



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:21 PM GMT

PDB ID : 1TAT
Title : CRYSTALLINE MITOCHONDRIAL ASPARTATE AMINOTRANSFERASE EXISTS IN ONLY TWO CONFORMATIONS
Authors : Hohenester, E.; Jansonius, J.N.
Deposited on : 1993-10-04
Resolution : 3.00 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

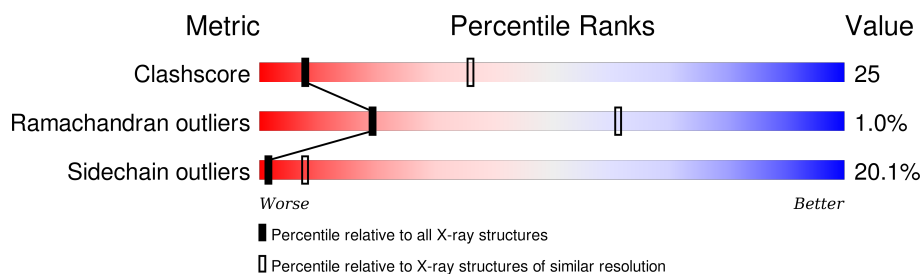
1 Overall quality at a glance

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	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (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 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	401	 40% 44% 15% •
1	B	401	 41% 44% 13% •

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6352 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.

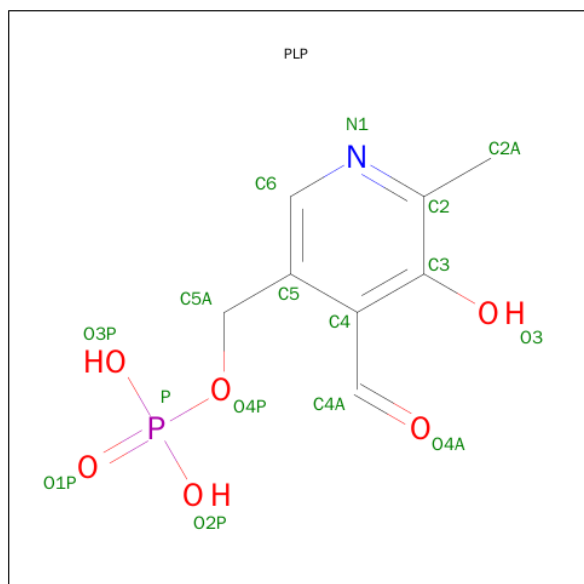
- Molecule 1 is a protein called ASPARTATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	129	0	0
			3161	2004	558	581	18			
1	B	401	Total	C	N	O	S	125	0	0
			3161	2004	558	581	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	PRO	SER	CONFLICT	UNP P00508
B	47	PRO	SER	CONFLICT	UNP P00508

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



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

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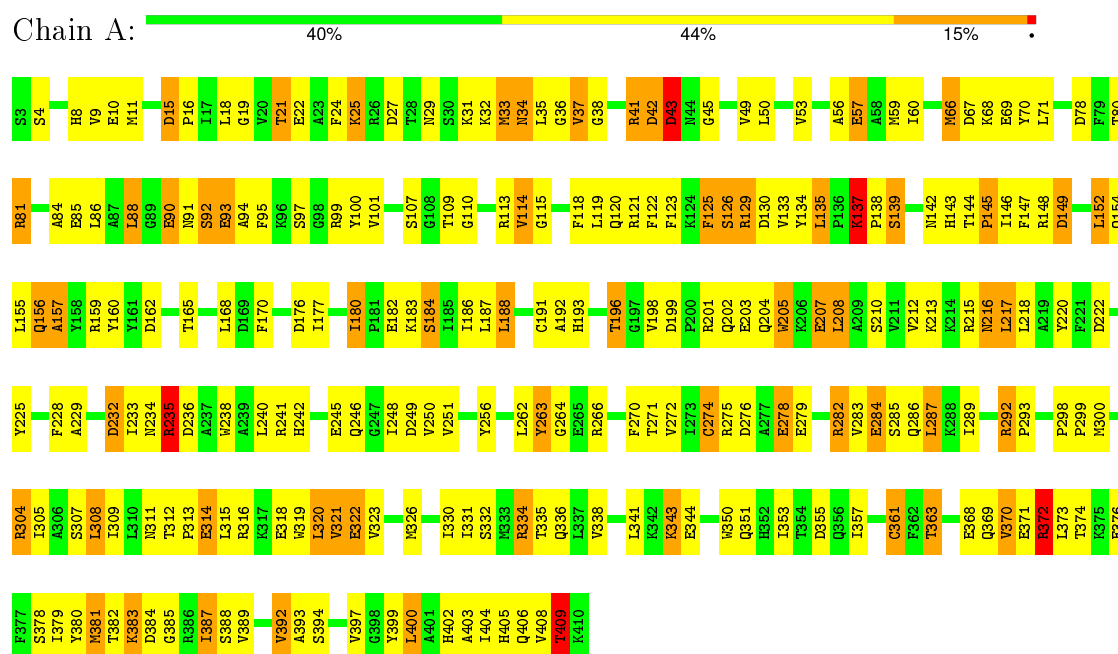
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

3 Residue-property plots

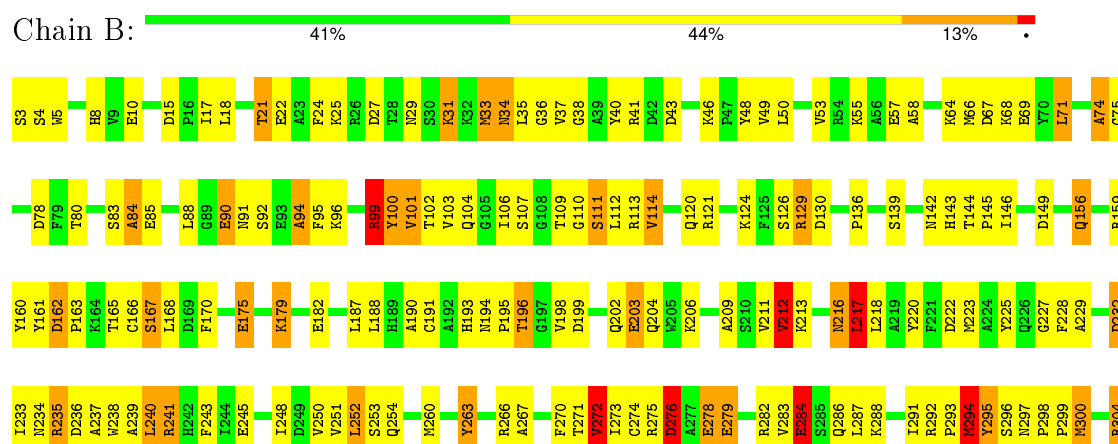
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

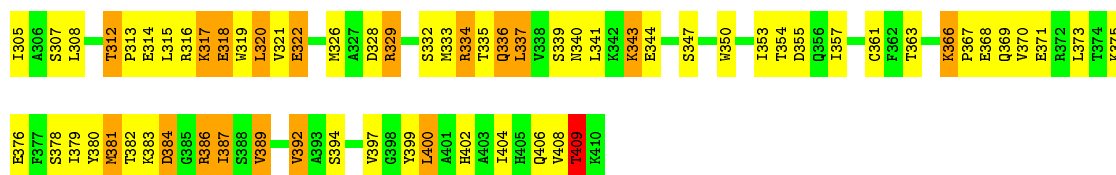
Note EDS was not executed.

• Molecule 1: ASPARTATE AMINOTRANSFERASE



• Molecule 1: ASPARTATE AMINOTRANSFERASE





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.50Å 89.60Å 144.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.150 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6352	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

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: 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	1.20	20/3231 (0.6%)	1.74	73/4360 (1.7%)
1	B	1.24	20/3231 (0.6%)	1.78	70/4360 (1.6%)
All	All	1.22	40/6462 (0.6%)	1.76	143/8720 (1.6%)

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	2	0

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	57	GLU	CD-OE2	12.88	1.39	1.25
1	B	182	GLU	CD-OE1	8.31	1.34	1.25
1	A	57	GLU	CD-OE1	7.79	1.34	1.25
1	B	376	GLU	CD-OE1	7.50	1.33	1.25
1	A	318	GLU	CD-OE2	6.79	1.33	1.25
1	B	85	GLU	CD-OE2	6.70	1.33	1.25
1	A	343	LYS	CE-NZ	-6.55	1.32	1.49
1	B	245	GLU	CD-OE1	6.42	1.32	1.25
1	B	22	GLU	CD-OE1	6.40	1.32	1.25
1	B	344	GLU	CD-OE1	6.23	1.32	1.25
1	A	376	GLU	CD-OE1	6.15	1.32	1.25
1	A	322	GLU	CD-OE1	6.12	1.32	1.25
1	A	93	GLU	CD-OE2	6.06	1.32	1.25
1	A	203	GLU	CD-OE2	5.90	1.32	1.25
1	B	279	GLU	CD-OE2	5.90	1.32	1.25
1	B	322	GLU	CD-OE1	5.83	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	279	GLU	CD-OE1	5.73	1.31	1.25
1	A	344	GLU	CD-OE1	5.55	1.31	1.25
1	A	85	GLU	CD-OE2	5.50	1.31	1.25
1	B	318	GLU	CD-OE2	5.50	1.31	1.25
1	B	175	GLU	CD-OE1	5.39	1.31	1.25
1	A	278	GLU	CD-OE1	5.38	1.31	1.25
1	A	10	GLU	CD-OE1	5.37	1.31	1.25
1	A	245	GLU	CD-OE1	5.32	1.31	1.25
1	B	368	GLU	CD-OE2	5.31	1.31	1.25
1	A	90	GLU	CD-OE2	5.30	1.31	1.25
1	B	10	GLU	CD-OE1	5.26	1.31	1.25
1	B	278	GLU	CD-OE1	5.26	1.31	1.25
1	B	314	GLU	CD-OE1	5.25	1.31	1.25
1	A	149	ASP	CG-OD2	5.25	1.37	1.25
1	B	90	GLU	CD-OE2	5.24	1.31	1.25
1	A	368	GLU	CD-OE2	5.24	1.31	1.25
1	A	371	GLU	CD-OE2	5.22	1.31	1.25
1	B	203	GLU	CD-OE2	5.21	1.31	1.25
1	A	69	GLU	CD-OE1	5.14	1.31	1.25
1	A	314	GLU	CD-OE1	5.14	1.31	1.25
1	B	371	GLU	CD-OE2	5.07	1.31	1.25
1	B	284	GLU	CD-OE1	5.05	1.31	1.25
1	B	69	GLU	CD-OE1	5.03	1.31	1.25
1	A	22	GLU	CD-OE1	5.02	1.31	1.25

All (143) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	386	ARG	NE-CZ-NH2	17.04	128.82	120.30
1	B	121	ARG	NE-CZ-NH1	11.37	125.99	120.30
1	B	355	ASP	CB-CG-OD2	-9.72	109.56	118.30
1	B	67	ASP	CB-CG-OD2	-9.37	109.87	118.30
1	A	67	ASP	CB-CG-OD2	-9.17	110.05	118.30
1	B	294	MET	CG-SD-CE	-9.09	85.66	100.20
1	A	304	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	B	27	ASP	CB-CG-OD1	8.66	126.09	118.30
1	A	15	ASP	CB-CG-OD2	-8.66	110.51	118.30
1	A	43	ASP	CB-CG-OD2	-8.57	110.58	118.30
1	B	328	ASP	CB-CG-OD1	8.55	126.00	118.30
1	B	232	ASP	CB-CG-OD1	8.49	125.94	118.30
1	B	295	TYR	CB-CG-CD2	-8.25	116.05	121.00
1	A	67	ASP	CB-CG-OD1	8.10	125.59	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	ASP	CB-CG-OD1	8.04	125.54	118.30
1	A	113	ARG	NE-CZ-NH1	8.01	124.31	120.30
1	A	276	ASP	CB-CG-OD1	7.96	125.46	118.30
1	B	111	SER	N-CA-CB	7.96	122.43	110.50
1	B	222	ASP	CB-CG-OD2	-7.93	111.16	118.30
1	A	43	ASP	CB-CG-OD1	7.93	125.43	118.30
1	B	232	ASP	CB-CG-OD2	-7.85	111.24	118.30
1	A	355	ASP	CB-CG-OD2	-7.83	111.25	118.30
1	B	317	LYS	N-CA-CB	7.82	124.67	110.60
1	B	27	ASP	CB-CG-OD2	-7.80	111.28	118.30
1	A	361	CYS	CA-CB-SG	-7.79	99.97	114.00
1	A	276	ASP	CB-CG-OD2	-7.78	111.30	118.30
1	B	99	ARG	NE-CZ-NH2	7.78	124.19	120.30
1	B	386	ARG	NE-CZ-NH1	-7.75	116.42	120.30
1	A	78	ASP	CB-CG-OD1	-7.75	111.33	118.30
1	B	99	ARG	NE-CZ-NH1	-7.73	116.43	120.30
1	A	232	ASP	CB-CG-OD1	7.69	125.22	118.30
1	B	159	ARG	NE-CZ-NH1	-7.67	116.47	120.30
1	B	67	ASP	CB-CG-OD1	7.31	124.88	118.30
1	B	328	ASP	CB-CG-OD2	-7.24	111.78	118.30
1	A	130	ASP	CB-CG-OD1	7.17	124.76	118.30
1	A	380	TYR	CB-CG-CD1	7.17	125.30	121.00
1	A	27	ASP	CB-CG-OD1	7.14	124.73	118.30
1	B	304	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	A	184	SER	N-CA-CB	7.07	121.11	110.50
1	A	27	ASP	CB-CG-OD2	-7.02	111.98	118.30
1	A	249	ASP	CB-CG-OD1	-7.01	111.99	118.30
1	A	130	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	A	372	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	B	222	ASP	CB-CG-OD1	6.99	124.59	118.30
1	A	81	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	B	355	ASP	CB-CG-OD1	6.89	124.50	118.30
1	A	78	ASP	CB-CG-OD2	6.88	124.49	118.30
1	B	384	ASP	CB-CG-OD2	-6.88	112.11	118.30
1	A	165	THR	N-CA-CB	-6.86	97.27	110.30
1	B	78	ASP	CB-CG-OD2	6.85	124.47	118.30
1	B	239	ALA	CB-CA-C	-6.84	99.83	110.10
1	B	175	GLU	N-CA-CB	6.81	122.85	110.60
1	B	149	ASP	CB-CG-OD2	-6.77	112.20	118.30
1	B	267	ALA	N-CA-CB	6.76	119.57	110.10
1	A	121	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	A	236	ASP	CB-CG-OD2	6.76	124.38	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	355	ASP	CB-CG-OD1	6.74	124.36	118.30
1	B	241	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	A	137	LYS	N-CA-CB	6.69	122.65	110.60
1	A	157	ALA	N-CA-CB	-6.67	100.77	110.10
1	B	216	ASN	N-CA-CB	-6.65	98.63	110.60
1	A	232	ASP	CB-CG-OD2	-6.62	112.34	118.30
1	A	156	GLN	N-CA-CB	6.59	122.46	110.60
1	A	256	TYR	CB-CG-CD2	6.55	124.93	121.00
1	B	240	LEU	CB-CA-C	-6.52	97.81	110.20
1	B	78	ASP	CB-CG-OD1	-6.49	112.46	118.30
1	A	321	VAL	CB-CA-C	6.46	123.68	111.40
1	B	288	LYS	N-CA-CB	-6.45	98.99	110.60
1	A	409	THR	N-CA-CB	-6.45	98.05	110.30
1	B	129	ARG	CD-NE-CZ	6.37	132.51	123.60
1	A	304	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	A	272	VAL	CG1-CB-CG2	-6.31	100.81	110.90
1	B	74	ALA	N-CA-CB	6.29	118.90	110.10
1	B	21	THR	CA-CB-CG2	-6.25	103.65	112.40
1	B	111	SER	CB-CA-C	6.25	121.97	110.10
1	B	334	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	B	143	HIS	CA-CB-CG	-6.22	103.03	113.60
1	B	312	THR	CA-CB-CG2	-6.20	103.72	112.40
1	B	329	ARG	NE-CZ-NH2	6.19	123.39	120.30
1	B	217	LEU	CB-CA-C	-6.16	98.50	110.20
1	B	361	CYS	CA-CB-SG	-6.16	102.91	114.00
1	A	249	ASP	CB-CG-OD2	6.15	123.83	118.30
1	A	148	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	B	276	ASP	CB-CG-OD2	-6.11	112.81	118.30
1	B	33	MET	CG-SD-CE	-6.02	90.56	100.20
1	A	41	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	B	212	VAL	CB-CA-C	5.94	122.68	111.40
1	B	48	TYR	CB-CG-CD1	5.93	124.56	121.00
1	B	241	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	B	384	ASP	CB-CG-OD1	5.89	123.60	118.30
1	A	207	GLU	CB-CA-C	-5.85	98.70	110.40
1	A	81	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	B	121	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	A	236	ASP	CB-CG-OD1	-5.82	113.07	118.30
1	A	316	ARG	NE-CZ-NH2	5.81	123.20	120.30
1	A	384	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	B	335	THR	N-CA-CB	-5.80	99.28	110.30
1	A	162	ASP	CB-CG-OD2	-5.79	113.09	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	409	THR	N-CA-CB	-5.75	99.37	110.30
1	A	121	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	A	372	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	A	235	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	21	THR	CA-CB-CG2	-5.60	104.56	112.40
1	B	40	TYR	CA-C-N	-5.59	104.91	117.20
1	A	42	ASP	CB-CG-OD1	-5.58	113.28	118.30
1	A	282	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	A	380	TYR	CB-CG-CD2	-5.50	117.70	121.00
1	B	179	LYS	N-CA-CB	5.50	120.50	110.60
1	A	145	PRO	N-CA-CB	5.46	109.86	103.30
1	A	33	MET	CA-CB-CG	5.46	122.58	113.30
1	B	260	MET	CG-SD-CE	-5.44	91.49	100.20
1	B	354	THR	CA-CB-CG2	-5.43	104.80	112.40
1	A	80	THR	CA-CB-CG2	-5.43	104.80	112.40
1	A	149	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	A	41	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	A	90	GLU	N-CA-CB	5.37	120.27	110.60
1	B	238	TRP	CA-CB-CG	-5.36	103.53	113.70
1	B	276	ASP	CB-CG-OD1	5.32	123.09	118.30
1	B	130	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	216	ASN	N-CA-CB	-5.27	101.12	110.60
1	B	94	ALA	N-CA-CB	-5.21	102.81	110.10
1	A	70	TYR	CB-CG-CD2	-5.21	117.88	121.00
1	B	84	ALA	CB-CA-C	5.21	117.91	110.10
1	A	334	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	A	250	VAL	CA-CB-CG2	-5.18	103.12	110.90
1	B	162	ASP	CB-CG-OD1	5.18	122.96	118.30
1	A	70	TYR	N-CA-CB	5.17	119.91	110.60
1	A	199	ASP	CB-CG-OD1	-5.16	113.66	118.30
1	A	250	VAL	CB-CA-C	-5.15	101.62	111.40
1	A	284	GLU	CB-CA-C	5.14	120.68	110.40
1	B	100	TYR	CA-CB-CG	-5.14	103.64	113.40
1	A	49	VAL	CA-CB-CG1	-5.12	103.21	110.90
1	A	100	TYR	CB-CG-CD2	-5.12	117.92	121.00
1	B	300	MET	N-CA-C	5.12	124.81	111.00
1	A	162	ASP	CB-CG-OD1	5.11	122.90	118.30
1	B	304	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	B	272	VAL	CA-CB-CG1	5.10	118.55	110.90
1	B	49	VAL	CB-CA-C	-5.07	101.76	111.40
1	B	149	ASP	CB-CG-OD1	5.06	122.85	118.30
1	A	251	VAL	N-CA-CB	5.03	122.57	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	SER	N-CA-CB	5.02	118.03	110.50
1	B	101	VAL	CB-CA-C	-5.02	101.86	111.40
1	A	274	CYS	CA-CB-SG	-5.02	104.97	114.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	60	ILE	CB
1	B	370	VAL	CA

There are no planarity outliers.

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	3161	0	3151	166	0
1	B	3161	0	3151	149	0
2	A	15	0	6	0	0
2	B	15	0	6	0	0
All	All	6352	0	6314	302	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 25.

All (302) 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:196:THR:HG22	1:B:198:VAL:H	1.09	1.11
1:B:33:MET:HE3	1:B:379:ILE:HG12	1.40	1.04
1:B:234:ASN:HD22	1:B:241:ARG:HH12	1.06	1.01
1:B:156:GLN:HE21	1:B:156:GLN:HA	1.25	0.99
1:B:370:VAL:HB	1:B:381:MET:HE2	1.45	0.98
1:A:234:ASN:HD22	1:A:241:ARG:HH12	1.04	0.96
1:B:193:HIS:ND1	1:B:196:THR:HB	1.83	0.94
1:A:370:VAL:HB	1:A:381:MET:HE3	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ALA:HA	1:A:99:ARG:HD3	1.53	0.90
1:B:370:VAL:HB	1:B:381:MET:CE	2.05	0.85
1:A:361:CYS:HB3	1:A:387:ILE:CD1	2.07	0.85
1:A:234:ASN:ND2	1:A:241:ARG:HH12	1.73	0.84
1:B:350:TRP:HB3	1:B:353:ILE:HD12	1.57	0.84
1:B:373:LEU:HD23	1:B:408:VAL:HG21	1.59	0.82
1:A:361:CYS:HB3	1:A:387:ILE:HD13	1.60	0.81
1:A:369:GLN:HB3	1:A:408:VAL:CG1	2.10	0.81
1:B:196:THR:CG2	1:B:198:VAL:HB	2.11	0.81
1:B:196:THR:HG22	1:B:198:VAL:N	1.94	0.80
1:A:144:THR:HG23	1:A:155:LEU:HD13	1.63	0.79
1:A:370:VAL:HB	1:A:381:MET:CE	2.15	0.77
1:B:156:GLN:NE2	1:B:156:GLN:HA	2.01	0.75
1:A:144:THR:HG23	1:A:155:LEU:CD1	2.17	0.74
1:A:41:ARG:HG2	1:A:41:ARG:HH11	1.50	0.74
1:A:234:ASN:HD22	1:A:241:ARG:NH1	1.83	0.73
1:A:292:ARG:HB3	1:A:293:PRO:HD3	1.69	0.73
1:B:292:ARG:HB3	1:B:293:PRO:HD3	1.72	0.72
1:A:404:ILE:O	1:A:409:THR:HB	1.90	0.71
1:A:24:PHE:CD2	1:A:34:ASN:HB2	2.26	0.71
1:A:369:GLN:HB3	1:A:408:VAL:HG13	1.73	0.71
1:B:170:PHE:CE1	1:B:204:GLN:HB3	2.26	0.71
1:A:293:PRO:HB3	1:B:145:PRO:HB2	1.73	0.70
1:B:212:VAL:HA	1:B:217:LEU:HD22	1.73	0.70
1:A:379:ILE:HD13	1:A:400:LEU:HD23	1.73	0.69
1:A:142:ASN:O	1:A:146:ILE:HG13	1.92	0.69
1:A:196:THR:CG2	1:A:198:VAL:H	2.07	0.68
1:A:196:THR:HG23	1:A:198:VAL:N	2.08	0.68
1:A:177:ILE:HA	1:A:180:ILE:HD12	1.76	0.68
1:B:24:PHE:CD1	1:B:34:ASN:HB2	2.30	0.67
1:A:129:ARG:HE	1:A:129:ARG:HA	1.57	0.67
1:B:300:MET:O	1:B:304:ARG:HG3	1.95	0.67
1:A:135:LEU:HD22	1:A:155:LEU:HD22	1.75	0.66
1:A:402:HIS:O	1:A:406:GLN:HG2	1.95	0.66
1:A:34:ASN:HD22	1:A:36:GLY:H	1.43	0.66
1:B:196:THR:CG2	1:B:198:VAL:H	1.98	0.66
1:A:34:ASN:ND2	1:A:36:GLY:H	1.94	0.66
1:B:225:TYR:HB3	1:B:228:PHE:HB2	1.76	0.66
1:B:33:MET:HE1	1:B:399:TYR:HD2	1.61	0.66
1:A:196:THR:HG23	1:A:198:VAL:H	1.62	0.65
1:A:286:GLN:NE2	1:A:286:GLN:HA	2.09	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:ILE:HG23	1:A:389:VAL:HG12	1.78	0.65
1:B:229:ALA:HB3	1:B:236:ASP:OD1	1.97	0.65
1:A:110:GLY:O	1:A:114:VAL:HG13	1.96	0.64
1:A:92:SER:HB3	1:A:95:PHE:HB3	1.79	0.64
1:A:285:SER:O	1:A:289:ILE:HG13	1.98	0.64
1:B:74:ALA:CB	1:B:103:VAL:HG12	2.27	0.64
1:B:160:TYR:CE1	1:B:168:LEU:HD11	2.32	0.64
1:A:147:PHE:HD1	1:A:152:LEU:HD12	1.63	0.64
1:A:182:GLU:HG2	1:A:215:ARG:O	1.98	0.64
1:A:37:VAL:HG13	1:A:38:GLY:N	2.13	0.63
1:A:307:SER:O	1:A:311:ASN:HB2	1.99	0.63
1:A:101:VAL:O	1:A:271:THR:HA	1.98	0.62
1:A:56:ALA:O	1:A:60:ILE:HD12	1.99	0.62
1:B:196:THR:HG23	1:B:198:VAL:HB	1.82	0.62
1:A:405:HIS:O	1:A:409:THR:HG22	2.01	0.61
1:A:205:TRP:CE3	1:A:205:TRP:HA	2.34	0.61
1:B:33:MET:CE	1:B:379:ILE:HG12	2.25	0.60
1:B:50:LEU:N	1:B:50:LEU:HD12	2.16	0.60
1:A:299:PRO:HA	1:B:266:ARG:HG2	1.82	0.60
1:A:394:SER:O	1:A:397:VAL:HG12	2.01	0.60
1:A:305:ILE:O	1:A:309:ILE:HG13	2.01	0.60
1:B:366:LYS:HB3	1:B:367:PRO:CD	2.32	0.60
1:B:279:GLU:O	1:B:283:VAL:HG13	2.02	0.60
1:A:29:ASN:O	1:A:32:LYS:HG2	2.01	0.60
1:A:33:MET:CE	1:A:399:TYR:HD2	2.15	0.60
1:A:266:ARG:HG2	1:B:299:PRO:HA	1.82	0.60
1:B:193:HIS:CE1	1:B:196:THR:HB	2.36	0.59
1:B:35:LEU:N	1:B:380:TYR:O	2.32	0.59
1:B:404:ILE:O	1:B:409:THR:HB	2.01	0.59
1:B:94:ALA:HA	1:B:99:ARG:HD3	1.84	0.59
1:A:35:LEU:HB3	1:A:388:SER:H	1.68	0.59
1:B:278:GLU:HG2	1:B:278:GLU:O	2.02	0.59
1:A:101:VAL:HG21	1:A:283:VAL:HG22	1.85	0.58
1:A:400:LEU:O	1:A:404:ILE:HG13	2.04	0.58
1:B:92:SER:HB3	1:B:95:PHE:CB	2.34	0.58
1:A:99:ARG:HB3	1:A:274:CYS:O	2.04	0.58
1:A:264:GLY:O	1:B:300:MET:HG2	2.03	0.57
1:A:263:TYR:HB2	1:B:68:LYS:O	2.04	0.57
1:A:160:TYR:CE1	1:A:168:LEU:HD11	2.40	0.57
1:A:238:TRP:O	1:A:242:HIS:N	2.37	0.56
1:A:225:TYR:HB3	1:A:228:PHE:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:LEU:HD12	1:A:381:MET:HE1	1.86	0.56
1:A:15:ASP:OD1	1:A:18:LEU:N	2.37	0.56
1:B:50:LEU:H	1:B:50:LEU:HD12	1.71	0.56
1:A:334:ARG:HD3	1:A:353:ILE:O	2.04	0.56
1:B:74:ALA:HB2	1:B:103:VAL:HG12	1.87	0.56
1:A:43:ASP:O	1:A:393:ALA:HB1	2.06	0.56
1:A:389:VAL:O	1:A:392:VAL:HG13	2.06	0.56
1:A:160:TYR:O	1:A:168:LEU:HD12	2.06	0.56
1:B:50:LEU:HB2	1:B:53:VAL:HG23	1.87	0.55
1:A:374:THR:O	1:A:378:SER:HA	2.07	0.55
1:A:319:TRP:O	1:A:323:VAL:HG13	2.06	0.55
1:A:361:CYS:HB3	1:A:387:ILE:HD11	1.88	0.55
1:A:33:MET:CE	1:A:379:ILE:HD11	2.36	0.55
1:B:234:ASN:HD22	1:B:241:ARG:NH1	1.90	0.55
1:A:123:PHE:O	1:A:129:ARG:NH2	2.39	0.55
1:B:142:ASN:O	1:B:146:ILE:HD12	2.07	0.55
1:A:134:TYR:CD2	1:A:156:GLN:HB2	2.42	0.55
1:A:170:PHE:CE1	1:A:204:GLN:HB3	2.42	0.55
1:B:234:ASN:ND2	1:B:241:ARG:HH12	1.90	0.55
1:B:101:VAL:HG21	1:B:283:VAL:HG22	1.88	0.54
1:B:363:THR:HG21	1:B:387:ILE:CD1	2.36	0.54
1:A:9:VAL:O	1:B:282:ARG:HD2	2.07	0.54
1:B:202:GLN:O	1:B:206:LYS:HG3	2.08	0.54
1:A:42:ASP:O	1:A:45:GLY:N	2.41	0.54
1:B:101:VAL:HG11	1:B:284:GLU:HB3	1.91	0.53
1:B:402:HIS:O	1:B:406:GLN:HG2	2.07	0.53
1:B:165:THR:HG22	1:B:167:SER:OG	2.08	0.53
1:A:323:VAL:O	1:A:326:MET:HB2	2.08	0.53
1:B:29:ASN:OD1	1:B:31:LYS:HB2	2.07	0.53
1:B:21:THR:O	1:B:25:LYS:HG3	2.09	0.53
1:A:118:PHE:CD2	1:A:287:LEU:HD13	2.44	0.53
1:B:37:VAL:HG22	1:B:38:GLY:N	2.24	0.53
1:B:209:ALA:HB2	1:B:243:PHE:CE1	2.43	0.53
1:A:101:VAL:HG21	1:A:283:VAL:CG2	2.39	0.53
1:A:193:HIS:HB3	1:A:196:THR:HG22	1.90	0.53
1:B:227:GLY:N	1:B:236:ASP:OD2	2.42	0.53
1:A:8:HIS:CD2	1:A:8:HIS:H	2.27	0.52
1:B:209:ALA:HA	1:B:212:VAL:HG13	1.92	0.52
1:B:106:ILE:HD11	1:B:295:TYR:CZ	2.44	0.52
1:A:147:PHE:HD1	1:A:152:LEU:CD1	2.23	0.52
1:B:21:THR:O	1:B:24:PHE:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:TYR:CZ	1:B:168:LEU:HD11	2.45	0.52
1:B:286:GLN:HA	1:B:286:GLN:NE2	2.25	0.52
1:B:329:ARG:O	1:B:332:SER:HB3	2.10	0.52
1:A:373:LEU:CD2	1:A:403:ALA:HB1	2.40	0.52
1:A:41:ARG:NH1	1:A:41:ARG:HG2	2.20	0.52
1:A:233:ILE:HG13	1:A:234:ASN:H	1.74	0.52
1:A:350:TRP:HB3	1:A:353:ILE:HD12	1.91	0.52
1:A:145:PRO:O	1:A:149:ASP:HB2	2.09	0.52
1:A:160:TYR:CZ	1:A:168:LEU:HD13	2.45	0.51
1:A:86:LEU:HD12	1:A:86:LEU:O	2.10	0.51
1:A:292:ARG:CB	1:A:293:PRO:HD3	2.38	0.51
1:B:113:ARG:O	1:B:113:ARG:HG3	2.09	0.51
1:B:319:TRP:CE3	1:B:320:LEU:HD13	2.44	0.51
1:B:334:ARG:HD3	1:B:353:ILE:O	2.11	0.51
1:A:8:HIS:CD2	1:B:124:LYS:NZ	2.79	0.51
1:A:300:MET:O	1:A:304:ARG:HG3	2.11	0.51
1:B:252:LEU:HD12	1:B:253:SER:O	2.11	0.51
1:A:50:LEU:HB2	1:A:53:VAL:HG23	1.93	0.51
1:A:369:GLN:HB3	1:A:408:VAL:HG12	1.93	0.51
1:B:312:THR:HB	1:B:315:LEU:HB2	1.93	0.51
1:B:366:LYS:HB3	1:B:367:PRO:HD2	1.91	0.50
1:B:92:SER:HB3	1:B:95:PHE:HB3	1.93	0.50
1:A:233:ILE:HG13	1:A:234:ASN:N	2.25	0.50
1:A:33:MET:HE1	1:A:399:TYR:HD2	1.75	0.50
1:B:74:ALA:HB1	1:B:103:VAL:HG12	1.93	0.50
1:A:21:THR:O	1:A:25:LYS:HG2	2.11	0.50
1:A:304:ARG:O	1:A:308:LEU:HB2	2.12	0.50
1:A:24:PHE:CG	1:A:34:ASN:HB2	2.46	0.50
1:A:215:ARG:O	1:A:216:ASN:HB3	2.11	0.50
1:B:5:TRP:HA	1:B:5:TRP:CE3	2.46	0.50
1:A:144:THR:O	1:A:155:LEU:HD11	2.12	0.50
1:A:134:TYR:CE2	1:A:156:GLN:HB2	2.47	0.50
1:B:297:ASN:HB2	1:B:298:PRO:HD2	1.93	0.50
1:B:190:ALA:HB3	1:B:223:MET:HG3	1.93	0.50
1:A:363:THR:CG2	1:A:387:ILE:HD12	2.41	0.49
1:B:50:LEU:H	1:B:50:LEU:CD1	2.24	0.49
1:B:384:ASP:N	1:B:384:ASP:OD1	2.42	0.49
1:B:100:TYR:CD1	1:B:100:TYR:N	2.79	0.49
1:B:336:GLN:HB3	1:B:397:VAL:HG21	1.93	0.49
1:B:250:VAL:HG23	1:B:251:VAL:N	2.26	0.49
1:B:191:CYS:SG	1:B:236:ASP:HB3	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:THR:HG21	1:B:387:ILE:HD13	1.93	0.49
1:B:33:MET:HE1	1:B:399:TYR:CD2	2.43	0.49
1:A:186:ILE:HG12	1:A:188:LEU:CD1	2.43	0.49
1:B:33:MET:HE3	1:B:379:ILE:CG1	2.26	0.49
1:B:101:VAL:CG1	1:B:284:GLU:HB3	2.43	0.49
1:A:93:GLU:OE1	1:A:99:ARG:NH1	2.46	0.49
1:A:92:SER:HB3	1:A:95:PHE:CB	2.42	0.49
1:B:251:VAL:HG12	1:B:272:VAL:HB	1.94	0.48
1:A:135:LEU:O	1:A:157:ALA:HA	2.13	0.48
1:B:389:VAL:O	1:B:392:VAL:HG13	2.13	0.48
1:B:373:LEU:CD2	1:B:408:VAL:HG21	2.37	0.48
1:B:162:ASP:O	1:B:166:CYS:N	2.45	0.48
1:B:84:ALA:O	1:B:88:LEU:HB2	2.14	0.48
1:B:292:ARG:CB	1:B:293:PRO:HD3	2.39	0.48
1:B:228:PHE:CZ	1:B:326:MET:HE3	2.49	0.48
1:A:34:ASN:C	1:A:34:ASN:HD22	2.17	0.48
1:A:11:MET:HB2	1:B:282:ARG:HG2	1.96	0.47
1:A:115:GLY:O	1:A:119:LEU:HG	2.14	0.47
1:B:198:VAL:O	1:B:198:VAL:HG12	2.14	0.47
1:B:33:MET:CE	1:B:399:TYR:HD2	2.27	0.47
1:B:213:LYS:HB2	1:B:248:ILE:HD11	1.96	0.47
1:A:373:LEU:HD12	1:A:381:MET:CE	2.44	0.47
1:B:144:THR:HB	1:B:145:PRO:CD	2.44	0.47
1:A:246:GLN:HB2	1:A:248:ILE:HD12	1.95	0.47
1:A:217:LEU:HD13	1:A:217:LEU:N	2.29	0.47
1:B:295:TYR:O	1:B:296:SER:HB3	2.15	0.47
1:B:75:GLY:HA3	1:B:104:GLN:HB3	1.97	0.47
1:B:292:ARG:N	1:B:293:PRO:CD	2.78	0.47
1:A:8:HIS:CD2	1:B:124:LYS:HZ3	2.33	0.47
1:B:273:ILE:N	1:B:273:ILE:HD13	2.30	0.47
1:B:109:THR:HA	1:B:112:LEU:HD12	1.96	0.47
1:B:136:PRO:O	1:B:139:SER:HB2	2.15	0.47
1:B:322:GLU:O	1:B:326:MET:HG3	2.14	0.46
1:B:15:ASP:OD2	1:B:18:LEU:N	2.48	0.46
1:B:110:GLY:O	1:B:114:VAL:HG13	2.15	0.46
1:A:335:THR:HG22	1:A:336:GLN:N	2.29	0.46
1:B:37:VAL:CG2	1:B:38:GLY:N	2.79	0.46
1:A:160:TYR:CZ	1:A:168:LEU:CD1	2.99	0.46
1:A:182:GLU:O	1:A:183:LYS:HB2	2.15	0.46
1:B:287:LEU:O	1:B:291:ILE:HG13	2.15	0.46
1:A:84:ALA:O	1:A:88:LEU:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:GLU:O	1:B:321:VAL:HG22	2.15	0.46
1:B:291:ILE:O	1:B:294:MET:HB2	2.15	0.46
1:B:237:ALA:O	1:B:241:ARG:HG3	2.16	0.46
1:A:160:TYR:CE1	1:A:168:LEU:CD1	2.99	0.46
1:B:71:LEU:HD22	1:B:300:MET:HB3	1.98	0.46
1:B:160:TYR:CZ	1:B:168:LEU:CD1	2.98	0.46
1:A:196:THR:HG23	1:A:198:VAL:HB	1.96	0.46
1:B:333:MET:O	1:B:337:LEU:HB2	2.16	0.46
1:B:233:ILE:HG13	1:B:234:ASN:N	2.31	0.45
1:A:196:THR:HG22	1:A:198:VAL:H	1.80	0.45
1:A:372:ARG:HB3	1:A:408:VAL:HG22	1.98	0.45
1:B:228:PHE:CZ	1:B:326:MET:CE	2.99	0.45
1:B:337:LEU:HD23	1:B:337:LEU:HA	1.61	0.45
1:A:322:GLU:O	1:A:326:MET:HG3	2.16	0.45
1:A:196:THR:HG23	1:A:198:VAL:CB	2.47	0.45
1:A:143:HIS:NE2	1:A:222:ASP:OD2	2.47	0.45
1:B:106:ILE:CD1	1:B:295:TYR:CE2	2.99	0.45
1:A:115:GLY:HA2	1:A:270:PHE:CZ	2.52	0.45
1:B:55:LYS:O	1:B:58:ALA:HB3	2.16	0.45
1:A:193:HIS:ND1	1:A:196:THR:HB	2.32	0.45
1:A:217:LEU:N	1:A:217:LEU:CD1	2.79	0.45
1:A:202:GLN:HG3	1:A:238:TRP:CZ3	2.52	0.45
1:A:308:LEU:HA	1:A:308:LEU:HD23	1.67	0.45
1:A:33:MET:HE3	1:A:379:ILE:CD1	2.47	0.45
1:A:109:THR:OG1	1:B:296:SER:HB2	2.16	0.45
1:B:287:LEU:HA	1:B:287:LEU:HD12	1.55	0.45
1:A:232:ASP:HB3	1:A:235:ARG:HB3	1.99	0.44
1:A:33:MET:HE2	1:A:399:TYR:HD2	1.80	0.44
1:A:159:ARG:HH21	1:A:176:ASP:CG	2.18	0.44
1:B:165:THR:O	1:B:166:CYS:HB2	2.18	0.44
1:B:187:LEU:HD13	1:B:187:LEU:C	2.38	0.44
1:B:33:MET:CE	1:B:399:TYR:CD2	3.00	0.44
1:B:400:LEU:HA	1:B:400:LEU:HD23	1.68	0.44
1:A:160:TYR:HE2	1:A:196:THR:HG21	1.83	0.44
1:A:187:LEU:O	1:A:188:LEU:HD12	2.18	0.44
1:A:125:PHE:O	1:A:126:SER:HB2	2.16	0.43
1:A:315:LEU:HD23	1:A:315:LEU:HA	1.40	0.43
1:A:29:ASN:OD1	1:A:31:LYS:HB2	2.18	0.43
1:B:41:ARG:HA	1:B:46:LYS:O	2.17	0.43
1:B:318:GLU:O	1:B:322:GLU:HG3	2.17	0.43
1:A:68:LYS:O	1:B:263:TYR:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:CYS:O	1:A:192:ALA:HB3	2.17	0.43
1:B:370:VAL:HB	1:B:381:MET:HE3	1.95	0.43
1:B:102:THR:HA	1:B:270:PHE:O	2.18	0.43
1:A:71:LEU:HD23	1:A:298:PRO:HG2	2.01	0.43
1:B:106:ILE:HD11	1:B:295:TYR:CE2	2.54	0.43
1:A:309:ILE:HA	1:A:315:LEU:HB3	2.01	0.43
1:A:88:LEU:HA	1:A:88:LEU:HD12	1.64	0.43
1:A:287:LEU:HA	1:A:287:LEU:HD12	1.81	0.42
1:A:147:PHE:HB2	1:A:155:LEU:HD21	2.00	0.42
1:A:24:PHE:CE2	1:A:34:ASN:HB2	2.55	0.42
1:B:92:SER:HB3	1:B:95:PHE:HB2	1.99	0.42
1:A:363:THR:HG23	1:A:363:THR:H	1.55	0.42
1:A:180:ILE:HG22	1:A:217:LEU:HD11	2.01	0.42
1:A:400:LEU:HA	1:A:400:LEU:HD23	1.80	0.42
1:A:177:ILE:HD12	1:A:208:LEU:HD11	2.02	0.42
1:A:266:ARG:HA	1:A:266:ARG:HD2	1.59	0.42
1:B:382:THR:OG1	1:B:386:ARG:HB3	2.19	0.42
1:B:161:TYR:O	1:B:163:PRO:HD3	2.19	0.42
1:B:274:CYS:HB3	1:B:279:GLU:HB3	2.02	0.42
1:A:363:THR:HG23	1:A:385:GLY:O	2.20	0.41
1:A:15:ASP:O	1:A:19:GLY:N	2.50	0.41
1:B:232:ASP:HB3	1:B:235:ARG:HB3	2.02	0.41
1:B:292:ARG:N	1:B:293:PRO:HD2	2.36	0.41
1:A:186:ILE:HG12	1:A:188:LEU:HD11	2.02	0.41
1:A:119:LEU:HD23	1:A:119:LEU:HA	1.76	0.41
1:A:133:VAL:HG22	1:A:155:LEU:HD23	2.01	0.41
1:B:300:MET:HE2	1:B:300:MET:HB2	1.87	0.41
1:A:266:ARG:NH2	1:B:296:SER:HB3	2.36	0.41
1:B:194:ASN:HA	1:B:195:PRO:HA	1.90	0.41
1:A:229:ALA:HB1	1:A:357:ILE:HD13	2.02	0.41
1:B:363:THR:CG2	1:B:387:ILE:CD1	2.99	0.41
1:A:373:LEU:HG	1:A:408:VAL:HG21	2.03	0.41
1:A:225:TYR:CD1	1:A:225:TYR:N	2.88	0.41
1:B:340:ASN:HA	1:B:343:LYS:HB3	2.01	0.41
1:B:276:ASP:HB3	1:B:278:GLU:H	1.85	0.41
1:A:122:PHE:O	1:B:8:HIS:HE1	2.04	0.41
1:B:5:TRP:HA	1:B:5:TRP:HE3	1.86	0.41
1:A:66:MET:HE2	1:A:66:MET:HB3	1.77	0.41
1:A:93:GLU:O	1:A:93:GLU:HG2	2.20	0.41
1:A:57:GLU:HA	1:A:60:ILE:HD12	2.01	0.41
1:B:8:HIS:CD2	1:B:8:HIS:H	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:THR:HA	1:A:313:PRO:HD3	1.86	0.41
1:A:320:LEU:HD12	1:A:320:LEU:HA	1.77	0.41
1:A:137:LYS:HA	1:A:138:PRO:HA	1.76	0.41
1:B:101:VAL:O	1:B:271:THR:HG23	2.21	0.41
1:B:144:THR:CB	1:B:145:PRO:CD	3.00	0.40
1:A:160:TYR:CD1	1:A:168:LEU:HD11	2.57	0.40
1:A:282:ARG:HD2	1:A:282:ARG:HH11	1.75	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	399/401 (100%)	363 (91%)	32 (8%)	4 (1%)	19	61
1	B	399/401 (100%)	364 (91%)	31 (8%)	4 (1%)	19	61
All	All	798/802 (100%)	727 (91%)	63 (8%)	8 (1%)	19	61

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	TYR
1	B	263	TYR
1	A	4	SER
1	A	43	ASP
1	A	383	LYS
1	B	99	ARG
1	B	313	PRO
1	B	36	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	335/335 (100%)	269 (80%)	66 (20%)	1	9
1	B	335/335 (100%)	266 (79%)	69 (21%)	1	7
All	All	670/670 (100%)	535 (80%)	135 (20%)	1	8

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	PRO
1	A	25	LYS
1	A	34	ASN
1	A	37	VAL
1	A	43	ASP
1	A	59	MET
1	A	66	MET
1	A	81	ARG
1	A	88	LEU
1	A	90	GLU
1	A	91	ASN
1	A	92	SER
1	A	97	SER
1	A	107	SER
1	A	114	VAL
1	A	120	GLN
1	A	125	PHE
1	A	126	SER
1	A	129	ARG
1	A	135	LEU
1	A	137	LYS
1	A	139	SER
1	A	152	LEU
1	A	154	GLN
1	A	180	ILE
1	A	184	SER
1	A	188	LEU

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Mol	Chain	Res	Type
1	A	196	THR
1	A	201	ARG
1	A	205	TRP
1	A	207	GLU
1	A	208	LEU
1	A	210	SER
1	A	212	VAL
1	A	213	LYS
1	A	217	LEU
1	A	218	LEU
1	A	220	TYR
1	A	235	ARG
1	A	240	LEU
1	A	262	LEU
1	A	275	ARG
1	A	278	GLU
1	A	284	GLU
1	A	287	LEU
1	A	292	ARG
1	A	308	LEU
1	A	314	GLU
1	A	320	LEU
1	A	321	VAL
1	A	331	ILE
1	A	332	SER
1	A	338	VAL
1	A	341	LEU
1	A	343	LYS
1	A	351	GLN
1	A	363	THR
1	A	370	VAL
1	A	372	ARG
1	A	381	MET
1	A	382	THR
1	A	383	LYS
1	A	387	ILE
1	A	392	VAL
1	A	400	LEU
1	A	409	THR
1	B	3	SER
1	B	4	SER
1	B	17	ILE

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Mol	Chain	Res	Type
1	B	31	LYS
1	B	34	ASN
1	B	43	ASP
1	B	64	LYS
1	B	66	MET
1	B	71	LEU
1	B	80	THR
1	B	83	SER
1	B	90	GLU
1	B	91	ASN
1	B	96	LYS
1	B	99	ARG
1	B	107	SER
1	B	111	SER
1	B	114	VAL
1	B	120	GLN
1	B	126	SER
1	B	129	ARG
1	B	156	GLN
1	B	167	SER
1	B	175	GLU
1	B	179	LYS
1	B	188	LEU
1	B	196	THR
1	B	199	ASP
1	B	203	GLU
1	B	211	VAL
1	B	212	VAL
1	B	216	ASN
1	B	217	LEU
1	B	218	LEU
1	B	220	TYR
1	B	235	ARG
1	B	240	LEU
1	B	252	LEU
1	B	254	GLN
1	B	272	VAL
1	B	275	ARG
1	B	276	ASP
1	B	284	GLU
1	B	294	MET
1	B	305	ILE

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Mol	Chain	Res	Type
1	B	307	SER
1	B	308	LEU
1	B	316	ARG
1	B	317	LYS
1	B	320	LEU
1	B	336	GLN
1	B	337	LEU
1	B	339	SER
1	B	341	LEU
1	B	343	LYS
1	B	347	SER
1	B	357	ILE
1	B	366	LYS
1	B	369	GLN
1	B	375	LYS
1	B	378	SER
1	B	381	MET
1	B	383	LYS
1	B	387	ILE
1	B	389	VAL
1	B	392	VAL
1	B	394	SER
1	B	400	LEU
1	B	409	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	34	ASN
1	A	120	GLN
1	A	234	ASN
1	A	286	GLN
1	A	336	GLN
1	B	8	HIS
1	B	34	ASN
1	B	120	GLN
1	B	156	GLN
1	B	216	ASN
1	B	234	ASN
1	B	254	GLN
1	B	286	GLN

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 ⓘ

2 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	411	1	15,15,16	1.86	4 (26%)	21,22,23	2.99	7 (33%)
2	PLP	B	411	1	15,15,16	1.69	3 (20%)	21,22,23	2.72	9 (42%)

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	411	1	-	0/6/6/8	0/1/1/1
2	PLP	B	411	1	-	0/6/6/8	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	411	PLP	C4A-C4	-4.56	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	411	PLP	C3-C2	-3.67	1.38	1.40
2	B	411	PLP	C4A-C4	-3.51	1.44	1.51
2	A	411	PLP	C3-C4	-2.74	1.33	1.40
2	B	411	PLP	P-O2P	-2.31	1.46	1.54
2	A	411	PLP	C3-C2	-2.16	1.39	1.40
2	A	411	PLP	C5A-C5	2.43	1.57	1.50

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	411	PLP	C3-C2-N1	-4.41	114.52	120.61
2	A	411	PLP	C5-C6-N1	-4.40	116.23	123.86
2	B	411	PLP	C5-C6-N1	-4.17	116.61	123.86
2	B	411	PLP	C3-C2-N1	-4.07	114.98	120.61
2	B	411	PLP	O3-C3-C2	-2.46	113.39	117.66
2	B	411	PLP	C4A-C4-C5	-2.25	118.53	120.88
2	A	411	PLP	C4A-C4-C5	-2.25	118.54	120.88
2	A	411	PLP	C6-C5-C4	2.62	120.37	118.15
2	B	411	PLP	O3-C3-C4	2.75	125.85	118.12
2	B	411	PLP	C6-C5-C4	2.79	120.52	118.15
2	A	411	PLP	C6-N1-C2	4.45	128.35	119.28
2	B	411	PLP	C6-N1-C2	4.56	128.58	119.28
2	B	411	PLP	C2A-C2-C3	5.39	127.53	121.04
2	B	411	PLP	O4P-C5A-C5	6.21	119.26	108.99
2	A	411	PLP	C2A-C2-C3	6.82	129.26	121.04
2	A	411	PLP	O4P-C5A-C5	7.68	121.69	108.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.