



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 4, 2026 – 11:09 PM UTC

PDB ID : 1WDW / pdb_00001wdw
Title : Structural basis of mutual activation of the tryptophan synthase a2b2 complex from a hyperthermophile, *Pyrococcus furiosus*
Authors : Lee, S.J.; Ogasahara, K.; Ma, J.; Nishio, K.; Ishida, M.; Yamagata, Y.; Tsukihara, T.; Yutani, K.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2004-05-19
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

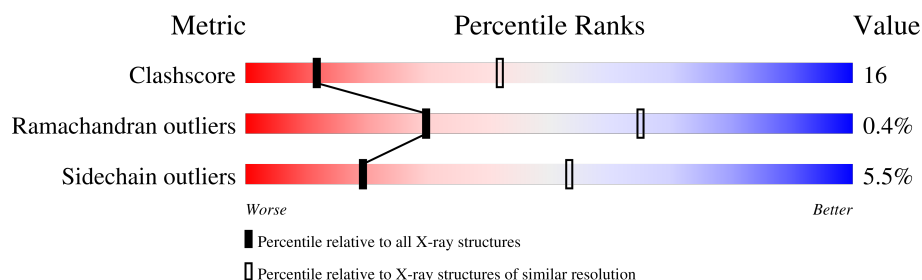
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	248	65% 31% ..
1	C	248	66% 30% ..
1	E	248	67% 31% .
1	G	248	68% 28% ..
1	I	248	67% 30% ..
1	K	248	66% 28% . 6%
2	B	385	68% 27% .
2	D	385	66% 30% .

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Mol	Chain	Length	Quality of chain
2	F	385	 69% 27% .
2	H	385	 67% 29% .
2	J	385	 68% 28% 5%
2	L	385	 66% 31% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 29563 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.

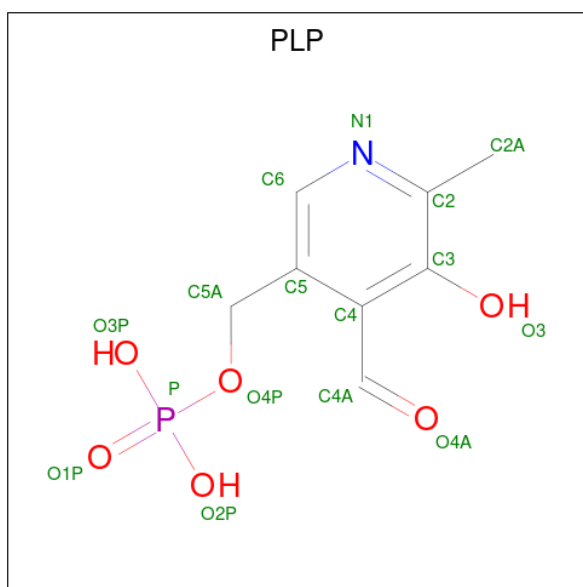
- Molecule 1 is a protein called Tryptophan synthase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	0	0	0
			1895	1224	321	346	4			
1	C	241	Total	C	N	O	S	0	0	0
			1895	1225	321	345	4			
1	E	248	Total	C	N	O	S	0	0	0
			1942	1251	331	356	4			
1	G	242	Total	C	N	O	S	0	0	0
			1904	1230	322	348	4			
1	I	244	Total	C	N	O	S	0	0	0
			1919	1238	327	350	4			
1	K	234	Total	C	N	O	S	0	0	0
			1835	1184	313	334	4			

- Molecule 2 is a protein called Tryptophan synthase beta chain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	385	Total	C	N	O	S	0	0	0
			2977	1902	512	551	12			
2	D	385	Total	C	N	O	S	0	0	0
			2977	1902	512	551	12			
2	F	385	Total	C	N	O	S	0	0	0
			2977	1902	512	551	12			
2	H	385	Total	C	N	O	S	0	0	0
			2977	1902	512	551	12			
2	J	385	Total	C	N	O	S	0	0	0
			2977	1902	512	551	12			
2	L	385	Total	C	N	O	S	0	0	0
			2977	1902	512	551	12			

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	F	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	H	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	J	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	L	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	23	Total	O	0	0
			23	23		
4	C	2	Total	O	0	0
			2	2		
4	D	23	Total	O	0	0
			23	23		
4	E	4	Total	O	0	0
			4	4		
4	F	33	Total	O	0	0
			33	33		
4	G	9	Total	O	0	0
			9	9		

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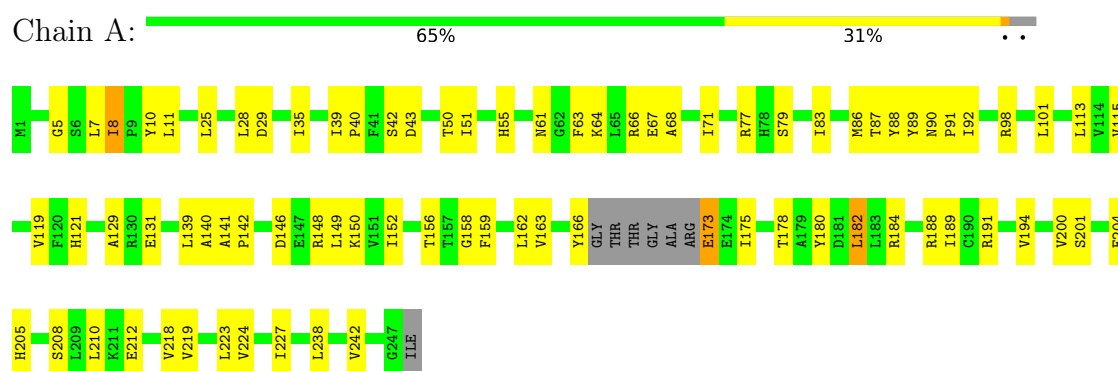
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	36	Total 36	O 36	0	0
4	I	13	Total 13	O 13	0	0
4	J	43	Total 43	O 43	0	0
4	L	35	Total 35	O 35	0	0

3 Residue-property plots

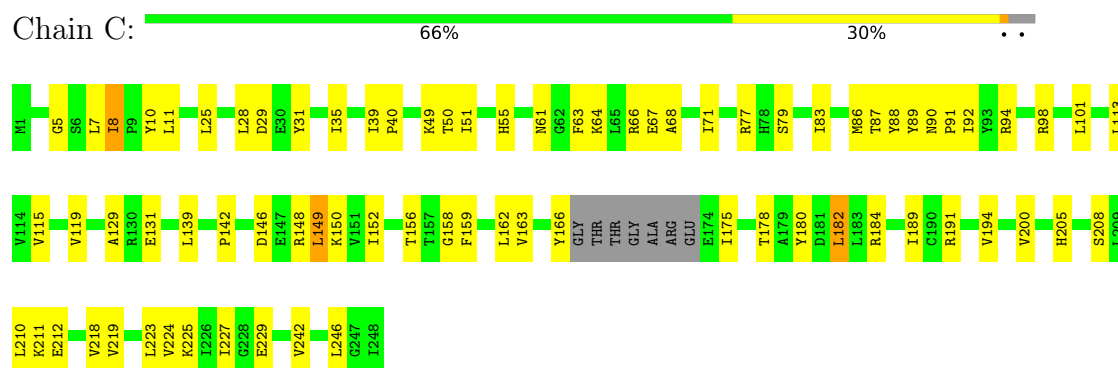
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

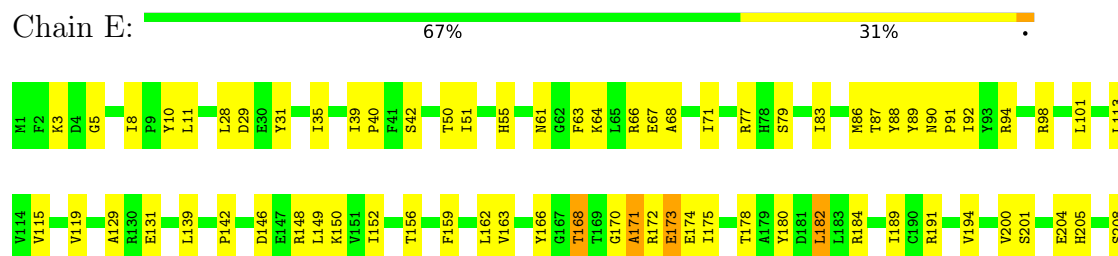
- Molecule 1: Tryptophan synthase alpha chain



- Molecule 1: Tryptophan synthase alpha chain



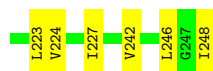
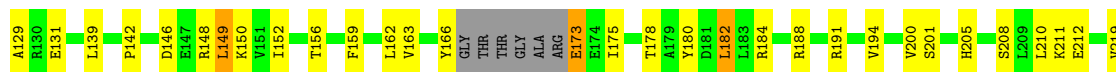
- Molecule 1: Tryptophan synthase alpha chain





- Molecule 1: Tryptophan synthase alpha chain

Chain G: 68% 28% ..



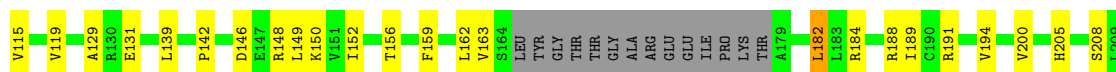
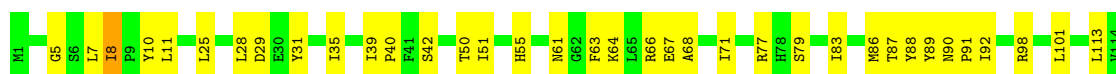
- Molecule 1: Tryptophan synthase alpha chain

Chain I: 67% 30% ..



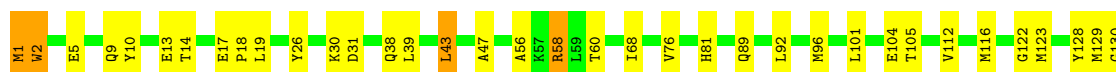
- Molecule 1: Tryptophan synthase alpha chain

Chain K: 66% 28% • 6%



- Molecule 2: Tryptophan synthase beta chain 1

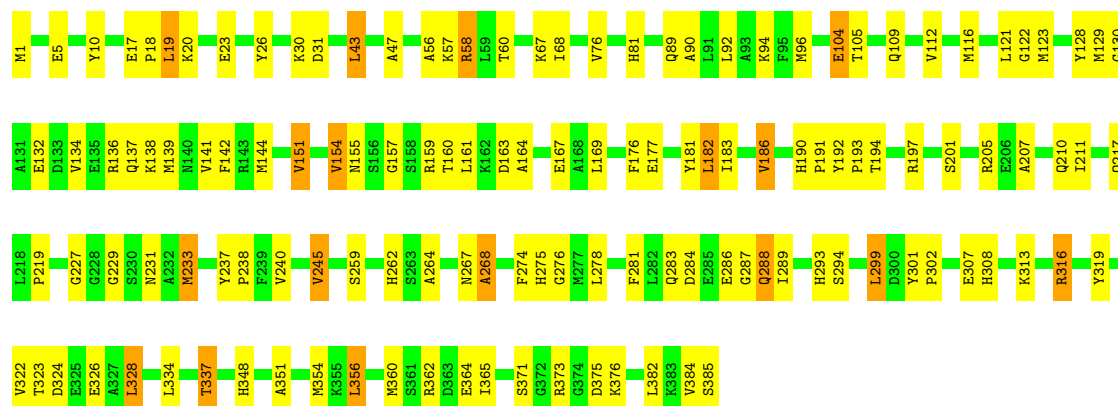
Chain B: 68% 27% •





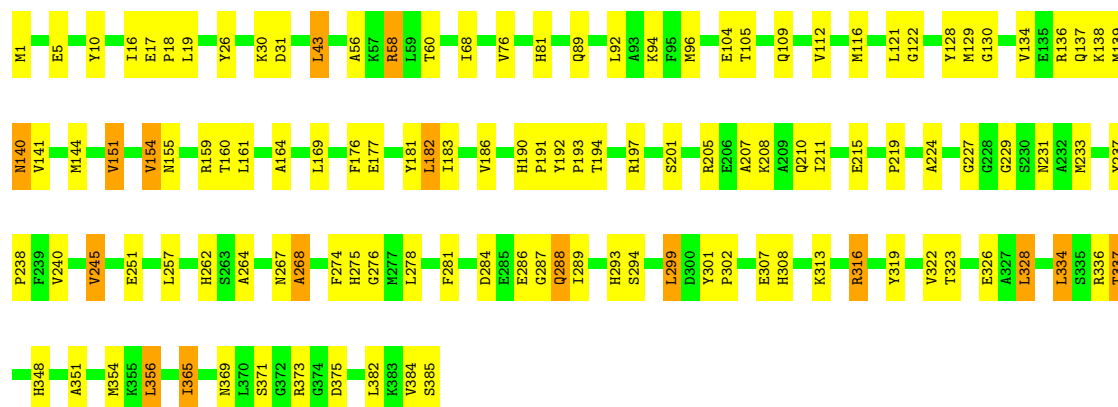
• Molecule 2: Tryptophan synthase beta chain 1

Chain D: 66% 30% •



• Molecule 2: Tryptophan synthase beta chain 1

Chain F: 69% 27% •



• Molecule 2: Tryptophan synthase beta chain 1

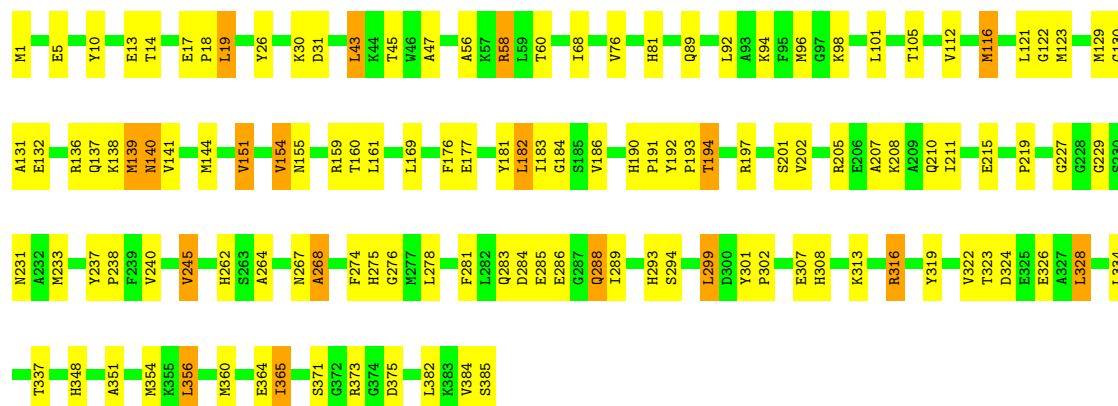
Chain H: 67% 29% •





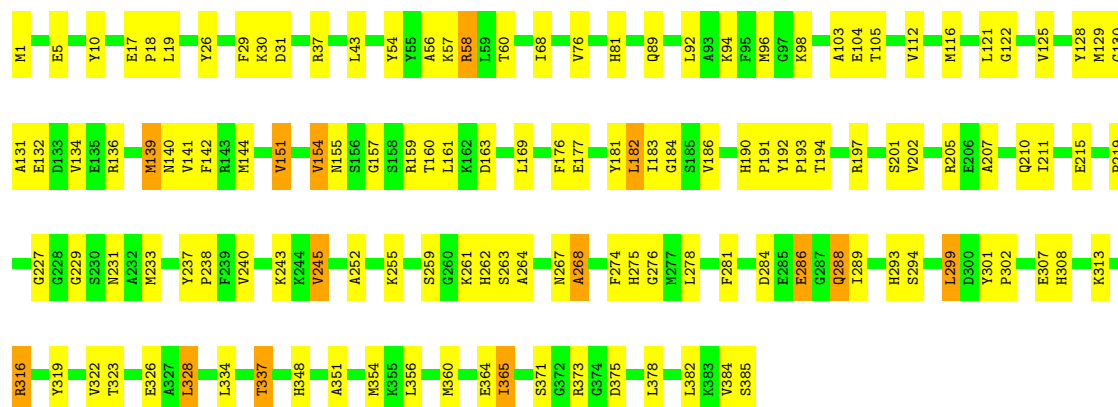
• Molecule 2: Tryptophan synthase beta chain 1

Chain J: 68% 28% 5%



• Molecule 2: Tryptophan synthase beta chain 1

Chain L: 66% 31% 3%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.06Å 220.26Å 292.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.17 – 3.00	Depositor
% Data completeness (in resolution range)	97.7 (89.17-3.00)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.196 , 0.231	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	29563	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.42	0/1931	0.92	5/2605 (0.2%)
1	C	0.46	0/1931	0.90	5/2604 (0.2%)
1	E	0.46	0/1979	0.91	5/2670 (0.2%)
1	G	0.45	0/1940	0.89	4/2616 (0.2%)
1	I	0.46	0/1955	0.89	4/2635 (0.2%)
1	K	0.43	0/1869	0.91	5/2519 (0.2%)
2	B	0.50	0/3038	0.93	6/4099 (0.1%)
2	D	0.51	1/3038 (0.0%)	0.93	5/4099 (0.1%)
2	F	0.50	0/3038	0.92	6/4099 (0.1%)
2	H	0.51	0/3038	0.92	5/4099 (0.1%)
2	J	0.50	1/3038 (0.0%)	0.93	7/4099 (0.2%)
2	L	0.47	0/3038	0.92	7/4099 (0.2%)
All	All	0.48	2/29833 (0.0%)	0.92	64/40243 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	116	MET	SD-CE	5.99	1.94	1.79
2	D	233	MET	SD-CE	-5.50	1.65	1.79

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	TRP	N-CA-C	8.76	122.81	109.23
1	I	115	VAL	N-CA-C	7.96	118.72	110.36
1	A	115	VAL	N-CA-C	7.88	118.64	110.36
1	K	115	VAL	N-CA-C	7.69	118.44	110.36
2	D	245	VAL	N-CA-C	7.11	118.23	108.84

There are no chirality outliers.

There are no planarity outliers.

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	1895	0	1948	57	0
1	C	1895	0	1953	56	0
1	E	1942	0	1998	62	0
1	G	1904	0	1959	55	1
1	I	1919	0	1975	60	0
1	K	1835	0	1889	51	0
2	B	2977	0	2999	113	0
2	D	2977	0	2999	124	0
2	F	2977	0	2999	105	0
2	H	2977	0	2999	107	0
2	J	2977	0	2999	114	0
2	L	2977	0	2999	123	1
3	B	15	0	7	0	0
3	D	15	0	7	0	0
3	F	15	0	6	1	0
3	H	15	0	7	0	0
3	J	15	0	7	0	0
3	L	15	0	7	0	0
4	B	23	0	0	2	0
4	C	2	0	0	0	0
4	D	23	0	0	4	0
4	E	4	0	0	1	0
4	F	33	0	0	6	0
4	G	9	0	0	1	0
4	H	36	0	0	2	0
4	I	13	0	0	3	0
4	J	43	0	0	5	0
4	L	35	0	0	9	0
All	All	29563	0	29757	939	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 16.

The worst 5 of 939 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)
2:J:122:GLY:CA	2:L:58:ARG:HH22	1.25	1.49
2:F:122:GLY:CA	2:H:58:ARG:HH22	1.31	1.40
2:B:122:GLY:CA	2:D:58:ARG:HH22	1.44	1.30
2:F:122:GLY:HA2	2:H:58:ARG:NH2	1.45	1.27
2:B:58:ARG:HH22	2:D:122:GLY:CA	1.46	1.27

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:G:66:ARG:NH2	2:L:98:LYS:O[4_466]	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	237/248 (96%)	226 (95%)	11 (5%)	0	100	100
1	C	237/248 (96%)	226 (95%)	11 (5%)	0	100	100
1	E	246/248 (99%)	230 (94%)	15 (6%)	1 (0%)	30	65
1	G	238/248 (96%)	228 (96%)	10 (4%)	0	100	100
1	I	240/248 (97%)	228 (95%)	12 (5%)	0	100	100
1	K	230/248 (93%)	219 (95%)	11 (5%)	0	100	100
2	B	383/385 (100%)	352 (92%)	29 (8%)	2 (0%)	24	60
2	D	383/385 (100%)	355 (93%)	25 (6%)	3 (1%)	16	50
2	F	383/385 (100%)	354 (92%)	27 (7%)	2 (0%)	24	60
2	H	383/385 (100%)	358 (94%)	22 (6%)	3 (1%)	16	50
2	J	383/385 (100%)	357 (93%)	24 (6%)	2 (0%)	24	60
2	L	383/385 (100%)	356 (93%)	24 (6%)	3 (1%)	16	50
All	All	3726/3798 (98%)	3489 (94%)	221 (6%)	16 (0%)	30	65

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	171	ALA
2	J	268	ALA
2	L	268	ALA
2	B	268	ALA
2	D	186	VAL

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	201/205 (98%)	193 (96%)	8 (4%)	28	62
1	C	201/205 (98%)	194 (96%)	7 (4%)	32	65
1	E	205/205 (100%)	196 (96%)	9 (4%)	25	60
1	G	202/205 (98%)	194 (96%)	8 (4%)	28	62
1	I	203/205 (99%)	195 (96%)	8 (4%)	28	62
1	K	194/205 (95%)	189 (97%)	5 (3%)	40	72
2	B	306/306 (100%)	286 (94%)	20 (6%)	15	47
2	D	306/306 (100%)	286 (94%)	20 (6%)	15	47
2	F	306/306 (100%)	286 (94%)	20 (6%)	15	47
2	H	306/306 (100%)	284 (93%)	22 (7%)	13	43
2	J	306/306 (100%)	286 (94%)	20 (6%)	15	47
2	L	306/306 (100%)	286 (94%)	20 (6%)	15	47
All	All	3042/3066 (99%)	2875 (94%)	167 (6%)	19	53

5 of 167 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	139	LEU
1	K	139	LEU
1	I	178	THR
2	J	169	LEU

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Mol	Chain	Res	Type
2	L	76	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 104 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	36	ASN
1	I	52	GLN
2	L	275	HIS
2	H	137	GLN
2	H	275	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PLP	H	400	2	15,15,16	1.75	5 (33%)	21,22,23	2.02	7 (33%)
3	PLP	B	400	2	15,15,16	1.68	4 (26%)	21,22,23	2.04	7 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PLP	J	400	2	15,15,16	1.72	4 (26%)	21,22,23	1.99	4 (19%)
3	PLP	F	400	2	15,15,16	1.57	4 (26%)	21,22,23	2.07	6 (28%)
3	PLP	L	400	2	15,15,16	1.66	4 (26%)	21,22,23	2.06	6 (28%)
3	PLP	D	400	2	15,15,16	1.65	3 (20%)	21,22,23	2.15	7 (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
3	PLP	H	400	2	-	0/6/6/8	0/1/1/1
3	PLP	B	400	2	-	0/6/6/8	0/1/1/1
3	PLP	J	400	2	-	0/6/6/8	0/1/1/1
3	PLP	F	400	2	-	0/6/6/8	0/1/1/1
3	PLP	L	400	2	-	0/6/6/8	0/1/1/1
3	PLP	D	400	2	-	0/6/6/8	0/1/1/1

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	400	PLP	C2-N1	3.20	1.39	1.33
3	H	400	PLP	C5-C4	3.08	1.44	1.40
3	B	400	PLP	C5-C4	3.07	1.44	1.40
3	D	400	PLP	C2-N1	3.04	1.39	1.33
3	L	400	PLP	C2-N1	2.83	1.38	1.33

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	400	PLP	O4P-C5A-C5	6.03	120.66	109.36
3	F	400	PLP	O4P-C5A-C5	5.87	120.36	109.36
3	L	400	PLP	O4P-C5A-C5	5.85	120.31	109.36
3	J	400	PLP	O4P-C5A-C5	5.67	119.99	109.36
3	H	400	PLP	O4P-C5A-C5	5.58	119.82	109.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	400	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.