



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2018 – 09:42 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

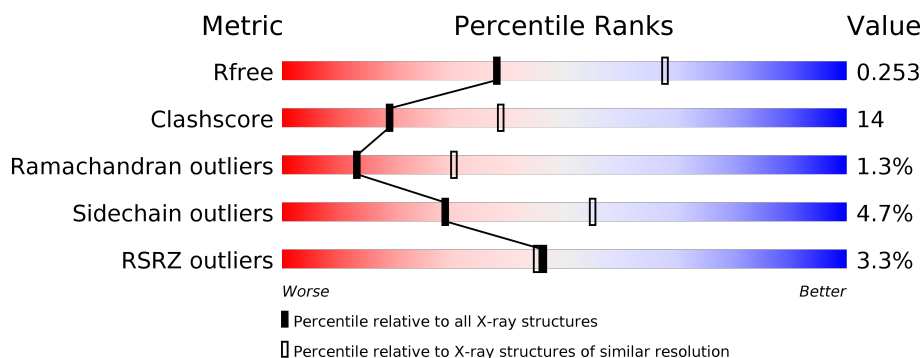
1 Overall quality at a glance

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}	111664	3333 (2.70-2.66)
Clashscore	122126	3672 (2.70-2.66)
Ramachandran outliers	120053	3620 (2.70-2.66)
Sidechain outliers	120020	3620 (2.70-2.66)
RSRZ outliers	108989	3248 (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 $\leq 5\%$. 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	 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	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11693 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ADENOSYLMETHIONINE-8-AMINO-7-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:

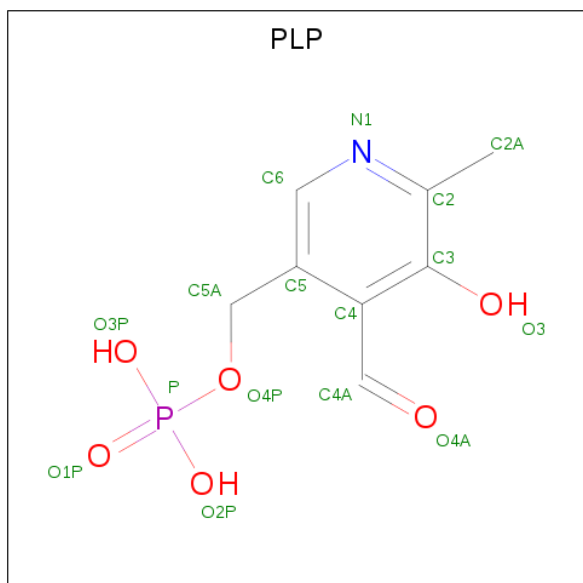
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	GLY	-	expression tag	UNP B0F481
A	-18	SER	-	expression tag	UNP B0F481
A	-17	SER	-	expression tag	UNP B0F481
A	-16	HIS	-	expression tag	UNP B0F481
A	-15	HIS	-	expression tag	UNP B0F481
A	-14	HIS	-	expression tag	UNP B0F481
A	-13	HIS	-	expression tag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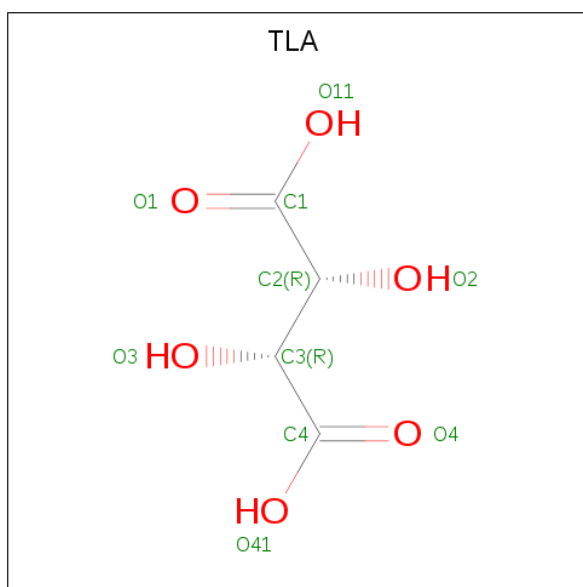
Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	HIS	-	expression tag	UNP B0F481
B	-14	HIS	-	expression tag	UNP B0F481
B	-13	HIS	-	expression tag	UNP B0F481
B	-12	HIS	-	expression tag	UNP B0F481
B	-11	HIS	-	expression tag	UNP B0F481
B	-10	SER	-	expression tag	UNP B0F481
B	-9	SER	-	expression tag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



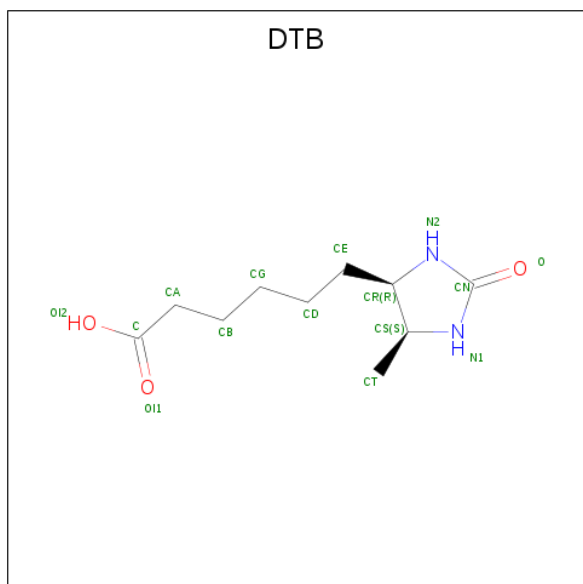
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- 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		

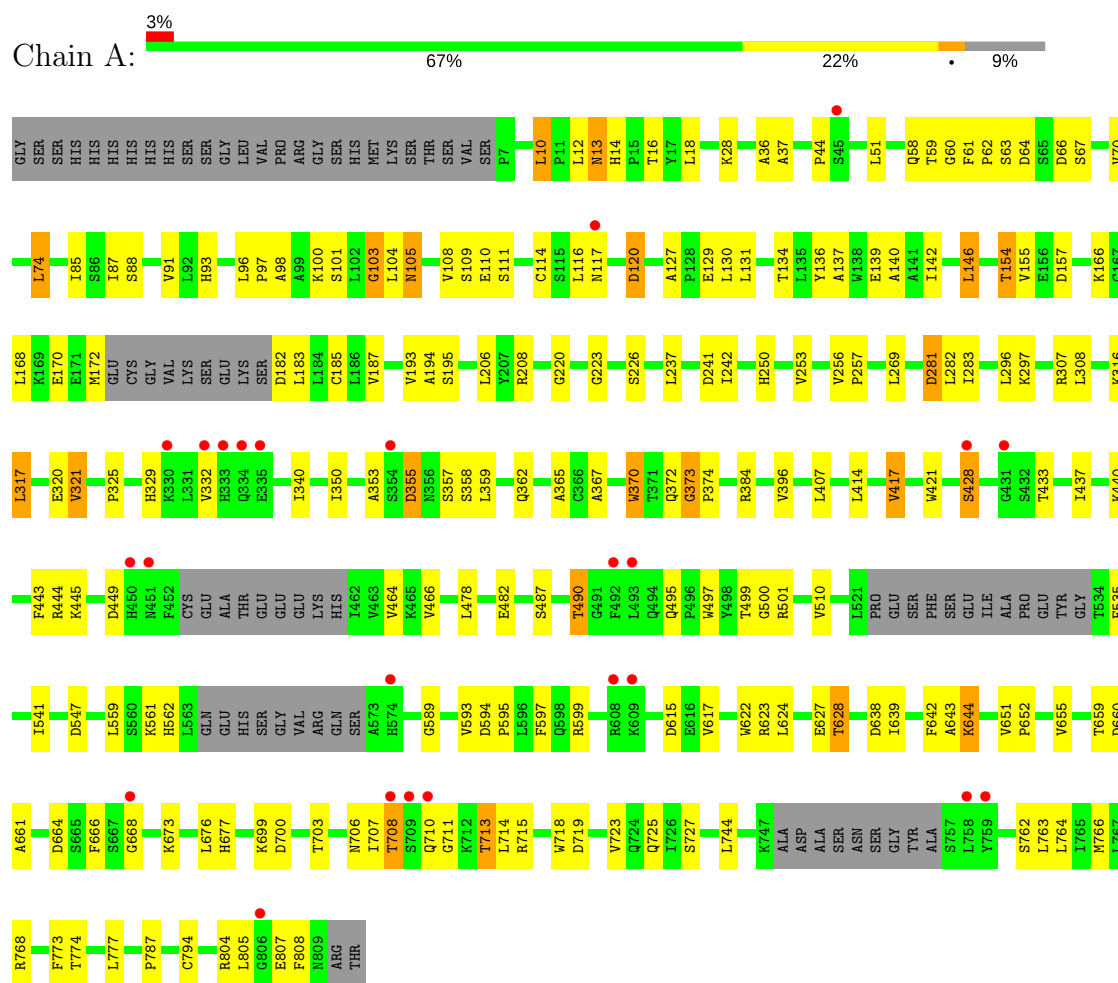
- Molecule 5 is water.

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

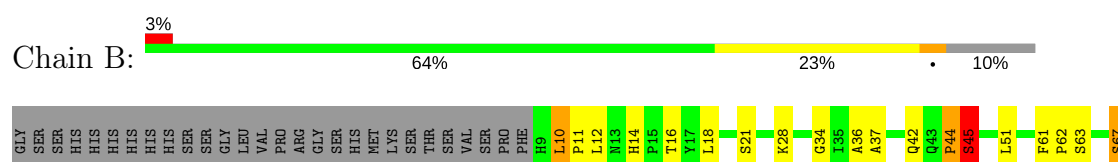
3 Residue-property plots

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

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



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



ASP	L758	L759	L760	L761	L762	L763	L764	L765	L766	L767	L768	F773	T774	R775	P776	L777	P787	Y802	R803	R804	L805	G806	E807	PHE	ASN	ARG	THR																					
K644	L645	T647	G648	G649	M650	V651	P652	L653	A654	V655	T656	L657	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
E540	I541	F542	D547	S556	A557	Y558	L559	S560	K561	H562	L563	Q564	HIS	SER	GLY	VAL	ARG	GLN	SER	A573	H574	V575	G589	V593	D594	P595	L596	F597	Q598	R599	R607	R608	R609	F614	V617	F618	T619	R623	L624	G625	V626	E627	T628	P637	D638	I639	F642	A643
D449	F452	CYS	GLU	ALA	THR	GLU	GLU	LYS	HIS	L462	V463	V464	K465	V466	L478	E482	S487	P488	Y489	T490	G491	F492	L493	Q494	Q495	P496	W497	R501	Q502	V510	N514	Q515	S516	V517	P522	P525	S526	GLU	ILE	ALA	PRO	GLU	TYR	GLY	T534	F535	R538	D539
V321	H329	V332	I340	I350	S354	D355	V356	S357	L358	L359	Q362	A365	W370	T371	Q372	G373	P374	L382	V396	M397	F398	P399	L407	K408	L414	V417	W421	R424	S428	T433	I437	K440	M441	A442	F443	R444	K445	F446	C447	V448								
L168	M172	GLU	CYS	GLY	VAL	LYS	SER	GLU	LYS	SER	D182	L183	L184	C185	L186	V187	G191	G192	V193	A194	L206	Y207	P209	L222	I225	S226	D241	I242	V256	P257	L269	D281	L282	I283	E284	F293	L296	K297	R307	L308	T154	V155	K316	L317	E320			
L74	R80	I85	S86	I87	S88	N89	S90	GLU	V91	L92	H93	S94	S95	L96	P97	A98	A99	K100	S101	L102	GLY	LEU	ASN	VAL	GLU	VAL	SER	GLU	SER	G112	M113	L116	D120	A127	L130	T134	L135	Y136	E139	L146	E151	N152	A153	T154	V155	E156	D157	M163

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 40.72 – 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
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.69Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.184 , 0.259 0.179 , 0.253	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)	0.38 , 65.7	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: 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	24
1	B	736/831 (89%)	696 (95%)	33 (4%)	7 (1%)	17	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1481/1662 (89%)	1383 (93%)	79 (5%)	19 (1%)	13 30

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%)	28 54
1	B	605/704 (86%)	575 (95%)	30 (5%)	27 52
All	All	1227/1408 (87%)	1167 (95%)	60 (5%)	29 53

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	1.85	3 (20%)	20,22,23	1.67	2 (10%)
3	TLA	A	1810	-	3,9,9	1.97	1 (33%)	6,12,12	3.07	3 (50%)
4	DTB	A	1811	-	12,15,15	0.83	1 (8%)	12,19,19	1.07	1 (8%)
2	PLP	B	1644	1	15,15,16	1.87	3 (20%)	20,22,23	1.74	1 (5%)
4	DTB	B	1808	-	12,15,15	0.83	0	12,19,19	1.73	2 (16%)
3	TLA	B	1809	-	3,9,9	1.72	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	-5.83	1.23	1.37
2	A	1644	PLP	O3-C3	-5.73	1.23	1.37
3	A	1810	TLA	O3-C3	-3.33	1.36	1.42
3	B	1809	TLA	O2-C2	-2.57	1.37	1.42
4	A	1811	DTB	CN-N1	-2.15	1.32	1.35
2	B	1644	PLP	C3-C2	-2.08	1.39	1.40
2	B	1644	PLP	C2-N1	2.10	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1644	PLP	C2-N1	2.40	1.38	1.33
2	A	1644	PLP	C6-N1	2.44	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	-3.73	106.26	113.96
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	5.44	119.86	109.39
2	B	1644	PLP	O4P-C5A-C5	6.18	121.27	109.39

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, 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%)	-0.02	24 (3%) 47 46	15, 31, 68, 94	0
1	B	748/831 (90%)	-0.03	25 (3%) 46 45	14, 30, 68, 94	0
All	All	1503/1662 (90%)	-0.03	49 (3%) 46 45	14, 31, 68, 94	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	488	PRO	5.1
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	3.1
1	A	708	THR	3.1
1	A	710	GLN	3.0
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	2.6
1	B	730	SER	2.6
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	2.4
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	A	806	GLY	2.2
1	B	96	LEU	2.2
1	B	761	LYS	2.2
1	A	45	SER	2.2
1	A	431	GLY	2.2
1	B	448	VAL	2.1
1	B	608	ARG	2.1
1	B	802	TYR	2.1
1	A	574	HIS	2.1
1	A	335	GLU	2.1
1	B	609	LYS	2.1
1	B	760	ALA	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. 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(\AA^2)	Q<0.9
3	TLA	B	1809	10/10	0.94	0.16	22,37,47,56	0
3	TLA	A	1810	10/10	0.94	0.16	7,28,39,45	0
4	DTB	B	1808	15/15	0.95	0.20	2,23,45,51	0
4	DTB	A	1811	15/15	0.97	0.18	5,33,64,71	0
2	PLP	A	1644	15/16	0.97	0.21	16,31,39,40	0
2	PLP	B	1644	15/16	0.97	0.18	15,31,36,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.