



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:44 AM UTC

PDB ID : 4A0R / pdb_00004a0r
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

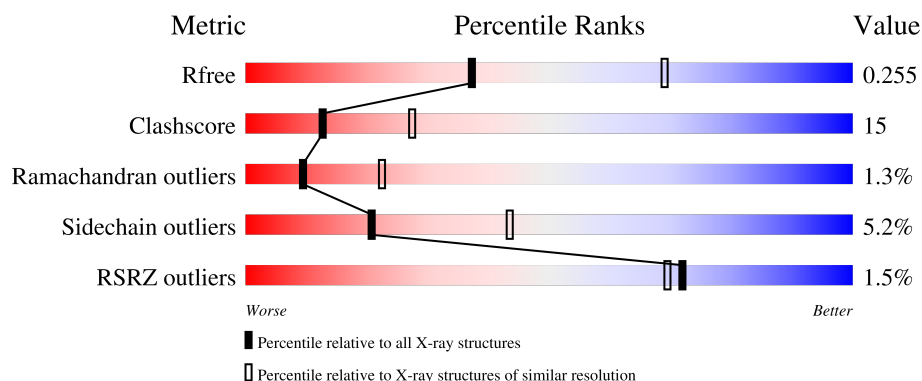
1 Overall quality at a glance

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}	180053	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (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 $\leq 5\%$. 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	% 64% 23% • 9%
1	B	831	% 63% 24% • 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	A	1810	-	X	-	-
3	TLA	B	1809	-	X	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:

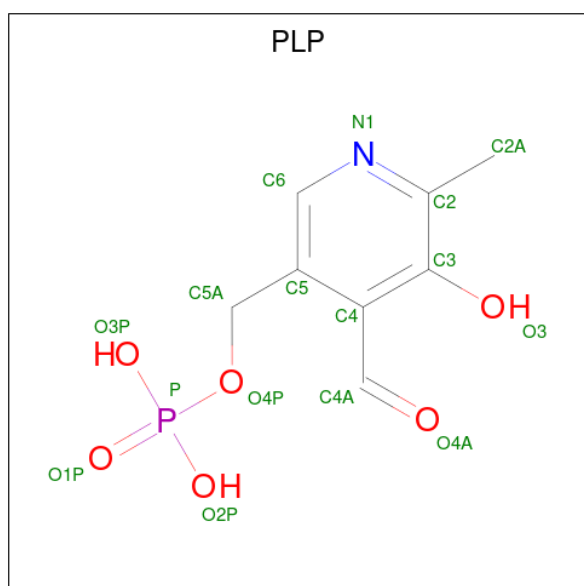
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	GLY	-	expression tag	UNP B0F481
A	-18	SER	-	expression tag	UNP B0F481
A	-17	SER	-	expression tag	UNP B0F481
A	-16	HIS	-	expression tag	UNP B0F481
A	-15	HIS	-	expression tag	UNP B0F481
A	-14	HIS	-	expression tag	UNP B0F481
A	-13	HIS	-	expression tag	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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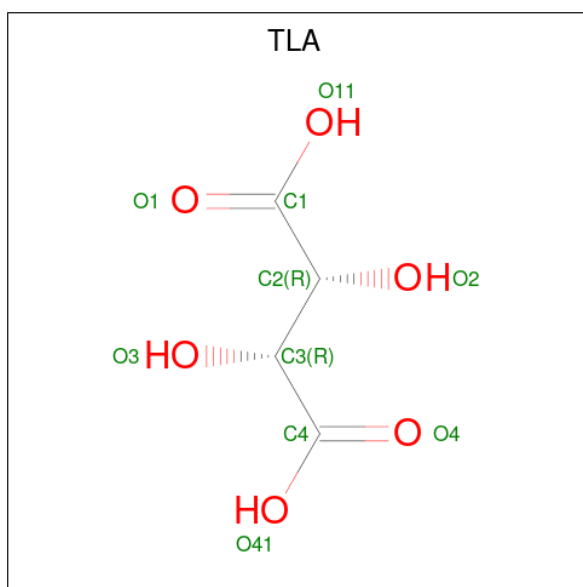
Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	HIS	-	expression tag	UNP B0F481
B	-14	HIS	-	expression tag	UNP B0F481
B	-13	HIS	-	expression tag	UNP B0F481
B	-12	HIS	-	expression tag	UNP B0F481
B	-11	HIS	-	expression tag	UNP B0F481
B	-10	SER	-	expression tag	UNP B0F481
B	-9	SER	-	expression tag	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 (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



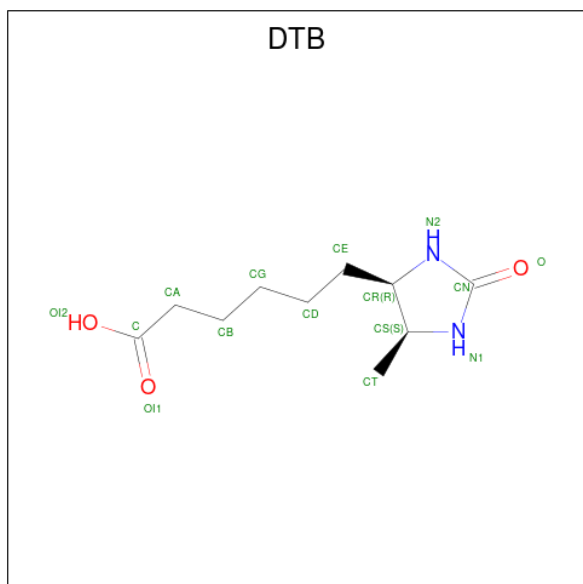
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is L(+)-TARTARIC ACID (CCD ID: 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 (CCD ID: 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		

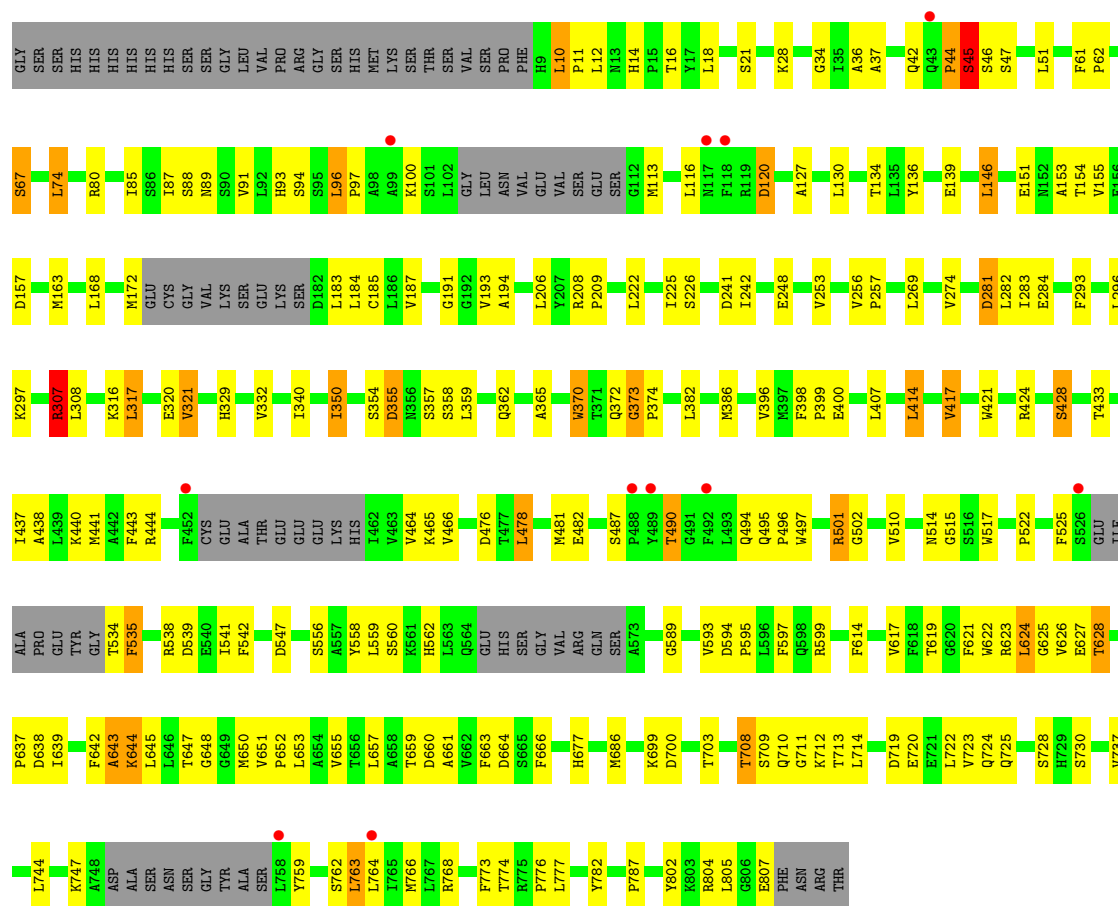
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			15	10	2	3		

- 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		



4 Data and refinement statistics

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 40.44 – 2.68	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.44-2.68) 99.6 (40.44-2.68)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.69Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.184 , 0.259 0.180 , 0.255	Depositor 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/Å ³), B_{sol} (Å ²)	0.39 , 64.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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 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.*

¹Intensities estimated from amplitudes.

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.

5 Model quality

5.1 Standard geometry

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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.60	1/5922 (0.0%)	0.91	10/8050 (0.1%)
1	B	0.60	2/5836 (0.0%)	0.91	8/7938 (0.1%)
All	All	0.60	3/11758 (0.0%)	0.91	18/15988 (0.1%)

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	-10.03	1.18	1.32
1	A	307	ARG	CZ-NH1	-8.87	1.20	1.32
1	B	307	ARG	CZ-NH2	-5.86	1.25	1.33

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	307	ARG	NE-CZ-NH2	10.99	129.09	119.20
1	B	307	ARG	NE-CZ-NH2	10.19	128.37	119.20
1	A	44	PRO	N-CA-CB	7.28	110.90	103.25
1	A	495	GLN	CA-C-N	7.24	127.86	119.47
1	A	495	GLN	C-N-CA	7.24	127.86	119.47
1	B	307	ARG	NH1-CZ-NH2	-7.01	110.19	119.30
1	B	44	PRO	N-CA-CB	6.71	110.29	103.25
1	B	46	SER	N-CA-C	6.71	119.74	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	47	SER	N-CA-C	-6.56	104.76	112.89
1	A	108	VAL	N-CA-C	6.04	116.63	108.17
1	B	414	LEU	N-CA-C	5.63	117.41	111.28
1	A	782	TYR	N-CA-C	5.45	117.96	109.52
1	B	478	LEU	N-CA-C	5.40	117.16	111.28
1	B	782	TYR	N-CA-C	5.31	117.75	109.52
1	A	280	ASP	N-CA-C	5.30	117.71	110.24
1	A	594	ASP	CA-C-N	5.08	124.52	119.24
1	A	594	ASP	C-N-CA	5.08	124.52	119.24
1	A	445	LYS	N-CA-C	-5.07	105.75	111.28

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	179	0
1	B	5704	0	5585	193	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	5	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	348	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 15.

All (348) 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:A:766:MET:HE1	1:A:807:GLU:HG3	1.39	1.01
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:766:MET:HE1	1:B:807:GLU:HG3	1.42	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
1:B:42:GLN:OE1	1:B:42:GLN:HA	1.75	0.84
1:B:766:MET:HE2	1:B:804:ARG:HH11	1.43	0.83
1:A:11:PRO:HB2	1:A:172:MET:HE2	1.60	0.82
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:766:MET:HE2	1:A:804:ARG:HH11	1.45	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:B:11:PRO:HB2	1:B:172:MET:HE2	1.65	0.79
1:B:659:THR:HG22	1:B:661:ALA:N	1.96	0.79
1:B:465:LYS:HE2	1:B:502:GLY:C	2.10	0.76
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:94:SER:N	1:B:113:MET:HE1	2.01	0.75
1:B:510:VAL:HG11	1:B:541:ILE:HD13	1.67	0.75
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:316:LYS:HE2	1:B:320:GLU:OE2	1.89	0.72
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:28:LYS:NZ	3:B:1809:TLA:H2	2.09	0.67
1:B:373:GLY:H	1:B:374:PRO:HD2	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:104:LEU:O	1:A:105:ASN:C	2.43	0.61
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:B:766:MET:CE	1:B:804:ARG:HH11	2.15	0.58
1:A:437:ILE:HD11	1:A:677:HIS:CD2	2.39	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:B:80:ARG:HH21	1:B:284:GLU:CD	2.13	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:A:28:LYS:HZ1	3:A:1810:TLA:H3	1.70	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:28:LYS:HZ3	3:B:1809:TLA:H2	1.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ILE:HD12	1:A:146:LEU:HB3	1.88	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:744:LEU:C	1:A:744:LEU:HD12	2.33	0.54
1:B:14:HIS:HB2	1:B:172:MET:HE1	1.88	0.54
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
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:A:766:MET:CE	1:A:804:ARG:HH11	2.18	0.52
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: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:A:100:LYS:C	1:A:103:GLY:H	2.18	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:441:MET:HE3	1:B:639:ILE:HG12	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:VAL:CG1	1:B:642:PHE:CZ	2.94	0.51
1:A:478:LEU:HA	1:A:481:MET:HE3	1.91	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:441:MET:HE1	1:A:656:THR:HG22	1.94	0.50
1:A:622:TRP:CE3	1:A:714:LEU:HD13	2.47	0.50
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: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: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:A:353:ALA:C	1:A:355:ASP:H	2.19	0.49
1:B:478:LEU:HA	1:B:481:MET:HE3	1.93	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:A:476:ASP:O	1:A:481:MET:HE2	2.13	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:14:HIS:HB2	1:A:172:MET:HE1	1.95	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:14:HIS:HB2	1:B:172:MET:CE	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:766:MET:HE2	1:B:804:ARG:HD2	1.96	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:476:ASP:O	1:B:481:MET:HE2	2.14	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:744:LEU:HD12	1:B:744:LEU:C	2.39	0.48
1:B:417:VAL:HG11	1:B:642:PHE:CZ	2.49	0.48
1:A:441:MET:HE3	1:A:639:ILE:HG12	1.96	0.47
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:A:627:GLU:CD	1:A:699:LYS:HE3	2.39	0.47
1:A:97:PRO:HA	1:A:100:LYS:HE2	1.95	0.47
1:B:97:PRO:HG2	1:B:151:GLU:HB3	1.96	0.47
1:A:700:ASP:OD1	1:A:700:ASP:C	2.57	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: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:353:ALA:C	1:A:355:ASP:N	2.71	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:B:627:GLU:CD	1:B:699:LYS:HE3	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:28:LYS:HZ1	3:B:1809:TLA:H2	1.78	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:A:324:TRP:CG	1:B:400:GLU:H	2.34	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:B:93:HIS:HB3	1:B:113:MET:HE2	1.96	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:A:269:LEU:CD1	1:A:296:LEU:HD13	2.46	0.45
1:A:638:ASP:C	1:A:639:ILE:HG13	2.41	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:615:ASP:OD1	1:A:615:ASP:C	2.58	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:B:638:ASP:C	1:B:639:ILE:HG13	2.42	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:SER:O	1:B:355:ASP:O	2.36	0.44
1:B:805:LEU:C	1:B:807:GLU:N	2.75	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:784:MET:HE3	1:A:784:MET:HB2	1.88	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:A:80:ARG:HH21	1:A:284:GLU:CD	2.25	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:438:ALA:HA	1:A:441:MET:HE2	2.00	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:438:ALA:HA	1:B:441:MET:HE2	2.00	0.43
1:B:556:SER:O	1:B:560:SER:HB2	2.18	0.43
1:A:545:SER:C	1:A:547:ASP:N	2.76	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:A:766:MET:HE2	1:A:804:ARG:CD	2.49	0.43
1:A:541:ILE:HG22	1:A:595:PRO:HG2	2.00	0.43
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:386:MET:HE2	1:B:686:MET:HE3	2.00	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:A:186:LEU:CD2	1:A:300:MET:HE1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:621:PHE:C	1:B:622:TRP:CD1	2.98	0.42
1:A:14:HIS:HB2	1:A:172:MET:CE	2.50	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
1:B:766:MET:HE2	1:B:804:ARG:CD	2.50	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:A:499:THR:O	1:A:500:GLY:C	2.63	0.41
1:B:10:LEU:O	1:B:358:SER:HB2	2.20	0.41
1:B:805:LEU:C	1:B:807:GLU:H	2.29	0.41
1:A:686:MET:HE3	1:B:386:MET:HE2	2.02	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:A:805:LEU:C	1:A:807:GLU:N	2.77	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:592:MET:HE3	1:A:736:VAL:HG13	2.03	0.41
1:A:744:LEU:HD12	1:A:744:LEU:O	2.20	0.41
1:B:14:HIS:HD2	1:B:172:MET:HE3	1.86	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
1:A:93:HIS:HA	1:A:114:CYS:O	2.19	0.41
1:A:621:PHE:C	1:A:622:TRP:CD1	2.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:102:LEU:O	1:A:103:GLY:C	2.63	0.40
1:A:146:LEU:HD23	1:A:146:LEU:HA	1.86	0.40
1:B:248:GLU:CD	1:B:274:VAL:HG23	2.47	0.40
1:A:129:GLU:HG2	1:A:131:LEU:CD1	2.51	0.40
1:B:626:VAL:HG12	1:B:713:THR:HG22	2.03	0.40
1:A:14:HIS:HD2	1:A:172:MET:HE3	1.86	0.40
1:B:191:GLY:N	3:B:1809:TLA:O11	2.46	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: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:643:ALA:O	1:B:644:LYS:C	2.63	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%)	7	18
1	B	736/831 (89%)	696 (95%)	33 (4%)	7 (1%)	12	28
All	All	1481/1662 (89%)	1383 (93%)	79 (5%)	19 (1%)	9	22

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%)	587 (94%)	35 (6%)	19	40
1	B	605/704 (86%)	575 (95%)	30 (5%)	22	45
All	All	1227/1408 (87%)	1162 (95%)	65 (5%)	21	43

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	13	ASN
1	A	67	SER
1	A	74	LEU
1	A	96	LEU

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Mol	Chain	Res	Type
1	A	109	SER
1	A	110	GLU
1	A	117	ASN
1	A	120	ASP
1	A	139	GLU
1	A	146	LEU
1	A	154	THR
1	A	193	VAL
1	A	253	VAL
1	A	279	SER
1	A	281[A]	ASP
1	A	281[B]	ASP
1	A	308	LEU
1	A	317	LEU
1	A	321	VAL
1	A	350	ILE
1	A	370	TRP
1	A	384	ARG
1	A	417	VAL
1	A	428	SER
1	A	466	VAL
1	A	534	THR
1	A	536	THR
1	A	624	LEU
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	67	SER
1	B	74	LEU
1	B	96	LEU
1	B	120	ASP
1	B	146	LEU
1	B	154	THR
1	B	193	VAL
1	B	253	VAL
1	B	281[A]	ASP
1	B	281[B]	ASP
1	B	307	ARG

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Mol	Chain	Res	Type
1	B	317	LEU
1	B	321	VAL
1	B	350	ILE
1	B	370	TRP
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	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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	HIS
1	A	250	HIS
1	A	347	ASN
1	A	362	GLN
1	B	14	HIS
1	B	250	HIS
1	B	329	HIS
1	B	347	ASN
1	B	362	GLN
1	B	395	HIS
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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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$
3	TLA	B	1809	-	9,9,9	2.09	5 (55%)	12,12,12	2.29	7 (58%)
2	PLP	B	1644	1	15,15,16	1.89	2 (13%)	21,22,23	1.75	1 (4%)
4	DTB	A	1811	-	15,15,15	0.93	0	16,19,19	0.91	1 (6%)
4	DTB	B	1808	-	15,15,15	0.92	1 (6%)	16,19,19	1.43	2 (12%)
2	PLP	A	1644	1	15,15,16	1.90	3 (20%)	21,22,23	1.68	2 (9%)
3	TLA	A	1810	-	9,9,9	2.05	4 (44%)	12,12,12	2.37	7 (58%)

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

All (15) 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	1.36
2	A	1644	PLP	O3-C3	-5.76	1.23	1.36
3	A	1810	TLA	C3-C4	-3.65	1.47	1.52
3	B	1809	TLA	C2-C1	-3.32	1.47	1.52
3	A	1810	TLA	O3-C3	-3.06	1.36	1.42
2	A	1644	PLP	C2-N1	2.72	1.38	1.33
2	A	1644	PLP	C6-N1	2.54	1.39	1.34
2	B	1644	PLP	C2-N1	2.38	1.38	1.33
3	B	1809	TLA	O2-C2	-2.30	1.37	1.42
3	B	1809	TLA	O11-C1	-2.26	1.23	1.30
4	B	1808	DTB	OI2-C	-2.26	1.23	1.30
3	B	1809	TLA	O41-C4	-2.22	1.23	1.30
3	B	1809	TLA	O1-C1	2.11	1.28	1.22
3	A	1810	TLA	O11-C1	-2.06	1.24	1.30
3	A	1810	TLA	O41-C4	-2.04	1.24	1.30

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1644	PLP	O4P-C5A-C5	6.36	121.27	109.36
2	A	1644	PLP	O4P-C5A-C5	5.60	119.86	109.36
3	A	1810	TLA	C3-C2-C1	-4.19	100.54	109.82
4	B	1808	DTB	CD-CE-CR	-4.03	106.26	113.94
3	B	1809	TLA	C2-C3-C4	-3.27	102.56	109.82
3	B	1809	TLA	O1-C1-C2	-3.26	112.94	121.62
3	B	1809	TLA	C3-C2-C1	-3.18	102.78	109.82
3	A	1810	TLA	O4-C4-C3	-3.14	113.25	121.62
3	B	1809	TLA	O4-C4-C3	-3.07	113.44	121.62
3	A	1810	TLA	O1-C1-C2	-3.02	113.58	121.62
3	A	1810	TLA	O11-C1-C2	2.79	121.06	113.31
3	B	1809	TLA	O41-C4-C3	2.72	120.86	113.31
3	A	1810	TLA	O2-C2-C1	2.61	116.27	110.69
3	B	1809	TLA	O11-C1-C2	2.59	120.50	113.31
2	A	1644	PLP	O3P-P-O4P	-2.55	100.01	106.67
3	A	1810	TLA	O41-C4-C3	2.52	120.31	113.31
3	A	1810	TLA	C2-C3-C4	-2.31	104.70	109.82
4	B	1808	DTB	CR-N2-CN	-2.09	109.31	112.38
4	A	1811	DTB	CS-CR-N2	-2.01	99.63	102.19
3	B	1809	TLA	O3-C3-C4	2.01	114.98	110.69

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1810	TLA	O3-C3-C4-O4
3	A	1810	TLA	O3-C3-C4-O41
3	B	1809	TLA	O1-C1-C2-O2
3	B	1809	TLA	O11-C1-C2-O2
4	A	1811	DTB	C-CA-CB-CG
4	B	1808	DTB	CG-CD-CE-CR
4	A	1811	DTB	CE-CD-CG-CB
4	A	1811	DTB	CA-CB-CG-CD
3	B	1809	TLA	O1-C1-C2-C3
4	B	1808	DTB	CE-CD-CG-CB
3	B	1809	TLA	O11-C1-C2-C3
2	A	1644	PLP	C5A-O4P-P-O1P
2	B	1644	PLP	C5A-O4P-P-O1P
4	B	1808	DTB	OI1-C-CA-CB
3	A	1810	TLA	O1-C1-C2-C3
4	A	1811	DTB	CG-CD-CE-CR
4	B	1808	DTB	OI2-C-CA-CB
4	A	1811	DTB	OI2-C-CA-CB
4	A	1811	DTB	OI1-C-CA-CB
4	A	1811	DTB	CD-CE-CR-CS
4	B	1808	DTB	CD-CE-CR-CS
3	A	1810	TLA	O11-C1-C2-C3

There are no ring outliers.

6 monomers are involved in 16 short contacts:

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

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	755/831 (90%)	-0.18	11 (1%) 72 69	15, 31, 68, 94	2 (0%)
1	B	748/831 (90%)	-0.21	11 (1%) 72 69	12, 30, 68, 94	2 (0%)
All	All	1503/1662 (90%)	-0.20	22 (1%) 72 69	12, 31, 68, 94	4 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	452	PHE	3.3
1	B	758	LEU	3.3
1	B	526	SER	3.2
1	A	63	SER	2.9
1	A	758	LEU	2.9
1	B	488	PRO	2.8
1	B	492	PHE	2.5
1	A	452	PHE	2.5
1	B	489	TYR	2.4
1	A	493	LEU	2.4
1	A	488	PRO	2.3
1	B	764	LEU	2.3
1	A	118	PHE	2.3
1	A	492	PHE	2.3
1	B	117	ASN	2.2
1	B	99	ALA	2.2
1	B	43	GLN	2.2
1	A	172	MET	2.1
1	A	333	HIS	2.0
1	B	118	PHE	2.0
1	A	462	ILE	2.0
1	A	518	ASN	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 oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	TLA	B	1809	10/10	0.89	0.12	22,37,47,56	0
3	TLA	A	1810	10/10	0.91	0.10	7,28,39,45	0
4	DTB	B	1808	15/15	0.93	0.10	2,23,45,51	0
4	DTB	A	1811	15/15	0.95	0.09	5,33,64,71	0
2	PLP	A	1644	15/16	0.97	0.07	16,31,39,40	0
2	PLP	B	1644	15/16	0.97	0.07	15,31,36,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.