



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:08 am GMT

PDB ID : 4A0G
Title : Structure of bifunctional DAPA aminotransferase-DTB synthetase from *Arabidopsis thaliana* in its apo form.
Authors : Cobessi, D.; Dumas, R.; Pautre, V.; Meinguet, C.; Ferrer, J.L.; Alban, C.
Deposited on : 2011-09-09
Resolution : 2.50 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

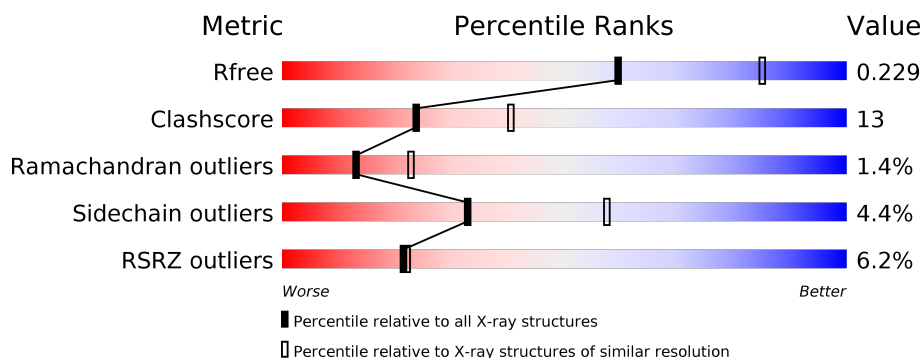
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>17%</div> <div>•</div> <div>7%</div> </div> </div>
1	B	831	<div> <div>3%</div> <div> <div></div> <div>71%</div> <div>18%</div> <div>•</div> <div>9%</div> </div> </div>
1	C	831	<div> <div>10%</div> <div> <div></div> <div>62%</div> <div>18%</div> <div>•</div> <div>18%</div> </div> </div>
1	D	831	<div> <div>7%</div> <div> <div></div> <div>64%</div> <div>19%</div> <div>•</div> <div>15%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	1813	-	-	-	X
3	SO4	A	1814	-	-	X	-
3	SO4	C	1808	-	-	-	X
3	SO4	C	1809	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22816 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	769	Total	C	N	O	S	0	14	0
			5943	3817	996	1098	32			
1	B	756	Total	C	N	O	S	0	7	0
			5789	3716	972	1070	31			
1	C	681	Total	C	N	O	S	0	4	0
			5160	3311	858	961	30			
1	D	709	Total	C	N	O	S	0	5	0
			5383	3457	901	996	29			

There are 80 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

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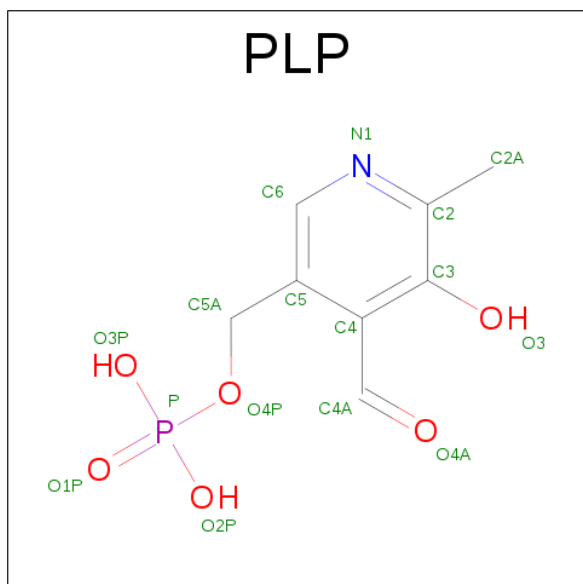
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	GLY	-	EXPRESSION TAG	UNP B0F481
B	-18	SER	-	EXPRESSION TAG	UNP B0F481
B	-17	SER	-	EXPRESSION TAG	UNP B0F481
B	-16	HIS	-	EXPRESSION TAG	UNP B0F481
B	-15	HIS	-	EXPRESSION TAG	UNP B0F481
B	-14	HIS	-	EXPRESSION TAG	UNP B0F481
B	-13	HIS	-	EXPRESSION TAG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

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

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



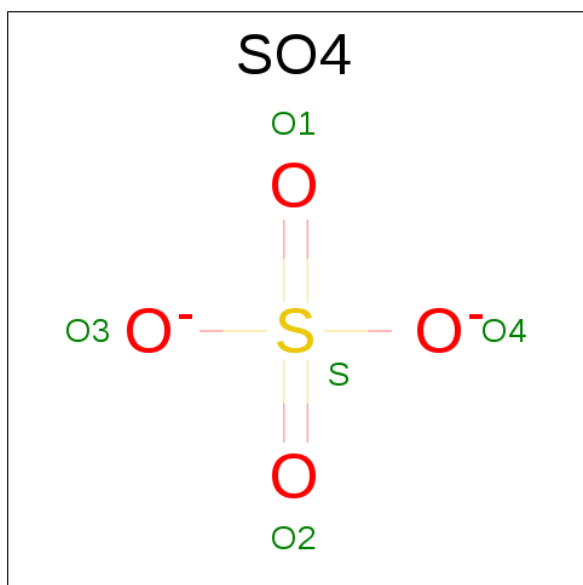
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		

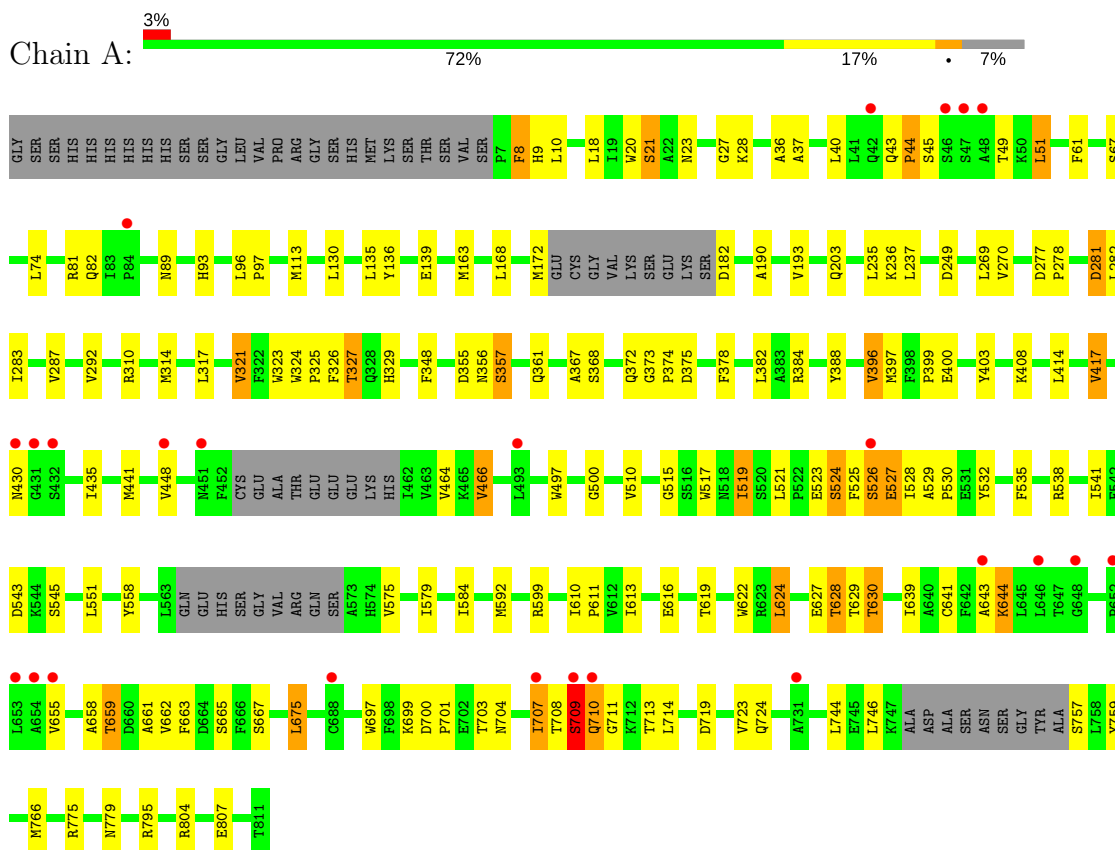
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	185	Total	O	0	0
			185	185		
5	B	123	Total	O	0	0
			123	123		
5	C	57	Total	O	0	0
			57	57		
5	D	64	Total	O	0	0
			64	64		

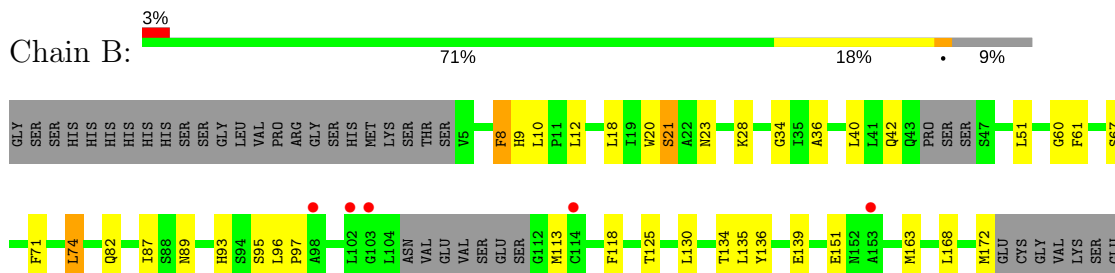
3 Residue-property plots [i](#)

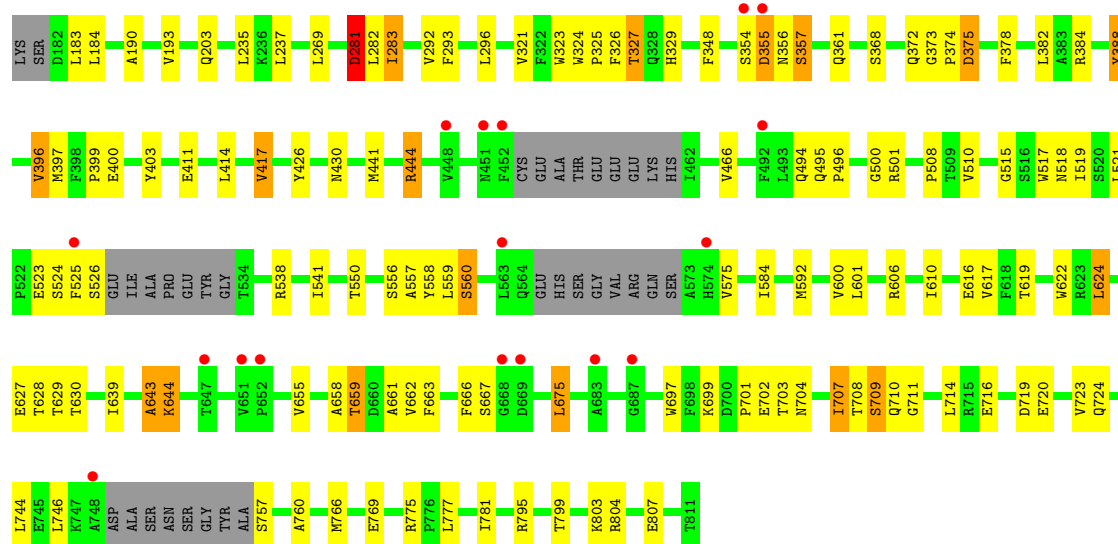
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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

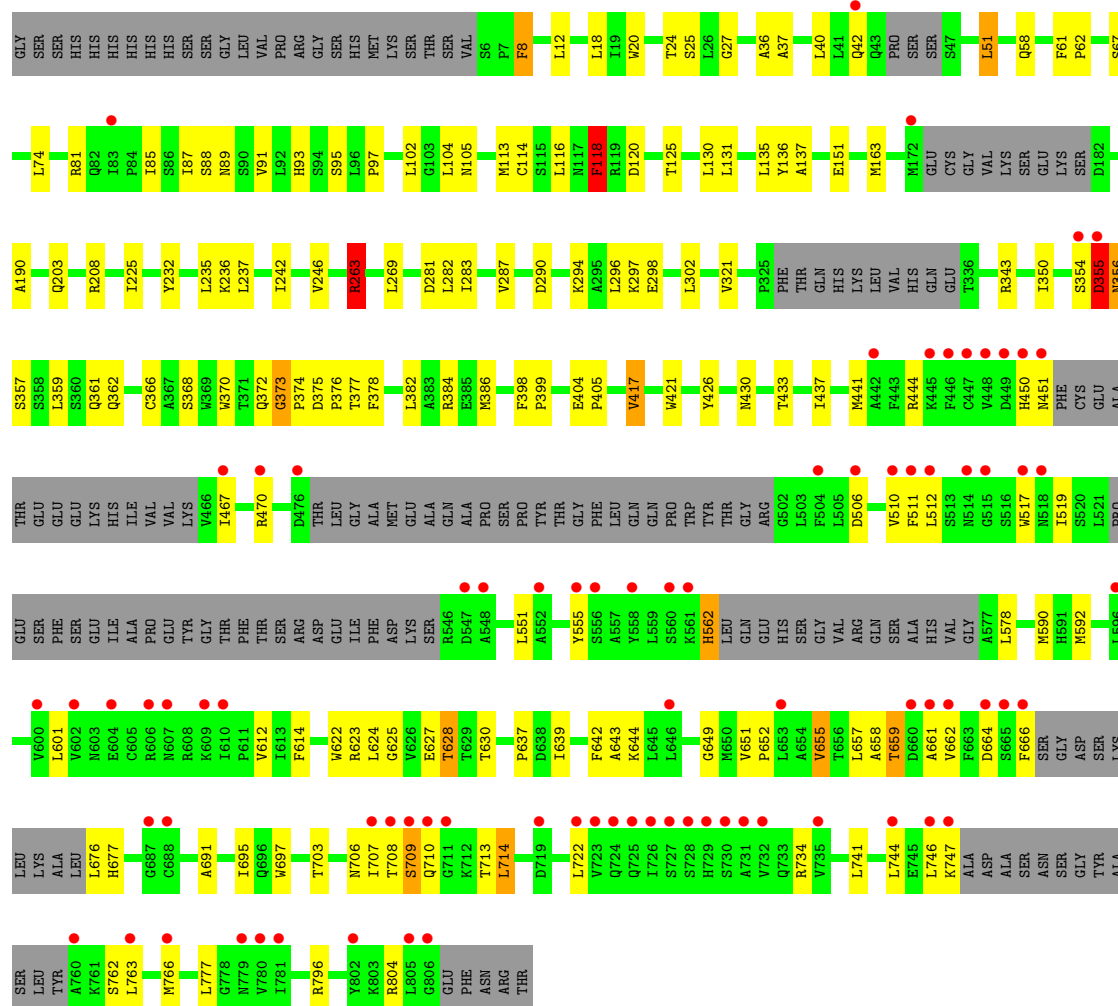


• Molecule 1: ADENOSYLMETHIONINE-8-AMINO-7-OXONONANOATE AMINOTRANSFERASE



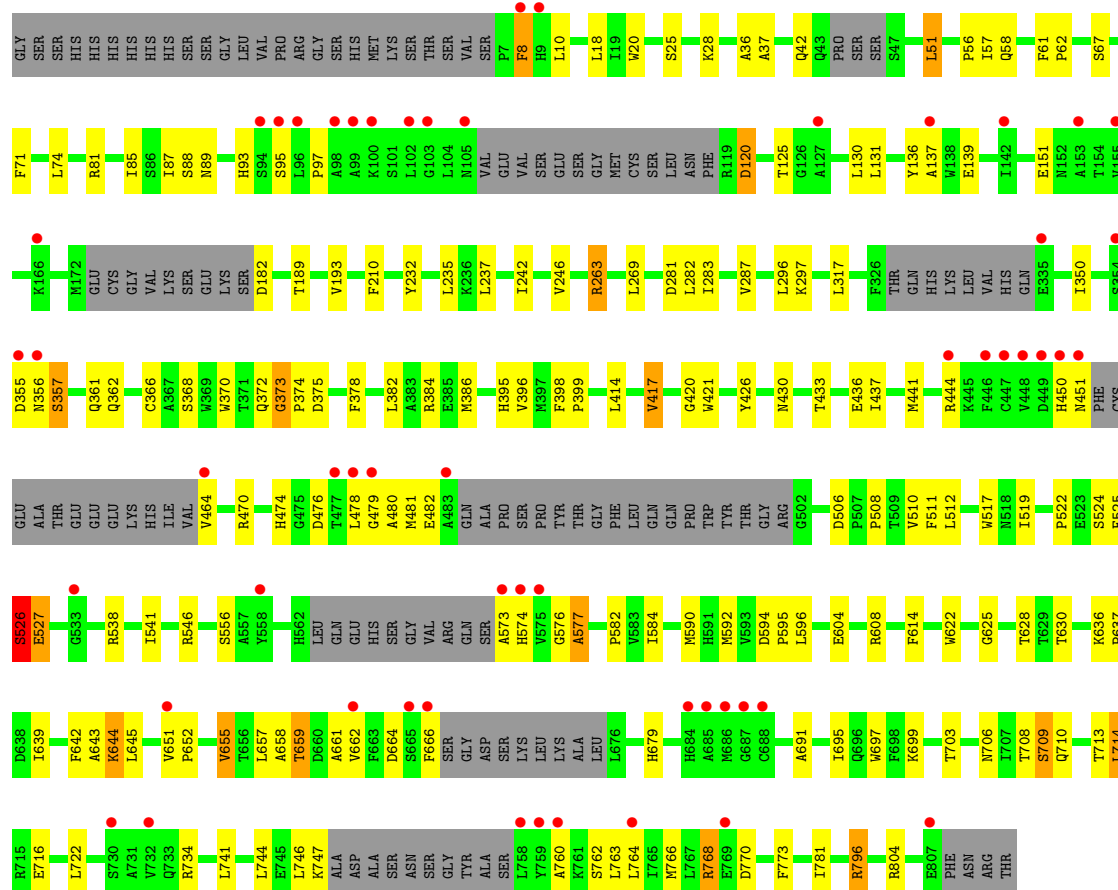


• Molecule 1: ADENOSYLMETHIONINE-8-AMINO-7-OXONONANOATE AMINOTRANSFERASE



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

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	79.44Å 80.07Å 136.94Å 99.96° 107.12° 97.25°	Depositor
Resolution (Å)	39.57 – 2.50 48.13 – 2.50	Depositor EDS
% Data completeness (in resolution range)	88.3 (39.57-2.50) 82.8 (48.13-2.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.51Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.177 , 0.239 0.165 , 0.229	Depositor DCC
R_{free} test set	4749 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	40.3	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 60.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.010 for k,h,-h-k-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22816	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SO4, 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	0.60	4/6119 (0.1%)	0.68	5/8324 (0.1%)
1	B	0.61	4/5942 (0.1%)	0.70	5/8081 (0.1%)
1	C	0.48	2/5283 (0.0%)	0.66	3/7189 (0.0%)
1	D	0.48	2/5516 (0.0%)	0.69	6/7505 (0.1%)
All	All	0.55	12/22860 (0.1%)	0.68	19/31099 (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	A	0	1
1	B	0	1
All	All	0	2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	388	TYR	CE1-CZ	-13.53	1.21	1.38
1	A	388	TYR	CE2-CZ	-12.80	1.22	1.38
1	B	388	TYR	CE2-CZ	-12.78	1.22	1.38
1	B	388	TYR	CE1-CZ	-12.54	1.22	1.38
1	B	388	TYR	CG-CD2	-11.50	1.24	1.39
1	A	388	TYR	CG-CD2	-10.86	1.25	1.39
1	B	388	TYR	CG-CD1	-10.40	1.25	1.39
1	A	388	TYR	CG-CD1	-10.09	1.26	1.39
1	C	796	ARG	CZ-NH1	-9.93	1.20	1.33
1	D	796	ARG	CZ-NH1	-9.57	1.20	1.33
1	D	263	ARG	CG-CD	-6.71	1.35	1.51
1	C	263	ARG	CG-CD	-5.83	1.37	1.51

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	796	ARG	NE-CZ-NH2	21.46	131.03	120.30
1	C	796	ARG	NE-CZ-NH2	20.18	130.39	120.30
1	D	796	ARG	NE-CZ-NH1	-14.34	113.13	120.30
1	C	796	ARG	NE-CZ-NH1	-13.95	113.33	120.30
1	D	263	ARG	CG-CD-NE	10.22	133.27	111.80
1	D	263	ARG	CB-CG-CD	-8.69	89.01	111.60
1	B	702	GLU	CA-CB-CG	-7.12	97.73	113.40
1	A	44	PRO	N-CA-CB	6.52	111.12	103.30
1	B	388	TYR	CZ-CE2-CD2	6.38	125.54	119.80
1	C	263	ARG	CB-CG-CD	-6.08	95.79	111.60
1	A	388	TYR	CZ-CE2-CD2	6.02	125.22	119.80
1	A	388	TYR	CB-CG-CD1	5.94	124.56	121.00
1	B	388	TYR	CB-CG-CD1	5.88	124.53	121.00
1	A	388	TYR	CD1-CG-CD2	-5.88	111.43	117.90
1	D	444	ARG	NE-CZ-NH1	-5.71	117.45	120.30
1	B	388	TYR	CD1-CG-CD2	-5.49	111.86	117.90
1	D	444	ARG	NE-CZ-NH2	5.17	122.88	120.30
1	B	444	ARG	CG-CD-NE	-5.06	101.17	111.80
1	A	388	TYR	CB-CG-CD2	5.00	124.00	121.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	374	PRO	Peptide
1	B	374	PRO	Peptide

5.2 Too-close contacts [\(i\)](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5943	0	5868	161	1
1	B	5789	0	5695	149	1
1	C	5160	0	5056	145	0
1	D	5383	0	5280	147	0
2	A	15	0	6	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	15	0	6	2	0
2	C	15	0	6	3	0
2	D	15	0	6	1	0
3	A	15	0	0	2	0
3	B	10	0	0	0	0
3	C	15	0	0	3	0
3	D	10	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	A	185	0	0	6	0
5	B	123	0	0	3	0
5	C	57	0	0	0	0
5	D	64	0	0	1	0
All	All	22816	0	21923	558	1

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 13.

All (558) 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:C:263:ARG:NH2	1:D:697:TRP:CZ3	2.08	1.22
1:C:697:TRP:CZ3	1:D:263:ARG:NH2	2.11	1.17
1:C:263:ARG:NH2	1:D:697:TRP:CH2	2.19	1.11
1:A:43:GLN:O	1:A:45:SER:N	1.89	1.03
1:C:441:MET:HE1	1:C:658:ALA:HB2	1.48	0.95
1:D:441:MET:HE1	1:D:658:ALA:HB2	1.49	0.95
1:D:768[A]:ARG:HG2	1:D:768[A]:ARG:HH11	1.32	0.94
1:D:355:ASP:O	1:D:357:SER:N	2.03	0.92
1:C:67:SER:HB3	1:C:89:ASN:HD21	1.35	0.92
1:A:704:ASN:O	1:A:707[B]:ILE:HG22	1.72	0.90
1:C:697:TRP:CH2	1:D:263:ARG:NH2	2.40	0.89
1:B:701:PRO:HA	1:B:707[B]:ILE:CG2	2.02	0.89
1:A:701:PRO:HA	1:A:707[B]:ILE:CG2	2.02	0.89
1:B:707[A]:ILE:HG23	1:B:708:THR:O	1.74	0.88
1:B:525:PHE:HE1	1:B:558:TYR:CD2	1.92	0.87
1:A:707[B]:ILE:HD11	1:A:711:GLY:HA2	1.55	0.86
1:D:464:VAL:HA	1:D:573:ALA:HB1	1.55	0.86
1:D:604:GLU:HG3	1:D:608:ARG:NH1	1.93	0.83
1:C:441:MET:CE	1:C:658:ALA:HB2	2.08	0.82
1:D:67:SER:HB3	1:D:89:ASN:HD21	1.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:704:ASN:O	1:B:707[B]:ILE:HG22	1.80	0.81
1:B:707[B]:ILE:HD12	1:B:708:THR:O	1.79	0.81
1:B:21:SER:HB3	1:B:28:LYS:HD3	1.63	0.81
1:C:697:TRP:HZ3	1:D:263:ARG:HH21	1.29	0.80
1:A:21:SER:HB3	1:A:28:LYS:HD3	1.63	0.80
1:A:323:TRP:HA	1:A:329:HIS:HE1	1.46	0.79
1:B:323:TRP:HA	1:B:329:HIS:HE1	1.48	0.79
1:B:67:SER:HG	1:B:134:THR:HG1	1.26	0.78
1:C:263:ARG:HH21	1:D:697:TRP:HZ3	1.32	0.78
1:C:708:THR:HG22	1:C:709:SER:H	1.49	0.77
1:D:441:MET:CE	1:D:658:ALA:HB2	2.14	0.77
1:C:659:THR:HG22	1:C:662:VAL:H	1.50	0.76
1:C:67:SER:HB3	1:C:89:ASN:ND2	2.00	0.76
1:B:441:MET:CE	1:B:658:ALA:HB2	2.16	0.75
1:B:74:LEU:HD13	1:B:130:LEU:HD22	1.66	0.75
1:C:467[A]:ILE:HD11	1:C:578:LEU:HD13	1.66	0.75
1:D:768[A]:ARG:CG	1:D:768[A]:ARG:HH11	2.01	0.74
1:A:701:PRO:HA	1:A:707[B]:ILE:HG21	1.70	0.74
1:C:375[B]:ASP:OD1	1:C:376:PRO:HD2	1.88	0.73
1:D:538:ARG:NH2	1:D:716:GLU:OE2	2.21	0.73
1:C:651:VAL:HG22	1:C:652:PRO:HD2	1.69	0.73
1:D:659:THR:HG22	1:D:662:VAL:H	1.53	0.73
1:A:708:THR:HG21	1:A:713:THR:HG22	1.69	0.72
1:D:706:ASN:HB3	1:D:714:LEU:HD23	1.72	0.72
1:C:375[B]:ASP:OD2	1:C:377:THR:HB	1.89	0.72
1:B:659:THR:HG22	1:B:662:VAL:H	1.52	0.72
1:A:526:SER:O	1:A:527:GLU:HB3	1.90	0.71
1:B:36:ALA:HA	1:B:51:LEU:HD13	1.70	0.71
1:D:436:GLU:HG2	1:D:479:GLY:HA3	1.71	0.71
1:B:659:THR:HG21	5:B:2107:HOH:O	1.90	0.71
1:B:707[B]:ILE:HD11	1:B:711:GLY:HA2	1.73	0.71
1:A:237:LEU:HD21	1:A:384[B]:ARG:HG2	1.73	0.71
1:A:659:THR:HG22	1:A:662:VAL:H	1.54	0.71
1:A:36:ALA:HA	1:A:51:LEU:HD13	1.73	0.70
1:D:538:ARG:HA	1:D:541:ILE:HD12	1.73	0.70
1:A:441:MET:CE	1:A:658:ALA:HB2	2.22	0.70
1:A:329:HIS:ND1	1:B:663:PHE:CE1	2.60	0.70
1:D:97:PRO:HG2	1:D:151:GLU:HG2	1.73	0.70
1:A:417:VAL:HG22	1:A:628:THR:HB	1.74	0.69
1:C:97:PRO:HG2	1:C:151:GLU:HG2	1.75	0.69
1:C:703:THR:CG2	1:D:263:ARG:HH22	2.06	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:651:VAL:HG22	1:D:652:PRO:HD2	1.74	0.68
1:A:417:VAL:HG23	1:A:627:GLU:HG2	1.75	0.68
1:A:707[B]:ILE:HD13	1:A:708:THR:H	1.57	0.68
1:D:67:SER:HB3	1:D:89:ASN:ND2	2.09	0.68
1:A:746:LEU:HD13	1:A:759:TYR:HB3	1.75	0.68
1:B:417:VAL:HG22	1:B:628:THR:HB	1.75	0.67
1:C:382:LEU:O	1:C:386:MET:HG3	1.94	0.67
1:B:701:PRO:HA	1:B:707[B]:ILE:HG21	1.76	0.67
1:B:525:PHE:HE1	1:B:558:TYR:CE2	2.12	0.66
1:C:706:ASN:HB3	1:C:714:LEU:HD23	1.77	0.66
1:B:525:PHE:CE1	1:B:558:TYR:CD2	2.81	0.66
1:B:325:PRO:O	1:B:327:THR:HG22	1.95	0.66
1:D:237:LEU:HD21	1:D:384:ARG:HG2	1.78	0.66
1:A:325:PRO:O	1:A:327:THR:HG22	1.96	0.66
1:D:417:VAL:HG22	1:D:628:THR:HB	1.78	0.65
1:C:697:TRP:HZ3	1:D:263:ARG:NH2	1.88	0.65
1:A:329:HIS:HD1	1:B:663:PHE:HZ	1.43	0.65
1:C:37:ALA:HA	1:C:74:LEU:HD21	1.79	0.65
1:D:382:LEU:O	1:D:386:MET:HG3	1.97	0.64
1:A:584:ILE:HG12	1:A:624:LEU:HD21	1.79	0.64
1:B:746:LEU:HD12	1:B:760:ALA:HB2	1.79	0.64
1:B:707[A]:ILE:HD13	1:B:714:LEU:HD23	1.77	0.64
1:A:356:ASN:O	1:A:357:SER:O	2.16	0.64
1:C:651:VAL:CG2	1:C:652:PRO:HD2	2.27	0.64
1:A:659:THR:HG23	1:A:661:ALA:H	1.61	0.64
1:A:707[B]:ILE:HD13	1:A:708:THR:N	2.11	0.64
1:B:96:LEU:HB3	1:B:97:PRO:HD3	1.80	0.63
1:D:517:TRP:CZ3	1:D:592:MET:HE1	2.33	0.63
1:D:426:TYR:CE1	1:D:437:ILE:HD13	2.32	0.63
1:A:766:MET:HE2	1:A:804:ARG:HD2	1.79	0.63
1:B:441:MET:HE3	1:B:658:ALA:HB2	1.80	0.63
1:A:67:SER:HB3	1:A:89:ASN:OD1	1.99	0.63
1:B:67:SER:HB3	1:B:89:ASN:OD1	1.98	0.63
1:A:37:ALA:HA	1:A:74[A]:LEU:HD21	1.80	0.63
1:D:430:ASN:OD1	1:D:433:THR:HG23	1.99	0.63
1:B:538:ARG:HA	1:B:541:ILE:HD12	1.81	0.62
1:B:584:ILE:HG12	1:B:624:LEU:HD21	1.81	0.62
1:A:510:VAL:HG12	1:A:592:MET:HE2	1.81	0.62
1:B:441:MET:HE1	1:B:658:ALA:HB2	1.81	0.62
1:B:659:THR:HG23	1:B:661:ALA:H	1.63	0.62
1:C:263:ARG:HH22	1:D:703:THR:HG22	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:GLY:HA2	3:C:1809:SO4:O4	2.00	0.62
1:C:237:LEU:HD21	1:C:384:ARG:HG2	1.82	0.62
1:D:281:ASP:O	1:D:282:LEU:HB2	1.99	0.62
1:C:510:VAL:HG22	1:C:519:ILE:HG12	1.82	0.62
1:A:521:LEU:HD22	1:A:525:PHE:HD2	1.63	0.62
1:C:470:ARG:HD3	1:C:506:ASP:OD1	2.00	0.62
5:A:2126:HOH:O	1:B:495:GLN:NE2	2.32	0.61
1:B:766:MET:HE2	1:B:804:ARG:HD2	1.82	0.61
1:A:528:ILE:HD12	1:A:529:ALA:H	1.64	0.61
1:C:426:TYR:CE1	1:C:437:ILE:HD13	2.36	0.61
1:B:744:LEU:O	1:B:744:LEU:HD12	2.00	0.61
1:A:707[B]:ILE:CD1	1:A:711:GLY:HA2	2.29	0.61
1:A:93:HIS:HB3	1:A:113:MET:CE	2.31	0.61
1:B:417:VAL:HG23	1:B:627:GLU:HG2	1.82	0.61
1:A:329:HIS:ND1	1:B:663:PHE:CZ	2.61	0.61
1:D:706:ASN:CB	1:D:714:LEU:HD23	2.31	0.60
1:D:8:PHE:C	1:D:8:PHE:CD1	2.73	0.60
1:D:36:ALA:HA	1:D:51:LEU:HD13	1.84	0.60
1:B:510:VAL:HG12	1:B:592:MET:HE2	1.82	0.60
1:B:707[B]:ILE:CD1	1:B:708:THR:N	2.65	0.60
1:C:74:LEU:HD13	1:C:130:LEU:HD22	1.84	0.60
1:A:441:MET:HE1	1:A:658:ALA:HB2	1.83	0.60
1:B:766:MET:HE2	1:B:807:GLU:OE1	2.02	0.60
1:D:622:TRP:HE3	1:D:714:LEU:HD12	1.66	0.60
1:B:707[B]:ILE:HD12	1:B:708:THR:N	2.17	0.60
1:C:36:ALA:HA	1:C:51:LEU:HD13	1.84	0.60
1:C:762:SER:O	1:C:766:MET:HG3	2.01	0.60
1:D:464:VAL:HG12	1:D:574:HIS:O	2.02	0.60
1:C:467[A]:ILE:CD1	1:C:578:LEU:HD13	2.32	0.59
1:D:450:HIS:O	1:D:451:ASN:HB2	2.02	0.59
1:D:708:THR:HG21	1:D:710:GLN:HG3	1.83	0.59
1:D:470:ARG:HD3	1:D:506:ASP:OD1	2.02	0.59
1:A:530:PRO:O	1:A:532:TYR:O	2.20	0.59
1:C:703:THR:HG22	1:D:263:ARG:HH22	1.66	0.59
1:B:559:LEU:HD13	1:B:601:LEU:HA	1.85	0.59
1:D:37:ALA:HA	1:D:74:LEU:HD21	1.83	0.59
1:B:93:HIS:HB3	1:B:113:MET:CE	2.32	0.59
1:C:263:ARG:HH22	1:D:703:THR:CG2	2.15	0.59
1:D:762:SER:O	1:D:766:MET:HG3	2.03	0.59
1:A:599:ARG:NH2	5:A:2144:HOH:O	2.35	0.58
1:B:237:LEU:HD21	1:B:384:ARG:HG2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:GLY:HA2	3:A:1814:SO4:O1	2.03	0.58
1:A:43:GLN:C	1:A:45:SER:N	2.56	0.58
1:D:768[A]:ARG:HH21	1:D:773:PHE:HE2	1.49	0.58
1:C:430:ASN:HB2	2:C:1644:PLP:O3P	2.03	0.58
1:C:8:PHE:C	1:C:8:PHE:CD1	2.76	0.58
1:D:713:THR:HG22	1:D:714:LEU:O	2.03	0.58
1:C:659:THR:CG2	1:C:662:VAL:H	2.16	0.58
1:A:709:SER:N	1:A:710:GLN:HE22	2.02	0.58
1:B:584:ILE:CG1	1:B:624:LEU:HD21	2.34	0.58
1:C:706:ASN:CB	1:C:714:LEU:HD23	2.33	0.58
1:A:644:LYS:NZ	2:A:1644:PLP:O3	2.34	0.58
1:A:775:ARG:HD3	1:B:397:MET:HE2	1.85	0.57
1:B:719:ASP:HB2	1:B:795:ARG:HG3	1.85	0.57
1:C:375[B]:ASP:OD1	1:C:376:PRO:CD	2.51	0.57
1:C:450:HIS:O	1:C:451:ASN:HB2	2.03	0.57
1:A:323:TRP:HA	1:A:329:HIS:CE1	2.33	0.57
1:A:707[B]:ILE:CD1	1:A:708:THR:N	2.67	0.57
1:A:543:ASP:OD2	1:A:545:SER:CB	2.52	0.57
1:C:263:ARG:HH12	1:D:703:THR:HG22	1.68	0.57
1:A:709:SER:N	1:A:710:GLN:NE2	2.52	0.57
1:D:651:VAL:CG2	1:D:652:PRO:HD2	2.34	0.57
1:B:707[B]:ILE:CD1	1:B:711:GLY:HA2	2.34	0.57
1:C:417:VAL:HG22	1:C:628:THR:HB	1.86	0.57
1:A:584:ILE:CG1	1:A:624:LEU:HD21	2.35	0.56
1:A:701:PRO:CA	1:A:707[B]:ILE:HG21	2.35	0.56
1:A:408:LYS:NZ	5:A:2117:HOH:O	2.38	0.56
1:C:373:GLY:H	1:C:374:PRO:CD	2.18	0.56
1:C:225:ILE:HB	3:C:1808:SO4:O4	2.05	0.56
1:A:397:MET:HE2	1:B:775:ARG:HD3	1.87	0.56
1:A:396[A]:VAL:HG22	1:B:348:PHE:CE1	2.41	0.56
1:A:190:ALA:O	1:A:203:GLN:NE2	2.39	0.56
1:A:8:PHE:C	1:A:8:PHE:CD1	2.79	0.56
1:B:323:TRP:HA	1:B:329:HIS:CE1	2.37	0.56
1:D:708:THR:HG21	1:D:710:GLN:OE1	2.06	0.56
1:D:510[B]:VAL:HG13	1:D:519:ILE:HG12	1.87	0.56
1:B:8:PHE:CD1	1:B:10:LEU:HG	2.41	0.55
1:B:193:VAL:HG22	1:B:235:LEU:HD21	1.89	0.55
1:D:74:LEU:HD13	1:D:130:LEU:HD22	1.87	0.55
1:D:659:THR:CG2	1:D:662:VAL:H	2.19	0.55
1:C:263:ARG:HH12	1:D:703:THR:CG2	2.19	0.55
1:A:40:LEU:CD1	1:A:130:LEU:HB2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:ARG:HA	1:A:541:ILE:HD12	1.88	0.55
1:B:622:TRP:HZ2	1:B:699:LYS:HG3	1.72	0.55
1:B:628:THR:OG1	1:B:630:THR:HG23	2.06	0.55
1:C:430:ASN:OD1	1:C:433:THR:HG23	2.06	0.55
1:C:625:GLY:HA2	1:C:714:LEU:CD1	2.36	0.55
1:C:93:HIS:HA	1:C:114:CYS:O	2.05	0.55
1:B:495:GLN:OE1	1:B:496:PRO:HD2	2.07	0.55
1:B:556:SER:O	1:B:560:SER:HB2	2.06	0.55
1:A:525:PHE:HE1	1:A:558:TYR:CD1	2.25	0.55
1:A:757:SER:HB3	1:A:779:ASN:OD1	2.07	0.55
1:A:8:PHE:CD1	1:A:10:LEU:HG	2.41	0.55
1:A:96:LEU:HB3	1:A:97:PRO:HD3	1.89	0.55
1:C:93:HIS:HB2	1:C:136:TYR:HD1	1.72	0.55
1:D:373:GLY:H	1:D:374:PRO:CD	2.19	0.55
1:B:559:LEU:HD12	1:B:600:VAL:HG12	1.87	0.55
1:D:510[B]:VAL:CG1	1:D:519:ILE:HG12	2.37	0.55
1:A:378:PHE:CE2	1:A:382:LEU:HD11	2.42	0.54
1:A:622:TRP:HZ2	1:A:699:LYS:HG3	1.71	0.54
1:A:441:MET:HE3	1:A:658:ALA:HB2	1.87	0.54
1:C:444:ARG:HD3	1:C:666:PHE:CE1	2.42	0.54
1:D:622:TRP:HE3	1:D:714:LEU:CD1	2.21	0.54
1:A:113:MET:HE2	1:A:136:TYR:HD1	1.72	0.54
1:B:708:THR:HG21	1:B:710:GLN:OE1	2.06	0.54
1:D:85:ILE:HG13	1:D:87:ILE:HG23	1.90	0.54
1:A:719:ASP:HB2	1:A:795:ARG:HG3	1.88	0.54
1:A:317:LEU:O	1:A:321[B]:VAL:HG22	2.08	0.54
1:A:321[A]:VAL:HG22	1:B:414:LEU:HD12	1.90	0.54
1:B:521:LEU:HD22	1:B:525:PHE:HD2	1.73	0.54
1:B:766:MET:CE	1:B:804:ARG:HD2	2.37	0.54
1:A:628:THR:OG1	1:A:630:THR:HG22	2.08	0.54
1:C:368:SER:HB2	1:C:372:GLN:HG2	1.89	0.54
1:A:616:GLU:OE2	1:A:629:THR:OG1	2.21	0.53
1:C:649:GLY:O	1:D:395:HIS:HB3	2.08	0.53
1:B:356:ASN:O	1:B:357:SER:O	2.26	0.53
1:A:414:LEU:CD1	1:B:321:VAL:HG13	2.39	0.53
1:D:645:LEU:HB2	5:D:2057:HOH:O	2.08	0.53
1:B:378:PHE:CE2	1:B:382:LEU:HD11	2.43	0.53
1:B:644:LYS:NZ	2:B:1644:PLP:O3	2.39	0.53
1:C:373:GLY:H	1:C:374:PRO:HD2	1.72	0.53
1:B:190:ALA:O	1:B:203:GLN:NE2	2.42	0.53
1:B:766:MET:CE	1:B:807:GLU:OE1	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:713:THR:HG22	1:C:714:LEU:O	2.08	0.53
1:A:74[A]:LEU:HD12	1:A:130:LEU:HD22	1.90	0.53
1:D:368:SER:HB2	1:D:372:GLN:HG2	1.91	0.53
1:C:677:HIS:HB2	1:D:476:ASP:HB3	1.91	0.53
1:D:525:PHE:O	1:D:527:GLU:N	2.42	0.53
1:A:329:HIS:HD1	1:B:663:PHE:HE1	1.53	0.53
1:A:766:MET:CE	1:A:804:ARG:HD2	2.39	0.53
1:A:766:MET:HE2	1:A:807:GLU:OE1	2.09	0.53
1:C:691:ALA:O	1:C:695:ILE:HG13	2.08	0.53
1:C:27:GLY:HA2	3:C:1809:SO4:S	2.50	0.52
1:C:85:ILE:HG13	1:C:87:ILE:HG23	1.90	0.52
1:A:269:LEU:HB3	1:A:292:VAL:HG13	1.92	0.52
1:B:517:TRP:C	1:B:518:ASN:HD22	2.12	0.52
1:B:113:MET:HE2	1:B:136:TYR:HD1	1.74	0.52
1:B:8:PHE:C	1:B:8:PHE:CD1	2.83	0.52
1:C:703:THR:HG21	1:D:263:ARG:HH22	1.74	0.52
1:C:625:GLY:HA2	1:C:714:LEU:HD12	1.91	0.52
1:A:348:PHE:CE1	1:B:396[A]:VAL:HG22	2.44	0.52
1:B:40:LEU:CD1	1:B:130:LEU:HB2	2.39	0.52
1:A:281[A]:ASP:O	1:A:282:LEU:HB2	2.10	0.52
1:B:523:GLU:O	1:B:525:PHE:N	2.43	0.52
1:A:575:VAL:HG12	1:A:610:ILE:HD13	1.91	0.52
1:B:444:ARG:HG3	1:B:666:PHE:CZ	2.45	0.52
1:A:628:THR:OG1	1:A:630:THR:CG2	2.58	0.52
1:B:744:LEU:HD12	1:B:744:LEU:C	2.29	0.52
1:D:768[A]:ARG:CG	1:D:768[A]:ARG:NH1	2.66	0.52
1:A:708:THR:HG21	1:A:713:THR:CG2	2.40	0.51
1:B:325:PRO:O	1:B:327:THR:CG2	2.58	0.51
1:B:441:MET:CE	1:B:639:ILE:HG12	2.40	0.51
1:D:622:TRP:CE3	1:D:714:LEU:CD1	2.93	0.51
1:A:766:MET:CE	1:A:807:GLU:OE1	2.58	0.51
1:D:622:TRP:CE3	1:D:714:LEU:HD12	2.44	0.51
1:A:193:VAL:HG22	1:A:235:LEU:HD21	1.92	0.51
1:A:74[A]:LEU:CD1	1:A:130:LEU:HD22	2.41	0.51
1:C:93:HIS:HB3	1:C:113:MET:CE	2.40	0.51
1:D:478:LEU:O	1:D:478:LEU:HG	2.10	0.51
1:D:478:LEU:O	1:D:482:GLU:HG2	2.11	0.51
1:B:95[B]:SER:OG	1:B:97:PRO:HD2	2.10	0.51
1:A:329:HIS:ND1	1:B:663:PHE:HE1	2.07	0.51
1:B:441:MET:HE2	1:B:639:ILE:HG12	1.91	0.51
1:D:232:TYR:HE1	1:D:242:ILE:HB	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:SER:O	1:A:527:GLU:CB	2.59	0.51
1:B:799:THR:HG22	1:B:803:LYS:HE3	1.92	0.51
1:D:590:MET:HE3	1:D:741:LEU:HD13	1.92	0.51
1:B:708:THR:HG22	1:B:709:SER:N	2.26	0.51
1:C:697:TRP:CE2	1:C:703:THR:HB	2.46	0.51
1:C:708:THR:HG21	1:C:710:GLN:OE1	2.11	0.51
1:B:708:THR:HG22	1:B:709:SER:H	1.76	0.50
1:D:235:LEU:HD13	1:D:242:ILE:HD11	1.93	0.50
1:A:659:THR:HG23	1:A:661:ALA:N	2.26	0.50
1:C:93:HIS:HB3	1:C:113:MET:HE2	1.91	0.50
1:B:525:PHE:CE1	1:B:558:TYR:CE2	2.96	0.50
1:C:93:HIS:HB2	1:C:136:TYR:CD1	2.47	0.50
1:C:622:TRP:HB3	1:C:714:LEU:HD11	1.94	0.50
1:C:511:PHE:HB2	1:C:734:ARG:HB2	1.92	0.50
1:A:708:THR:HG22	1:A:713:THR:O	2.12	0.50
1:C:444:ARG:HD3	1:C:666:PHE:CD1	2.47	0.50
1:D:708:THR:O	1:D:709:SER:CB	2.60	0.50
1:A:628:THR:CG2	1:A:630:THR:HG23	2.42	0.49
1:D:441:MET:HE2	1:D:639:ILE:HG12	1.94	0.49
1:A:441:MET:CE	1:A:639:ILE:HG12	2.41	0.49
1:B:430:ASN:HB2	2:B:1644:PLP:O3P	2.12	0.49
1:A:236:LYS:HE3	1:B:388:TYR:CD2	2.48	0.49
1:B:701:PRO:CA	1:B:707[B]:ILE:CG2	2.86	0.49
1:B:709:SER:O	1:B:710:GLN:C	2.49	0.49
1:B:93:HIS:HB3	1:B:113:MET:HE2	1.95	0.49
2:C:1644:PLP:O2P	1:D:679:HIS:ND1	2.45	0.49
1:A:430:ASN:HB2	2:A:1644:PLP:O3P	2.13	0.49
1:A:441:MET:HE2	1:A:639:ILE:HG12	1.95	0.49
1:A:414:LEU:HD12	1:B:321:VAL:HG13	1.94	0.49
1:B:659:THR:HG23	1:B:661:ALA:N	2.27	0.49
1:B:707[B]:ILE:HD13	1:B:708:THR:H	1.78	0.48
1:C:190:ALA:O	1:C:203:GLN:NE2	2.43	0.48
1:D:708:THR:O	1:D:709:SER:HB2	2.13	0.48
1:C:85:ILE:HG13	1:C:87:ILE:CG2	2.42	0.48
1:D:625:GLY:HA2	1:D:714:LEU:HD13	1.95	0.48
1:A:523:GLU:O	1:A:525:PHE:N	2.46	0.48
1:C:677:HIS:CB	1:D:476:ASP:HB3	2.43	0.48
1:B:515:GLY:HA2	1:B:724:GLN:OE1	2.14	0.48
1:D:61:PHE:CG	1:D:62:PRO:HA	2.48	0.48
1:D:697:TRP:CE2	1:D:703:THR:HB	2.48	0.48
1:B:384:ARG:NH2	5:B:2020:HOH:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:619:THR:HG22	1:B:624:LEU:HD11	1.95	0.48
1:C:441:MET:HE2	1:C:639:ILE:HG12	1.95	0.48
1:D:85:ILE:HG13	1:D:87:ILE:CG2	2.43	0.48
1:C:61:PHE:CG	1:C:62:PRO:HA	2.49	0.48
1:D:519:ILE:HD11	1:D:546:ARG:NH2	2.28	0.48
1:C:467[A]:ILE:CD1	1:C:601:LEU:HD11	2.44	0.48
1:D:510[B]:VAL:HG23	1:D:592:MET:HG2	1.95	0.48
1:A:28:LYS:N	3:A:1814:SO4:O3	2.47	0.47
1:A:515:GLY:HA2	1:A:724:GLN:OE1	2.14	0.47
1:B:269:LEU:CD1	1:B:296:LEU:HD13	2.45	0.47
1:B:8:PHE:CE2	1:B:361:GLN:HG3	2.48	0.47
1:C:298:GLU:O	1:C:302[B]:LEU:HG	2.14	0.47
1:C:659:THR:HG23	1:C:661:ALA:N	2.29	0.47
1:D:659:THR:HG22	1:D:662:VAL:HG23	1.95	0.47
1:A:327:THR:HB	5:A:2081:HOH:O	2.13	0.47
1:A:675:LEU:C	1:A:675:LEU:HD12	2.34	0.47
1:C:18:LEU:HD13	1:C:20:TRP:CZ2	2.50	0.47
1:D:511:PHE:HB2	1:D:734:ARG:HB2	1.95	0.47
1:A:744:LEU:C	1:A:744:LEU:HD12	2.34	0.47
1:D:770:ASP:O	1:D:796:ARG:NH2	2.48	0.47
1:A:321[A]:VAL:HG22	1:B:414:LEU:CD1	2.44	0.47
1:A:408:LYS:HG2	5:A:2116:HOH:O	2.15	0.47
1:D:10[A]:LEU:HD11	1:D:210:PHE:CD1	2.50	0.47
1:A:368:SER:HB2	1:A:372:GLN:HG2	1.97	0.47
1:C:517:TRP:CZ3	1:C:592:MET:HE1	2.50	0.47
1:C:95:SER:HB2	1:C:97:PRO:HD2	1.97	0.47
1:A:93:HIS:HB3	1:A:113:MET:HE3	1.96	0.47
1:A:325:PRO:O	1:A:327:THR:CG2	2.62	0.47
1:A:746:LEU:HD13	1:A:759:TYR:CB	2.44	0.47
1:A:397:MET:CE	1:B:775:ARG:HD3	2.44	0.47
1:C:81:ARG:HH21	1:C:287:VAL:HG22	1.79	0.47
1:A:40:LEU:HD11	1:A:130:LEU:HB2	1.96	0.47
1:D:604:GLU:HG3	1:D:608:ARG:HH12	1.76	0.47
1:D:766:MET:HE3	1:D:804:ARG:HH11	1.80	0.47
1:C:708:THR:HG22	1:C:709:SER:N	2.23	0.47
1:B:575:VAL:HG12	1:B:610:ILE:HD13	1.96	0.47
1:C:375[B]:ASP:OD1	1:C:376:PRO:N	2.48	0.47
1:B:538:ARG:HH22	1:B:716:GLU:CD	2.19	0.46
1:D:81:ARG:HH21	1:D:287:VAL:HG22	1.79	0.46
1:D:546:ARG:HB3	1:D:596:LEU:HD22	1.96	0.46
1:A:521:LEU:HD22	1:A:525:PHE:CD2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:ILE:HD13	1:A:641:CYS:SG	2.56	0.46
1:A:710:GLN:N	1:A:710:GLN:NE2	2.63	0.46
1:B:61:PHE:O	1:B:139:GLU:HA	2.14	0.46
1:D:746:LEU:HD12	1:D:760:ALA:HB2	1.98	0.46
1:D:56:PRO:C	1:D:57:ILE:HD12	2.36	0.46
1:D:71:PHE:CE2	1:D:87:ILE:HG13	2.50	0.46
1:D:8:PHE:CE2	1:D:361:GLN:HG3	2.50	0.46
1:B:183:LEU:HD23	1:B:184:LEU:N	2.31	0.46
1:B:378:PHE:CD1	1:B:697:TRP:CD2	3.03	0.46
1:B:701:PRO:CA	1:B:707[B]:ILE:HG21	2.42	0.46
1:D:508:PRO:HA	1:D:522:PRO:HD3	1.97	0.46
1:C:58:GLN:O	1:C:137:ALA:HA	2.16	0.46
1:C:708:THR:CG2	1:C:710:GLN:OE1	2.64	0.46
1:D:512:LEU:HD13	1:D:517:TRP:NE1	2.31	0.46
1:D:526:SER:O	1:D:527:GLU:CB	2.64	0.46
1:A:663:PHE:CE1	1:B:329:HIS:ND1	2.77	0.46
1:A:708:THR:HG23	1:A:710:GLN:HE21	1.81	0.46
1:C:246:VAL:HA	1:C:269:LEU:O	2.16	0.46
1:D:93:HIS:HB2	1:D:136:TYR:HD1	1.81	0.46
1:D:281:ASP:CG	1:D:283:ILE:HD13	2.37	0.46
1:A:707[B]:ILE:HD11	1:A:711:GLY:CA	2.37	0.45
1:A:744:LEU:O	1:A:744:LEU:HD12	2.16	0.45
1:C:614:PHE:CG	1:C:637:PRO:HB3	2.51	0.45
1:C:36:ALA:HB1	1:C:74:LEU:HD11	1.97	0.45
1:C:232:TYR:HE1	1:C:242:ILE:HB	1.80	0.45
1:C:659:THR:HG22	1:C:662:VAL:HG23	1.98	0.45
1:A:701:PRO:CA	1:A:707[B]:ILE:CG2	2.83	0.45
1:B:18:LEU:HD13	1:B:20:TRP:CZ2	2.52	0.45
1:C:426:TYR:OH	1:C:677:HIS:O	2.33	0.45
1:A:168:LEU:O	1:A:172:MET:HG2	2.16	0.45
1:A:628:THR:HG23	1:A:630:THR:HG23	1.99	0.45
1:C:281[B]:ASP:OD2	1:C:283:ILE:HB	2.17	0.45
1:D:95:SER:HB2	1:D:97:PRO:HD2	1.97	0.45
1:A:277:ASP:HA	1:A:278:PRO:HD3	1.81	0.45
1:A:613:ILE:HA	1:A:639:ILE:O	2.17	0.45
1:A:775:ARG:HD3	1:B:397:MET:CE	2.44	0.45
1:C:404:GLU:N	1:C:405:PRO:HD2	2.31	0.45
1:C:746:LEU:O	1:C:747:LYS:C	2.55	0.45
1:D:246:VAL:HA	1:D:269:LEU:O	2.17	0.45
1:A:281[A]:ASP:HB3	1:A:283:ILE:HD13	1.99	0.45
1:D:373:GLY:H	1:D:374:PRO:HD2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:HIS:CB	1:A:113:MET:CE	2.95	0.45
1:A:519:ILE:HG12	1:A:535:PHE:HE2	1.81	0.45
1:C:512:LEU:HD13	1:C:517:TRP:NE1	2.31	0.45
1:D:36:ALA:HB1	1:D:74:LEU:HD11	1.98	0.45
1:A:448:VAL:HG21	1:A:665:SER:HB2	1.98	0.44
1:A:708:THR:CG2	1:A:713:THR:HG22	2.41	0.44
1:C:642:PHE:HB2	1:C:655:VAL:HG12	1.99	0.44
1:A:707[A]:ILE:HD13	1:A:714:LEU:HD23	1.99	0.44
1:D:538:ARG:HH22	1:D:716:GLU:CD	2.17	0.44
1:A:18:LEU:HD13	1:A:20:TRP:CZ2	2.52	0.44
1:B:283:ILE:N	1:B:283:ILE:CD1	2.80	0.44
1:C:590:MET:HE3	1:C:741:LEU:HD13	2.00	0.44
1:C:91:VAL:O	1:C:116:LEU:HB2	2.17	0.44
1:B:60:GLY:HA2	1:B:139:GLU:O	2.17	0.44
1:B:616:GLU:OE2	1:B:629:THR:OG1	2.25	0.44
1:B:378:PHE:CD1	1:B:697:TRP:CE2	3.05	0.44
1:C:269:LEU:HD12	1:C:296:LEU:HD13	1.99	0.44
1:D:659:THR:HG23	1:D:661:ALA:N	2.33	0.44
1:A:517:TRP:HB3	1:A:541:ILE:HD11	1.99	0.44
1:A:619:THR:HG22	1:A:624:LEU:HD11	1.99	0.44
1:A:707[A]:ILE:HA	1:A:707[A]:ILE:HD13	1.90	0.44
1:B:324:TRP:HB3	1:B:327:THR:HG21	1.99	0.44
1:B:719:ASP:O	1:B:723:VAL:HG23	2.16	0.44
1:C:355:ASP:HB3	1:C:356:ASN:H	1.47	0.44
1:B:269:LEU:HB3	1:B:292:VAL:HG13	2.00	0.44
1:D:88:SER:HA	1:D:120:ASP:O	2.17	0.44
1:B:354:SER:O	1:B:355:ASP:O	2.36	0.44
1:B:399:PRO:O	1:B:400:GLU:HB2	2.17	0.44
1:C:562:HIS:ND1	1:C:562:HIS:N	2.65	0.44
1:C:676:LEU:HA	1:C:676:LEU:HD23	1.73	0.44
1:A:113:MET:CE	1:A:136:TYR:HD1	2.31	0.44
1:A:281[B]:ASP:O	1:A:282:LEU:HB2	2.17	0.44
1:C:91:VAL:HG12	1:C:116:LEU:HD12	2.00	0.44
1:D:766:MET:HB3	1:D:804:ARG:NH1	2.32	0.44
1:A:367:ALA:CA	1:A:372:GLN:HB2	2.48	0.43
1:B:525:PHE:HB3	1:B:526:SER:H	1.49	0.43
1:C:644:LYS:NZ	2:C:1644:PLP:O3	2.50	0.43
1:C:378:PHE:CE1	1:C:382:LEU:HG	2.53	0.43
1:A:8:PHE:CE2	1:A:361:GLN:HG3	2.53	0.43
1:C:61:PHE:CD1	1:C:62:PRO:HA	2.53	0.43
1:C:614:PHE:CD1	1:C:637:PRO:HB3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:PHE:CE2	1:C:361:GLN:HG3	2.52	0.43
1:D:691:ALA:O	1:D:695:ILE:HG13	2.18	0.43
1:A:766:MET:HE2	1:A:804:ARG:HH11	1.82	0.43
1:B:95[A]:SER:OG	1:B:151:GLU:OE1	2.25	0.43
1:D:474:HIS:O	1:D:480:ALA:HB1	2.19	0.43
1:D:614:PHE:CG	1:D:637:PRO:HB3	2.53	0.43
1:C:36:ALA:CB	1:C:74:LEU:HD11	2.48	0.43
1:D:764:LEU:HD21	1:D:768[B]:ARG:NH2	2.33	0.43
1:D:93:HIS:HB2	1:D:136:TYR:CD1	2.54	0.43
1:A:249:ASP:HB2	1:A:270:VAL:CG1	2.48	0.43
1:A:325:PRO:HA	1:B:426:TYR:OH	2.18	0.43
1:B:517:TRP:CZ3	1:B:592:MET:HE2	2.54	0.43
1:C:236:LYS:HD2	1:C:236:LYS:HA	1.81	0.43
1:C:321:VAL:HG22	1:D:414:LEU:CD1	2.48	0.43
1:C:102:LEU:HD13	1:C:118:PHE:CE1	2.53	0.43
1:D:417:VAL:CG1	1:D:642:PHE:CZ	3.02	0.43
1:A:136:TYR:OH	1:A:163:MET:HG3	2.19	0.43
1:D:297:LYS:HE2	1:D:297:LYS:HB3	1.75	0.43
1:A:310:ARG:O	1:A:314:MET:HG3	2.19	0.43
1:A:317:LEU:HD21	1:B:411:GLU:OE2	2.18	0.43
1:B:508:PRO:HG3	1:B:525:PHE:HE2	1.84	0.43
1:C:8:PHE:CD2	1:C:361:GLN:HG3	2.54	0.43
1:D:525:PHE:O	1:D:526:SER:C	2.57	0.43
1:A:61:PHE:O	1:A:139:GLU:HA	2.19	0.43
1:A:663:PHE:HZ	1:B:329:HIS:HD1	1.55	0.43
1:C:578:LEU:HD23	1:C:612:VAL:HG22	2.01	0.43
1:C:622:TRP:HE3	1:C:714:LEU:HD12	1.83	0.43
1:D:398:PHE:N	1:D:399:PRO:HD2	2.34	0.43
1:A:697:TRP:CE2	1:A:703:THR:HB	2.53	0.42
1:B:135:LEU:HD22	1:B:163:MET:HE2	2.01	0.42
1:D:350:ILE:HD12	1:D:362:GLN:HB2	2.00	0.42
1:D:744:LEU:HD12	1:D:744:LEU:C	2.39	0.42
1:D:746:LEU:O	1:D:747:LYS:C	2.57	0.42
1:D:95:SER:CB	1:D:97:PRO:HD2	2.49	0.42
1:A:700:ASP:HB2	5:A:2167:HOH:O	2.19	0.42
1:A:81:ARG:HH21	1:A:287:VAL:HG13	1.83	0.42
1:C:297:LYS:HB3	1:C:297:LYS:HE2	1.76	0.42
1:B:617:VAL:HG13	1:B:643:ALA:HB3	1.99	0.42
1:D:193:VAL:HG22	1:D:235:LEU:HD21	2.02	0.42
1:D:8:PHE:CD2	1:D:361:GLN:HG3	2.55	0.42
1:D:664:ASP:O	1:D:666:PHE:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:TRP:HB3	1:B:327:THR:CG2	2.50	0.42
1:C:707:ILE:HD13	1:C:707:ILE:HA	1.78	0.42
1:A:517:TRP:CZ3	1:A:592:MET:CE	3.02	0.42
1:C:235:LEU:HD13	1:C:242:ILE:HD11	2.01	0.42
1:C:651:VAL:HG22	1:C:652:PRO:CD	2.46	0.42
1:A:399:PRO:O	1:A:400:GLU:HB2	2.19	0.42
1:A:709:SER:CA	1:A:710:GLN:NE2	2.83	0.42
1:C:664:ASP:O	1:C:666:PHE:N	2.52	0.42
1:C:777:LEU:HA	1:C:777:LEU:HD23	1.78	0.42
1:D:18:LEU:HD13	1:D:20:TRP:CZ2	2.55	0.42
1:A:367:ALA:HB1	1:A:372:GLN:HB2	2.00	0.42
1:A:525:PHE:HE1	1:A:558:TYR:CG	2.37	0.42
1:D:576:GLY:O	1:D:577:ALA:HB2	2.19	0.42
1:A:324:TRP:HB3	1:A:327:THR:CG2	2.50	0.42
1:A:466[A]:VAL:CG2	1:A:579:ILE:HG22	2.49	0.42
1:B:707[B]:ILE:HD13	1:B:708:THR:N	2.33	0.42
1:C:135:LEU:HD13	1:C:163:MET:HB3	2.01	0.42
1:C:350:ILE:HD12	1:C:362:GLN:HB2	2.01	0.42
1:C:398:PHE:N	1:C:399:PRO:HD2	2.34	0.42
1:C:744:LEU:HD12	1:C:744:LEU:C	2.40	0.42
1:B:34:GLY:HA3	1:B:293:PHE:CE2	2.55	0.42
1:B:368:SER:HB2	1:B:372:GLN:HG2	2.02	0.42
1:C:40:LEU:HD11	1:C:130:LEU:HB2	2.02	0.42
1:D:420:GLY:O	1:D:636:LYS:HE3	2.20	0.42
1:D:655:VAL:HG13	1:D:657:LEU:CD1	2.49	0.42
1:B:168:LEU:O	1:B:172:MET:HG2	2.20	0.42
1:B:71:PHE:CE2	1:B:87:ILE:HG13	2.55	0.42
1:A:324:TRP:HB3	1:A:327:THR:HG21	2.00	0.41
1:C:551:LEU:HD22	1:C:555:TYR:CZ	2.55	0.41
1:D:317:LEU:HD12	1:D:317:LEU:HA	1.75	0.41
1:D:664:ASP:C	1:D:666:PHE:H	2.23	0.41
1:A:135:LEU:HD22	1:A:163:MET:HE2	2.02	0.41
1:B:441:MET:HE3	1:B:658:ALA:CB	2.48	0.41
1:D:644:LYS:NZ	2:D:1644:PLP:O3	2.51	0.41
1:D:594:ASP:HA	1:D:595:PRO:HD2	1.86	0.41
1:A:397:MET:CE	1:B:775:ARG:CD	2.98	0.41
1:B:675:LEU:HD12	1:B:675:LEU:C	2.40	0.41
1:B:707[B]:ILE:CD1	1:B:708:THR:H	2.30	0.41
1:C:655:VAL:HG13	1:C:657:LEU:CD1	2.51	0.41
1:D:269:LEU:HD12	1:D:296:LEU:HD13	2.01	0.41
1:D:61:PHE:CD1	1:D:62:PRO:HA	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:TRP:CD2	1:B:501:ARG:HD2	2.56	0.41
1:B:606:ARG:HA	5:B:2100:HOH:O	2.20	0.41
1:C:343:ARG:HD2	1:D:396:VAL:HG23	2.03	0.41
1:B:12:LEU:HD12	1:B:12:LEU:HA	1.72	0.41
1:B:701:PRO:HA	1:B:707[B]:ILE:HG22	1.96	0.41
1:B:375:ASP:HB3	1:B:378:PHE:H	1.85	0.41
1:D:58:GLN:O	1:D:137:ALA:HA	2.20	0.41
1:D:622:TRP:CE3	1:D:714:LEU:HD11	2.56	0.41
1:D:760:ALA:HA	1:D:781[A]:ILE:HD11	2.02	0.41
1:A:719:ASP:O	1:A:723:VAL:HG23	2.21	0.41
1:B:281:ASP:O	1:B:282:LEU:HB2	2.20	0.41
1:C:625:GLY:HA2	1:C:714:LEU:HD13	2.03	0.41
1:D:582:PRO:O	1:D:584:ILE:N	2.48	0.41
1:D:622:TRP:HZ2	1:D:699:LYS:HG3	1.85	0.41
1:C:290:ASP:O	1:C:294:LYS:HB2	2.21	0.41
1:C:664:ASP:C	1:C:666:PHE:N	2.74	0.41
1:A:329:HIS:CE1	1:B:663:PHE:HE1	2.39	0.41
1:A:397:MET:HE3	1:B:775:ARG:CD	2.51	0.41
1:C:208:ARG:HD2	1:C:208:ARG:O	2.21	0.41
1:D:61:PHE:O	1:D:139:GLU:HA	2.21	0.41
1:C:12:LEU:HD22	1:C:359:LEU:HG	2.03	0.41
1:C:417:VAL:HG23	1:C:627:GLU:HG2	2.03	0.41
1:A:610:ILE:HA	1:A:611:PRO:HD3	1.96	0.40
1:D:28:LYS:HE3	1:D:189:THR:O	2.21	0.40
1:B:766:MET:HE2	1:B:804:ARG:HH11	1.86	0.40
1:C:40:LEU:CD1	1:C:130:LEU:HB2	2.50	0.40
1:C:24:THR:O	1:C:25:SER:HB2	2.20	0.40
1:C:467[A]:ILE:HD12	1:C:601:LEU:HD11	2.03	0.40
1:C:664:ASP:C	1:C:666:PHE:H	2.23	0.40
1:C:766:MET:HB3	1:C:804:ARG:NH1	2.36	0.40
1:D:522:PRO:HG2	1:D:525:PHE:HE2	1.85	0.40
1:D:36:ALA:CB	1:D:74:LEU:HD11	2.51	0.40
1:B:40:LEU:HD11	1:B:130:LEU:HB2	2.04	0.40
1:C:88:SER:HA	1:C:120:ASP:O	2.21	0.40
1:C:622:TRP:HE3	1:C:714:LEU:CD1	2.34	0.40
1:D:476:ASP:C	1:D:481:MET:HG2	2.42	0.40
1:C:263:ARG:NH2	1:D:703:THR:HG22	2.35	0.40
1:A:49:THR:HA	1:A:182:ASP:O	2.21	0.40
1:A:282:LEU:HD23	1:A:282:LEU:HA	1.87	0.40
1:B:777:LEU:HA	1:B:777:LEU:HD23	1.86	0.40
1:C:623:ARG:HG3	1:C:624:LEU:CD1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:378:PHE:CE1	1:D:382:LEU:HG	2.56	0.40
1:B:760:ALA:HA	1:B:781:ILE:HD11	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:807:GLU:OE2	1:B:769:GLU:OE1[1_455]	2.11	0.09

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	773/831 (93%)	724 (94%)	37 (5%)	12 (2%)	11	19
1	B	747/831 (90%)	699 (94%)	37 (5%)	11 (2%)	12	21
1	C	665/831 (80%)	621 (93%)	37 (6%)	7 (1%)	17	29
1	D	694/831 (84%)	644 (93%)	40 (6%)	10 (1%)	13	23
All	All	2879/3324 (87%)	2688 (93%)	151 (5%)	40 (1%)	13	23

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	355	ASP
1	A	357	SER
1	A	709	SER
1	B	355	ASP
1	B	357	SER
1	C	118	PHE
1	C	355	ASP
1	D	356	ASN

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Mol	Chain	Res	Type
1	D	526	SER
1	A	44	PRO
1	B	118	PHE
1	C	105	ASN
1	C	643	ALA
1	D	357	SER
1	D	527	GLU
1	D	709	SER
1	A	373	GLY
1	A	375	ASP
1	A	500	GLY
1	A	524	SER
1	A	526	SER
1	A	527	GLU
1	A	644	LYS
1	B	281	ASP
1	B	373	GLY
1	B	524	SER
1	B	644	LYS
1	C	357	SER
1	D	577	ALA
1	D	644	LYS
1	A	643	ALA
1	D	643	ALA
1	B	375	ASP
1	B	500	GLY
1	B	557	ALA
1	C	373	GLY
1	D	421	TRP
1	B	643	ALA
1	C	421	TRP
1	D	373	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	637/704 (90%)	603 (95%)	34 (5%)	26	48
1	B	617/704 (88%)	585 (95%)	32 (5%)	27	49
1	C	549/704 (78%)	526 (96%)	23 (4%)	34	59
1	D	569/704 (81%)	546 (96%)	23 (4%)	36	62
All	All	2372/2816 (84%)	2260 (95%)	112 (5%)	33	54

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	PHE
1	A	9	HIS
1	A	21	SER
1	A	23	ASN
1	A	51	LEU
1	A	82	GLN
1	A	281[A]	ASP
1	A	281[B]	ASP
1	A	321[A]	VAL
1	A	321[B]	VAL
1	A	326	PHE
1	A	327	THR
1	A	396[A]	VAL
1	A	396[B]	VAL
1	A	403	TYR
1	A	417	VAL
1	A	464[A]	VAL
1	A	464[B]	VAL
1	A	466[A]	VAL
1	A	466[B]	VAL
1	A	519	ILE
1	A	524	SER
1	A	551	LEU
1	A	624	LEU
1	A	628	THR
1	A	630	THR
1	A	655	VAL
1	A	659	THR
1	A	667	SER
1	A	675	LEU
1	A	707[A]	ILE
1	A	707[B]	ILE
1	A	709	SER

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Mol	Chain	Res	Type
1	A	710	GLN
1	B	8	PHE
1	B	9	HIS
1	B	21	SER
1	B	23	ASN
1	B	42	GLN
1	B	74	LEU
1	B	82	GLN
1	B	125	THR
1	B	281	ASP
1	B	283	ILE
1	B	326	PHE
1	B	327	THR
1	B	396[A]	VAL
1	B	396[B]	VAL
1	B	403	TYR
1	B	417	VAL
1	B	466	VAL
1	B	494	GLN
1	B	519	ILE
1	B	550	THR
1	B	560	SER
1	B	624	LEU
1	B	655	VAL
1	B	659	THR
1	B	667	SER
1	B	675	LEU
1	B	703	THR
1	B	707[A]	ILE
1	B	707[B]	ILE
1	B	709	SER
1	B	720	GLU
1	B	757	SER
1	C	8	PHE
1	C	42	GLN
1	C	51	LEU
1	C	104	LEU
1	C	118	PHE
1	C	125	THR
1	C	131	LEU
1	C	263	ARG
1	C	354	SER

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Mol	Chain	Res	Type
1	C	355	ASP
1	C	356	ASN
1	C	366	CYS
1	C	370	TRP
1	C	417	VAL
1	C	562	HIS
1	C	628	THR
1	C	630	THR
1	C	655	VAL
1	C	659	THR
1	C	709	SER
1	C	714	LEU
1	C	722	LEU
1	C	763	LEU
1	D	8	PHE
1	D	25	SER
1	D	42	GLN
1	D	51	LEU
1	D	120	ASP
1	D	125	THR
1	D	131	LEU
1	D	182	ASP
1	D	366	CYS
1	D	370	TRP
1	D	375	ASP
1	D	417	VAL
1	D	524	SER
1	D	526	SER
1	D	556	SER
1	D	630	THR
1	D	655	VAL
1	D	659	THR
1	D	714	LEU
1	D	722	LEU
1	D	763	LEU
1	D	768[A]	ARG
1	D	768[B]	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	304	ASN

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Mol	Chain	Res	Type
1	A	710	GLN
1	B	304	ASN
1	B	518	ASN
1	C	14	HIS
1	C	89	ASN
1	C	451	ASN
1	C	677	HIS
1	C	725	GLN
1	D	14	HIS
1	D	89	ASN
1	D	451	ASN
1	D	725	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PLP	A	1644	1	15,15,16	1.84	3 (20%)	20,22,23	1.47	3 (15%)
3	SO4	A	1812	-	4,4,4	0.20	0	6,6,6	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	A	1813	-	4,4,4	0.22	0	6,6,6	0.25	0
3	SO4	A	1814	-	4,4,4	0.18	0	6,6,6	0.21	0
2	PLP	B	1644	1	15,15,16	1.75	2 (13%)	20,22,23	1.64	4 (20%)
3	SO4	B	1812	-	4,4,4	0.22	0	6,6,6	0.33	0
3	SO4	B	1813	4	4,4,4	0.28	0	6,6,6	0.59	0
2	PLP	C	1644	1	15,15,16	1.86	2 (13%)	20,22,23	1.75	5 (25%)
3	SO4	C	1807	-	4,4,4	0.15	0	6,6,6	0.15	0
3	SO4	C	1808	-	4,4,4	0.18	0	6,6,6	0.33	0
3	SO4	C	1809	-	4,4,4	0.24	0	6,6,6	0.46	0
2	PLP	D	1644	1	15,15,16	1.92	3 (20%)	20,22,23	1.65	2 (10%)
3	SO4	D	1808	-	4,4,4	0.14	0	6,6,6	0.32	0
3	SO4	D	1809	4	4,4,4	0.15	0	6,6,6	0.56	0

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	SO4	A	1812	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1813	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1814	-	-	0/0/0/0	0/0/0/0
2	PLP	B	1644	1	-	0/6/6/8	0/1/1/1
3	SO4	B	1812	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1813	4	-	0/0/0/0	0/0/0/0
2	PLP	C	1644	1	-	0/6/6/8	0/1/1/1
3	SO4	C	1807	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1808	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1809	-	-	0/0/0/0	0/0/0/0
2	PLP	D	1644	1	-	0/6/6/8	0/1/1/1
3	SO4	D	1808	-	-	0/0/0/0	0/0/0/0
3	SO4	D	1809	4	-	0/0/0/0	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1644	PLP	O3-C3	-5.86	1.23	1.37
2	C	1644	PLP	O3-C3	-5.81	1.23	1.37
2	A	1644	PLP	O3-C3	-5.74	1.23	1.37
2	B	1644	PLP	O3-C3	-5.60	1.24	1.37
2	D	1644	PLP	C6-N1	2.01	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1644	PLP	C6-N1	2.08	1.38	1.34
2	C	1644	PLP	C2-N1	2.18	1.38	1.33
2	D	1644	PLP	C2-N1	2.21	1.38	1.33
2	B	1644	PLP	C2-N1	2.22	1.38	1.33
2	A	1644	PLP	C2-N1	2.45	1.39	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1644	PLP	C5-C6-N1	-2.59	119.49	123.87
2	A	1644	PLP	C5-C6-N1	-2.48	119.66	123.87
2	B	1644	PLP	C5-C6-N1	-2.21	120.13	123.87
2	C	1644	PLP	O4P-P-O1P	-2.15	100.43	106.47
2	D	1644	PLP	C5-C6-N1	-2.06	120.38	123.87
2	B	1644	PLP	O3-C3-C2	2.03	122.03	117.78
2	A	1644	PLP	C6-C5-C4	2.18	120.00	118.18
2	C	1644	PLP	O3P-P-O1P	2.36	119.74	110.50
2	B	1644	PLP	C6-C5-C4	2.92	120.62	118.18
2	C	1644	PLP	C6-C5-C4	3.74	121.30	118.18
2	A	1644	PLP	O4P-C5A-C5	4.49	118.34	109.32
2	C	1644	PLP	O4P-C5A-C5	4.51	118.39	109.32
2	B	1644	PLP	O4P-C5A-C5	5.08	119.53	109.32
2	D	1644	PLP	O4P-C5A-C5	5.78	120.95	109.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1644	PLP	2	0
3	A	1814	SO4	2	0
2	B	1644	PLP	2	0
2	C	1644	PLP	3	0
3	C	1808	SO4	1	0
3	C	1809	SO4	2	0
2	D	1644	PLP	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	769/831 (92%)	-0.02	24 (3%)	49	52	19, 36, 74, 111	0
1	B	756/831 (90%)	-0.04	22 (2%)	52	55	19, 36, 74, 111	0
1	C	681/831 (81%)	0.42	81 (11%)	5	4	27, 53, 102, 144	0
1	D	709/831 (85%)	0.18	55 (7%)	14	14	24, 51, 90, 118	0
All	All	2915/3324 (87%)	0.13	182 (6%)	21	22	19, 43, 88, 144	0

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	446	PHE	6.7
1	C	448	VAL	5.9
1	C	708	THR	5.6
1	C	806	GLY	5.4
1	C	470	ARG	5.4
1	D	448	VAL	5.4
1	C	709	SER	5.4
1	D	100	LYS	5.3
1	C	728	SER	5.2
1	D	478	LEU	5.1
1	C	746	LEU	5.0
1	C	661	ALA	4.9
1	C	517	TRP	4.8
1	C	560	SER	4.7
1	A	48	ALA	4.7
1	C	450	HIS	4.6
1	C	726	ILE	4.5
1	D	98	ALA	4.5
1	C	449	ASP	4.5
1	C	442	ALA	4.4
1	C	512	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	758	LEU	4.2
1	A	709	SER	4.2
1	D	575	VAL	4.1
1	D	464	VAL	4.1
1	C	600	VAL	4.0
1	C	725	GLN	4.0
1	D	574	HIS	4.0
1	C	732	VAL	4.0
1	A	47	SER	3.8
1	D	483	ALA	3.8
1	C	548	ALA	3.8
1	C	763	LEU	3.7
1	C	805	LEU	3.7
1	D	479	GLY	3.7
1	A	451	ASN	3.6
1	C	476	ASP	3.6
1	D	444	ARG	3.6
1	B	102	LEU	3.5
1	C	729	HIS	3.5
1	D	96	LEU	3.5
1	C	722	LEU	3.4
1	C	447	CYS	3.4
1	C	504	PHE	3.4
1	D	102	LEU	3.4
1	B	114	CYS	3.4
1	C	665	SER	3.4
1	C	467[A]	ILE	3.3
1	D	446	PHE	3.3
1	C	445	LYS	3.3
1	C	723	VAL	3.3
1	B	748	ALA	3.3
1	C	719	ASP	3.3
1	C	727	SER	3.3
1	C	355	ASP	3.3
1	C	779	ASN	3.2
1	D	533	GLY	3.2
1	C	710	GLN	3.2
1	C	724	GLN	3.2
1	D	760	ALA	3.1
1	C	730	SER	3.1
1	C	781	ILE	3.1
1	D	477	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	450	HIS	3.1
1	C	802	TYR	3.1
1	D	666	PHE	3.1
1	C	514	ASN	3.0
1	D	730	SER	3.0
1	D	759	TYR	3.0
1	D	103	GLY	3.0
1	D	166	LYS	3.0
1	D	688	CYS	2.9
1	A	688	CYS	2.9
1	C	760	ALA	2.9
1	C	354	SER	2.9
1	A	493	LEU	2.9
1	D	447	CYS	2.9
1	D	155	VAL	2.9
1	B	355	ASP	2.9
1	D	105	ASN	2.8
1	C	688	CYS	2.8
1	B	98	ALA	2.8
1	B	354	SER	2.8
1	D	451	ASN	2.8
1	C	558	TYR	2.8
1	D	335	GLU	2.8
1	B	492	PHE	2.8
1	C	511	PHE	2.8
1	D	685	ALA	2.8
1	C	518	ASN	2.8
1	C	607	ASN	2.8
1	C	42	GLN	2.8
1	C	766	MET	2.8
1	A	448	VAL	2.7
1	B	153	ALA	2.7
1	D	686	MET	2.7
1	A	431	GLY	2.7
1	B	103	GLY	2.7
1	C	451	ASN	2.7
1	A	46	SER	2.7
1	C	610	ILE	2.7
1	C	735	VAL	2.7
1	C	606	ARG	2.7
1	D	356	ASN	2.7
1	A	42	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	660	ASP	2.6
1	A	526	SER	2.6
1	B	451	ASN	2.6
1	D	95	SER	2.6
1	C	687	GLY	2.6
1	C	731	ALA	2.5
1	A	652	PRO	2.5
1	C	609	LYS	2.5
1	D	665	SER	2.5
1	C	510	VAL	2.5
1	A	655	VAL	2.5
1	B	652	PRO	2.5
1	D	99	ALA	2.5
1	C	666	PHE	2.5
1	B	683	ALA	2.5
1	D	137	ALA	2.5
1	D	142	ILE	2.5
1	B	574	HIS	2.4
1	D	764	LEU	2.4
1	C	602	VAL	2.4
1	A	731	ALA	2.4
1	B	669	ASP	2.4
1	C	561	LYS	2.4
1	C	707	ILE	2.4
1	C	83	ILE	2.4
1	C	547	ASP	2.4
1	B	452	PHE	2.4
1	C	747	LYS	2.4
1	A	84	PRO	2.4
1	B	525	PHE	2.4
1	D	687	GLY	2.3
1	D	9	HIS	2.3
1	A	653	LEU	2.3
1	C	653	LEU	2.3
1	D	355	ASP	2.3
1	D	732	VAL	2.3
1	B	647	THR	2.3
1	B	448	VAL	2.3
1	A	648	GLY	2.3
1	D	8	PHE	2.3
1	A	710	GLN	2.3
1	C	604	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	558	TYR	2.3
1	C	780	VAL	2.2
1	C	556	SER	2.2
1	C	646	LEU	2.2
1	D	449	ASP	2.2
1	D	769	GLU	2.2
1	D	662	VAL	2.2
1	A	643	ALA	2.2
1	D	573	ALA	2.2
1	C	552	ALA	2.2
1	D	153	ALA	2.2
1	D	94	SER	2.2
1	A	707[A]	ILE	2.1
1	C	711	GLY	2.1
1	C	744	LEU	2.1
1	D	354	SER	2.1
1	C	515	GLY	2.1
1	A	646	LEU	2.1
1	D	684	HIS	2.1
1	A	430	ASN	2.1
1	B	668	GLY	2.1
1	A	654	ALA	2.1
1	C	555	TYR	2.1
1	C	662	VAL	2.1
1	B	563	LEU	2.1
1	B	687	GLY	2.1
1	D	807	GLU	2.1
1	C	506	ASP	2.1
1	C	664	ASP	2.1
1	D	127	ALA	2.1
1	A	432	SER	2.1
1	C	596	LEU	2.1
1	B	651	VAL	2.0
1	D	651	VAL	2.0
1	C	172	MET	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 [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, 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	LLDF	B-factors(Å ²)	Q<0.9
3	SO4	A	1813	5/5	0.99	0.20	2.42	39,40,59,63	0
3	SO4	C	1808	5/5	0.99	0.18	2.06	37,47,51,66	5
3	SO4	D	1808	5/5	0.98	0.19	1.95	36,38,46,58	5
3	SO4	B	1812	5/5	0.99	0.15	1.82	29,37,52,57	5
3	SO4	A	1814	5/5	0.93	0.14	0.32	56,58,73,86	5
3	SO4	A	1812	5/5	0.96	0.12	0.26	35,42,66,71	5
3	SO4	C	1809	5/5	0.95	0.14	0.04	25,31,67,79	5
3	SO4	D	1809	5/5	0.95	0.12	-0.31	17,31,74,99	5
2	PLP	D	1644	15/16	0.98	0.15	-0.47	27,51,59,64	0
2	PLP	B	1644	15/16	0.99	0.19	-0.47	19,25,38,39	0
2	PLP	A	1644	15/16	0.99	0.21	-0.49	14,27,34,35	0
2	PLP	C	1644	15/16	0.98	0.13	-0.87	42,56,77,91	0
3	SO4	B	1813	5/5	0.95	0.10	-1.29	32,38,71,81	5
3	SO4	C	1807	5/5	0.97	0.09	-1.57	30,45,66,83	5
4	MG	D	1810	1/1	0.94	0.06	-	45,45,45,45	0
4	MG	B	1814	1/1	0.97	0.17	-	58,58,58,58	1

6.5 Other polymers [i](#)

There are no such residues in this entry.