:HB2	2.12	0.49
1:A:805:LEU:O	1:A:808:PHE:N	2.45	0.49
1:B:534:THR:HG22	1:B:534:THR:O	2.10	0.49
1:A:195:SER:HB3	4:A:1811:DTB:HCA1	1.94	0.49
1:B:659:THR:CG2	1:B:660:ASP:N	2.75	0.49
1:B:623:ARG:HG3	1:B:624:LEU:HD13	1.92	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:B:93:HIS:HB2	1:B:136:TYR:CD1	2.48	0.49
1:A:93:HIS:HB2	1:A: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: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:B:437:ILE:O	1:B:441:MET:HG3	2.13	0.48
1:B:759:TYR:O	1:B:762:SER:HB2	2.13	0.48
1:A:497:TRP:O	1:A:499:THR:HG23	2.14	0.48
1:B:308:LEU:HD11	1:B:357:SER:HB3	1.95	0.48
1:A:804:ARG:O	1:A:807:GLU:HG2	2.12	0.48
1:A:623:ARG:HG3	1:A:624:LEU:HD13	1.95	0.48
1:B:350:ILE:HG12	1:B:362:GLN:HE21	1.79	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: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:510:VAL:HG11	1:A:541:ILE:HD13	1.95	0.48
1:B:720:GLU:O	1:B:724:GLN:HG2	2.14	0.48
1:B:478:LEU:O	1:B:482:GLU:HG2	2.14	0.48
1:A:589:GLY:HA2	1:A:777:LEU:HD22	1.95	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:374:PRO:HD3	1:B:648:GLY:O	2.15	0.47
1:B:297:LYS:HB3	1:B:297:LYS:HE2	1.72	0.47
1:B:91:VAL:HG22	1:B:134:THR:HB	1.97	0.47
1:B:93:HIS:HB3	1:B:113:MET:HE1	1.96	0.47
1:A:627:GLU:OE2	1:A:699:LYS:HE3	2.15	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:805:LEU:O	1:A:808:PHE:HD1	1.98	0.46
1:A:495:GLN:HE21	1:B:440:LYS:HE2	1.80	0.46
1:A:373:GLY:HA2	1:A:787:PRO:HD2	1.96	0.46
1:B:517:TRP:NE1	1:B:538:ARG:HB2	2.30	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:85:ILE:HA	1:A:127:ALA:HB1	1.97	0.46
1:A:700:ASP:HB3	1:A:703:THR:OG1	2.16	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:478:LEU:HD13	1:A:495:GLN:HG2	1.96	0.46
1:A:367:ALA:HB1	1:A:372:GLN:HB2	1.97	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:B:61:PHE:O	1:B:139:GLU:HA	2.17	0.45
1:A:478:LEU:O	1:A:482:GLU:HG2	2.16	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:HD13	1:A:296:LEU:HD13	1.99	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:B:398:PHE:HB3	1:B:399:PRO:HD3	1.99	0.45
1:B:208:ARG:HD2	1:B:208:ARG:O	2.17	0.45
1:A:226:SER:HA	1:B:194:ALA:HB3	1.98	0.45
1:B:708:THR:CG2	1:B:711:GLY:H	2.29	0.45
1:B:441:MET:CE	1:B:639:ILE:HG23	2.47	0.45
1:A:353:ALA:C	1:A:355:ASP:H	2.19	0.45
1:A:708:THR:CG2	1:A:711:GLY:H	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:LYS:HZ3	3:A:1810:TLA:H3	1.81	0.45
1:A:497:TRP:NE1	1:B:501:ARG:HD2	2.33	0.44
1:A:281[A]:ASP:HB3	1:A:283:ILE:HG12	1.99	0.44
1:A:763:LEU:HA	1:A:763:LEU:HD23	1.65	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:241:ASP:O	1:A:242:ILE:HD13	2.17	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:321:VAL:HG22	1:B:414:LEU:CD1	2.46	0.44
1:B:183:LEU:HD23	1:B:184:LEU:N	2.33	0.44
1:B:146:LEU:HA	1:B:146:LEU:HD23	1.82	0.44
1:A:220:GLY:O	1:A:250:HIS:HB2	2.18	0.44
1:B:354:SER:O	1:B:355:ASP:O	2.36	0.44
1:A:297:LYS:HE2	1:A:297:LYS:HB3	1.72	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:A:111:SER:HB2	1:A:154:THR:HG22	1.99	0.44
1:B:708:THR:CG2	1:B:710:GLN:HB2	2.48	0.44
1:B:136:TYR:OH	1:B:163:MET:HG3	2.18	0.44
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: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: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: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:617:VAL:HG11	2:A:1644:PLP:C5	2.48	0.43
1:A:417:VAL:HG11	1:A:642:PHE:CZ	2.54	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: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:91:VAL:HG22	1:A:134:THR:HB	2.00	0.43
1:A:808:PHE:CD1	1:A:808:PHE:N	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:725:GLN:HB3	1:B:802:TYR:CZ	2.54	0.43
1:A:541:ILE:HG22	1:A:595:PRO:HG2	2.00	0.43
1:B:281[A]:ASP:HB3	1:B:283:ILE:H	1.83	0.42
1:A:700:ASP:C	1:A:700:ASP:OD1	2.57	0.42
1:A:59:THR:HB	1:A:140:ALA:O	2.19	0.42
1:B:619:THR:HG22	1:B:624:LEU:HD22	2.01	0.42
1:A:487:SER:H	1:A:490:THR:CG2	2.32	0.42
1:A:325:PRO:HD3	5:A:2033:HOH:O	2.18	0.42
1:B:155:VAL:HG13	1:B:155:VAL:O	2.20	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: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:B:372:GLN:O	1:B:645:LEU:HD21	2.20	0.41
1:B:307:ARG:NH2	5:B:2018:HOH:O	2.45	0.41
1:A:157:ASP:HB3	1:A:206:LEU:HD13	2.02	0.41
1:B:424:ARG:HG3	1:B:663:PHE:CG	2.55	0.41
1:B:766:MET:HB3	1:B:804:ARG:NH1	2.35	0.41
1:B:225:ILE:HD13	1:B:257:PRO:HG2	2.01	0.41
3:A:1810:TLA:O41	3:A:1810:TLA:O2	2.38	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:B:487:SER:H	1:B:490:THR:CG2	2.33	0.41
1:A:807:GLU:HB2	1:A:808:PHE:CE1	2.55	0.41
1:B:766:MET:HE1	1:B:807:GLU:HG3	2.03	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:GLN:O	1:A:137:ALA:HA	2.21	0.41
1:B:593:VAL:CG1	1:B:594:ASP:N	2.84	0.41
4:A:1811:DTB:HCB1	1:B:222:LEU:CD1	2.50	0.41
1:A:93:HIS:HA	1:A:114:CYS:O	2.19	0.41
1:B:514:ASN:HD22	1:B:728:SER:HA	1.85	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:B:135:LEU:HD22	1:B:163:MET:HE2	2.04	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: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:535:PHE:CG	1:A:541:ILE:HG12	2.57	0.40
1:B:719:ASP:HB3	1:B:722:LEU:HB2	2.04	0.40
1:B:614:PHE:CG	1:B:637:PRO:HB3	2.56	0.40
1:A:237:LEU:HD12	1:A:237:LEU:HA	1.93	0.40
1:A:155:VAL:O	1:A:155:VAL:HG13	2.22	0.40
1:A:615:ASP:OD1	1:A:615:ASP:C	2.58	0.40
1:A:13:ASN:H	1:A:13:ASN:ND2	2.20	0.40
1:B:535:PHE:CD1	1:B:535:PHE:N	2.66	0.40
1:A:445:LYS:CE	1:A:449:ASP:OD2	2.69	0.40
1:A:182:ASP:HB3	1:A:183:LEU:H	1.81	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%)	12	28
1	B	736/831 (89%)	696 (95%)	33 (4%)	7 (1%)	19	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1481/1662 (89%)	1383 (93%)	79 (5%)	19 (1%)	15 35

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%)	31 59
1	B	605/704 (86%)	575 (95%)	30 (5%)	30 57
All	All	1227/1408 (87%)	1167 (95%)	60 (5%)	32 58

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 (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	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%)	21,22,23	1.84	3 (14%)
3	TLA	A	1810	-	3,9,9	1.88	1 (33%)	6,12,12	3.27	3 (50%)
4	DTB	A	1811	-	12,15,15	0.87	1 (8%)	14,19,19	1.18	3 (21%)
2	PLP	B	1644	1	15,15,16	1.87	2 (13%)	21,22,23	1.96	2 (9%)
4	DTB	B	1808	-	12,15,15	0.86	1 (8%)	14,19,19	1.94	2 (14%)
3	TLA	B	1809	-	3,9,9	1.64	1 (33%)	6,12,12	3.13	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	-5.78	1.23	1.37
2	A	1644	PLP	O3-C3	-5.68	1.23	1.37
3	A	1810	TLA	O3-C3	-3.18	1.36	1.42
3	B	1809	TLA	O2-C2	-2.45	1.37	1.42
4	A	1811	DTB	CN-N1	-2.27	1.32	1.35
2	B	1644	PLP	C3-C2	-2.13	1.39	1.40
4	B	1808	DTB	CN-N2	-2.08	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1644	PLP	C2-N1	2.19	1.38	1.34
2	A	1644	PLP	C6-N1	2.39	1.39	1.34

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1810	TLA	C1-C2-C3	-6.25	100.54	113.35
3	B	1809	TLA	C4-C3-C2	-5.26	102.56	113.35
3	B	1809	TLA	C1-C2-C3	-5.16	102.78	113.35
4	B	1808	DTB	CR-N2-CN	-4.24	109.31	112.49
3	A	1810	TLA	C4-C3-C2	-4.22	104.70	113.35
4	B	1808	DTB	CD-CE-CR	-3.71	106.26	114.10
4	A	1811	DTB	CS-CR-N2	-2.34	99.63	102.30
2	A	1644	PLP	O3P-P-O4P	-2.28	100.01	106.56
2	B	1644	PLP	O4P-P-O1P	-2.19	101.56	107.14
4	A	1811	DTB	CR-N2-CN	-2.07	110.94	112.49
4	A	1811	DTB	CT-CS-N1	-2.03	109.39	111.66
3	A	1810	TLA	O2-C2-C1	2.01	116.27	111.21
2	A	1644	PLP	O3P-P-O1P	2.07	117.26	110.58
2	A	1644	PLP	O4P-C5A-C5	6.57	119.86	108.99
2	B	1644	PLP	O4P-C5A-C5	7.43	121.27	108.99

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

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^{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>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	755/831 (90%)	0.01	24 (3%) 51 50	15, 31, 68, 94	0
1	B	748/831 (90%)	0.00	26 (3%) 48 47	14, 30, 68, 94	0
All	All	1503/1662 (90%)	0.01	50 (3%) 50 49	14, 31, 68, 94	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	488	PRO	5.2
1	A	709	SER	4.0
1	B	563	LEU	3.8
1	A	492	PHE	3.8
1	A	451	ASN	3.8
1	B	99	ALA	3.7
1	B	806	GLY	3.6
1	A	333	HIS	3.6
1	B	446	PHE	3.2
1	A	708	THR	3.2
1	A	710	GLN	3.1
1	B	559	LEU	3.0
1	B	661	ALA	3.0
1	A	493	LEU	2.9
1	A	758	LEU	2.8
1	B	463	VAL	2.8
1	A	759	TYR	2.8
1	B	575	VAL	2.8
1	B	668	GLY	2.8
1	A	117	ASN	2.7
1	A	450	HIS	2.7
1	B	669	ASP	2.6
1	B	607	ASN	2.6
1	B	730	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	334	GLN	2.6
1	B	489	TYR	2.6
1	A	332	VAL	2.5
1	B	449	ASP	2.5
1	B	807	GLU	2.4
1	A	354	SER	2.4
1	A	330	LYS	2.4
1	B	759	TYR	2.3
1	A	806	GLY	2.3
1	B	492	PHE	2.3
1	B	96	LEU	2.3
1	B	761	LYS	2.3
1	A	45	SER	2.2
1	A	431	GLY	2.2
1	B	608	ARG	2.2
1	A	335	GLU	2.2
1	B	448	VAL	2.2
1	B	802	TYR	2.2
1	B	760	ALA	2.2
1	B	609	LYS	2.2
1	A	574	HIS	2.2
1	A	668	GLY	2.1
1	A	608	ARG	2.1
1	A	428	SER	2.1
1	A	609	LYS	2.1
1	B	800	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å^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.