



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:38 AM UTC

PDB ID : 1AIC / pdb_00001aic
Title : STRUCTURAL BASIS FOR THE CATALYTIC ACTIVITY OF ASPARTATE AMINOTRANSFERASE K258H LACKING THE PYRIDOXAL-5'-PHOSPHATE BINDING LYSINE RESIDUE
Authors : Jaeger, J.; Jansonius, J.N.
Deposited on : 1994-05-10
Resolution : 2.40 Å(reported)

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

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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

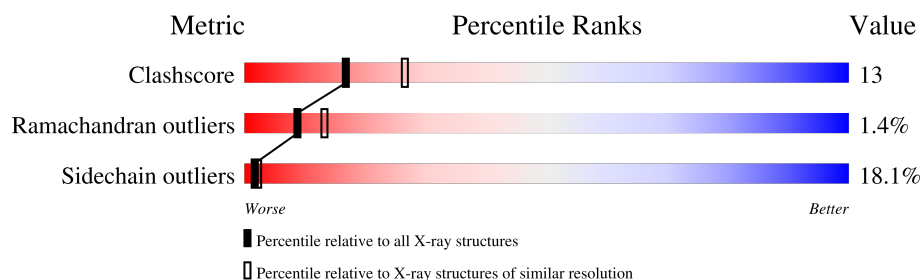
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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	396	 55% 27% 15% •
1	B	396	 58% 28% 11% •

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6182 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.

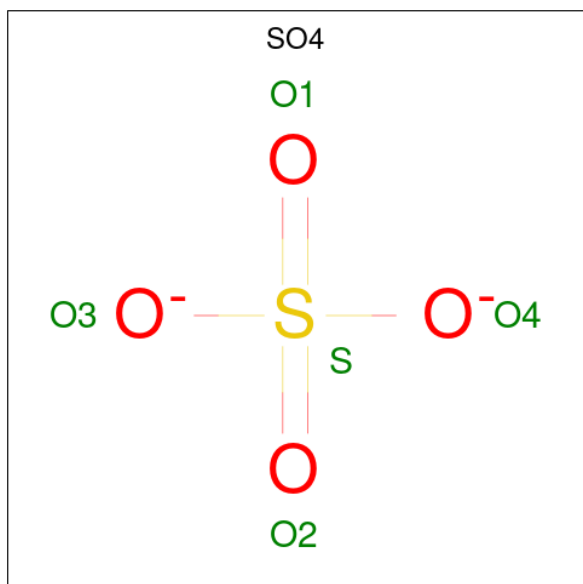
- Molecule 1 is a protein called ASPARTATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	0	0
			3070	1936	537	584	13			
1	B	396	Total	C	N	O	S	0	0	0
			3070	1936	537	584	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	258	HIS	LYS	engineered mutation	UNP P00509
B	258	HIS	LYS	engineered mutation	UNP P00509

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



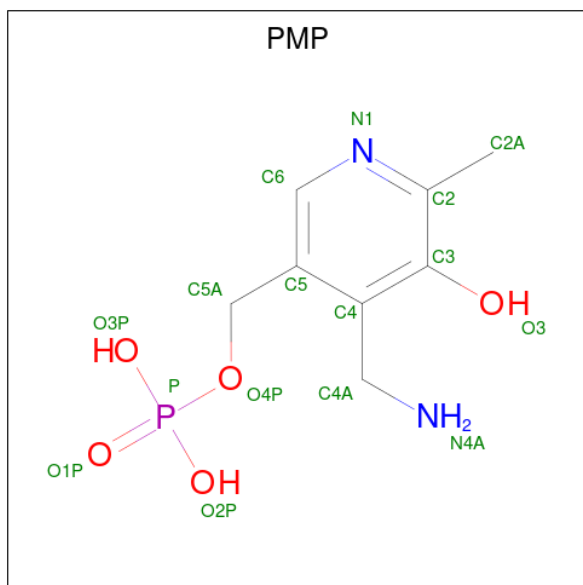
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	O S	0	0
			5	4 1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (CCD ID: PMP) (formula: $C_8H_{13}N_2O_5P$).



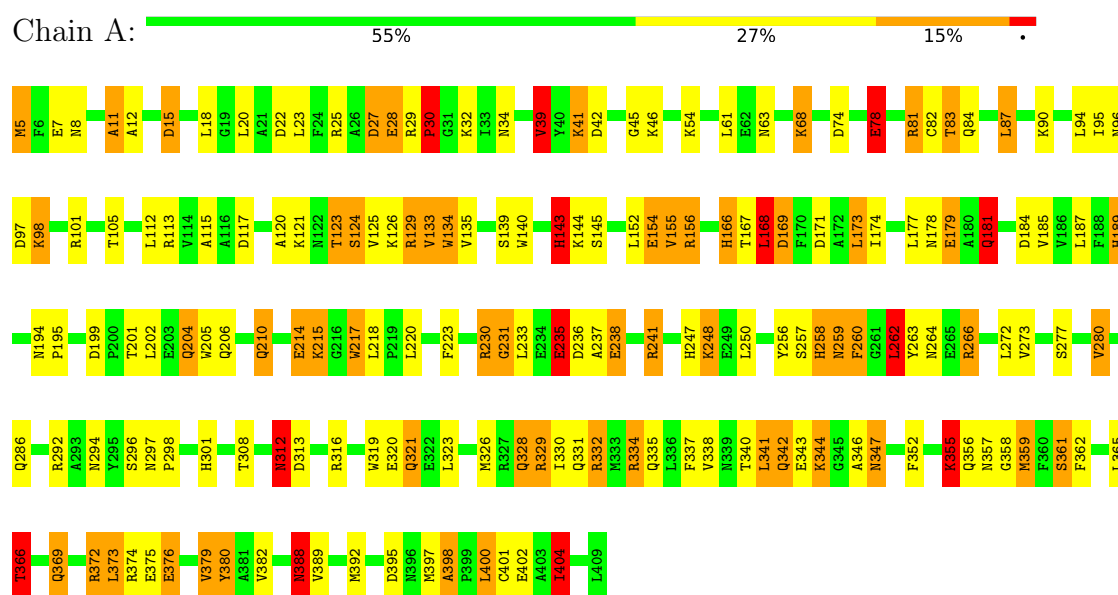
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
3	B	1	Total	C	N	O	P	0	0
			16	8	2	5	1		

3 Residue-property plots

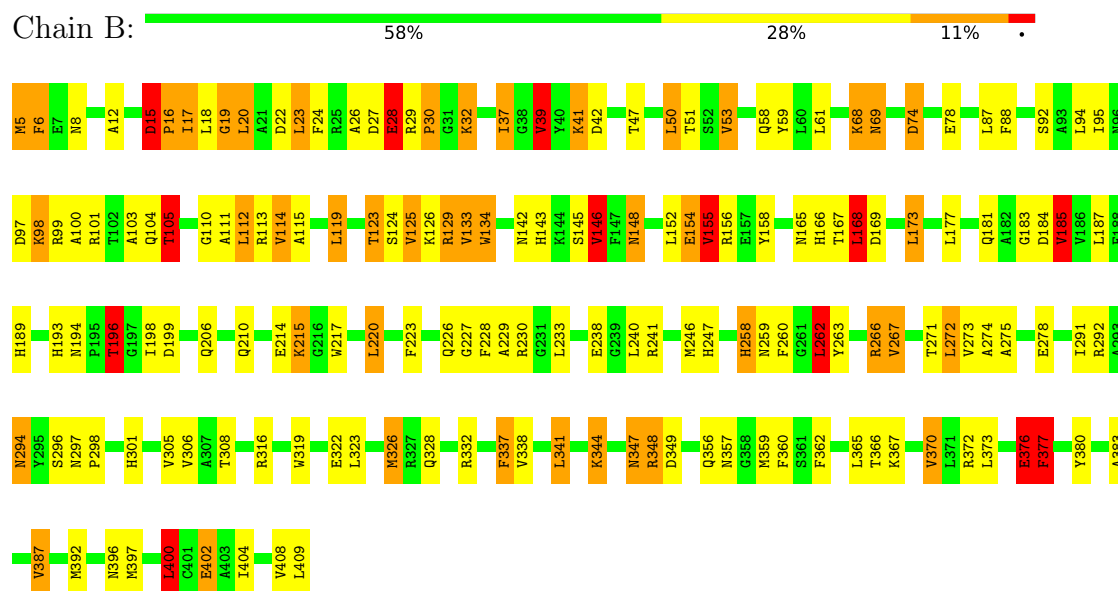
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 1: ASPARTATE AMINOTRANSFERASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.20Å 79.90Å 89.60Å 90.00° 119.10° 90.00°	Depositor
Resolution (Å)	10.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.191 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6182	wwPDB-VP
Average B, all atoms (Å ²)	25.0	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: PMP, SO4

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	1.29	20/3132 (0.6%)	2.20	152/4244 (3.6%)
1	B	1.66	23/3132 (0.7%)	2.15	129/4244 (3.0%)
All	All	1.49	43/6264 (0.7%)	2.18	281/8488 (3.3%)

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	2
1	B	0	3
All	All	0	5

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	19	GLY	N-CA	35.63	1.90	1.45
1	B	16	PRO	C-N	30.94	1.71	1.33
1	B	15	ASP	N-CA	25.47	1.89	1.46
1	B	17	ILE	CB-CG1	-21.02	1.11	1.53
1	B	155	VAL	CA-CB	9.96	1.66	1.54
1	A	231	GLY	C-N	8.77	1.45	1.33
1	B	15	ASP	C-N	-8.24	1.14	1.33
1	A	404	ILE	CA-CB	7.72	1.65	1.54
1	A	189	HIS	CD2-NE2	-7.42	1.29	1.37
1	B	226	GLN	CA-CB	-7.40	1.42	1.53
1	B	301	HIS	CD2-NE2	-7.21	1.29	1.37
1	A	120	ALA	C-N	7.01	1.44	1.33
1	B	247	HIS	CD2-NE2	-6.64	1.30	1.37
1	B	258	HIS	CD2-NE2	-6.42	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	301	HIS	CD2-NE2	-6.36	1.30	1.37
1	A	258	HIS	CD2-NE2	-6.31	1.30	1.37
1	B	143	HIS	CD2-NE2	-6.24	1.30	1.37
1	B	189	HIS	CD2-NE2	-6.16	1.31	1.37
1	B	367	LYS	CA-CB	-6.03	1.43	1.53
1	A	189	HIS	CG-ND1	-5.96	1.31	1.38
1	B	47	THR	N-CA	-5.79	1.40	1.46
1	B	189	HIS	CG-ND1	-5.78	1.31	1.38
1	A	143	HIS	CD2-NE2	-5.75	1.31	1.37
1	B	146	VAL	CA-CB	5.72	1.61	1.54
1	B	193	HIS	CD2-NE2	-5.67	1.31	1.37
1	B	166	HIS	CD2-NE2	-5.60	1.31	1.37
1	A	247	HIS	CD2-NE2	-5.59	1.31	1.37
1	B	185	VAL	CA-CB	5.55	1.61	1.54
1	A	124	SER	C-N	-5.53	1.26	1.33
1	B	143	HIS	CG-ND1	-5.52	1.32	1.38
1	B	247	HIS	CG-ND1	-5.51	1.32	1.38
1	A	166	HIS	CG-ND1	-5.40	1.32	1.38
1	A	258	HIS	CG-ND1	-5.39	1.32	1.38
1	A	298	PRO	CA-CB	-5.36	1.46	1.54
1	A	374	ARG	CA-CB	-5.21	1.45	1.53
1	A	134	TRP	NE1-CE2	-5.20	1.31	1.37
1	A	166	HIS	CD2-NE2	-5.19	1.32	1.37
1	B	134	TRP	NE1-CE2	-5.09	1.31	1.37
1	A	179	GLU	C-N	5.09	1.40	1.33
1	B	217	TRP	CG-CD2	-5.06	1.34	1.43
1	A	277	SER	CA-CB	-5.03	1.45	1.53
1	A	277	SER	N-CA	-5.03	1.40	1.46
1	A	320	GLU	CA-CB	-5.03	1.45	1.53

All (281) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	15	ASP	CA-C-N	15.23	138.88	119.84
1	B	15	ASP	C-N-CA	15.23	138.88	119.84
1	B	15	ASP	O-C-N	-13.58	108.98	121.20
1	B	39	VAL	N-CA-CB	-12.88	95.99	112.60
1	A	8	ASN	N-CA-CB	-12.64	92.72	111.43
1	B	17	ILE	CA-CB-CG1	12.60	131.82	110.40
1	A	8	ASN	CA-CB-CG	11.52	124.12	112.60
1	A	266	ARG	NE-CZ-NH2	-11.26	109.07	119.20
1	B	377	PHE	O-C-N	10.97	137.19	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	ASN	CB-CA-C	10.59	129.57	111.46
1	B	17	ILE	CB-CG1-CD1	9.67	134.11	113.80
1	A	312	ASN	OD1-CG-ND2	-9.65	112.95	122.60
1	A	199	ASP	CA-CB-CG	9.63	122.23	112.60
1	A	342	GLN	OE1-CD-NE2	-9.51	113.09	122.60
1	A	231	GLY	O-C-N	-9.40	112.80	123.61
1	A	11	ALA	N-CA-C	9.33	130.68	110.80
1	B	196	THR	N-CA-CB	-9.16	96.59	110.33
1	A	328	GLN	CA-CB-CG	-8.97	96.15	114.10
1	A	280	VAL	CB-CA-C	-8.94	97.78	112.26
1	A	366	THR	CA-CB-OG1	-8.88	96.28	109.60
1	A	347	ASN	CA-CB-CG	8.68	121.28	112.60
1	A	355	LYS	CA-CB-CG	8.65	131.40	114.10
1	A	169	ASP	CA-C-O	8.65	130.56	120.70
1	A	178	ASN	CA-CB-CG	-8.64	103.96	112.60
1	B	194	ASN	CA-CB-CG	8.61	121.21	112.60
1	A	259	ASN	OD1-CG-ND2	-8.60	114.00	122.60
1	A	374	ARG	CB-CA-C	-8.51	97.77	110.95
1	A	120	ALA	CA-C-N	-8.30	109.34	122.29
1	A	120	ALA	C-N-CA	-8.30	109.34	122.29
1	A	366	THR	CA-CB-CG2	8.29	124.60	110.50
1	A	133	VAL	O-C-N	8.24	131.97	123.07
1	B	113	ARG	CA-C-O	-8.22	112.19	120.82
1	B	206	GLN	OE1-CD-NE2	-8.18	114.42	122.60
1	A	28	GLU	CA-CB-CG	8.17	130.45	114.10
1	B	301	HIS	CB-CG-CD2	-8.15	120.61	131.20
1	B	69	ASN	OD1-CG-ND2	-8.10	114.50	122.60
1	B	229	ALA	O-C-N	-8.09	113.85	123.31
1	A	329	ARG	NE-CZ-NH2	-7.98	112.02	119.20
1	B	294	ASN	OD1-CG-ND2	-7.91	114.69	122.60
1	B	8	ASN	OD1-CG-ND2	-7.89	114.71	122.60
1	A	96	ASN	OD1-CG-ND2	-7.86	114.74	122.60
1	A	81	ARG	CA-CB-CG	7.80	129.70	114.10
1	B	226	GLN	OE1-CD-NE2	-7.79	114.81	122.60
1	B	74	ASP	CA-CB-CG	7.72	120.32	112.60
1	A	169	ASP	CA-CB-CG	7.70	120.30	112.60
1	A	39	VAL	N-CA-CB	-7.68	99.54	112.44
1	A	189	HIS	CB-CG-CD2	-7.66	121.25	131.20
1	B	199	ASP	CA-CB-CG	7.65	120.25	112.60
1	A	329	ARG	CG-CD-NE	-7.60	95.27	112.00
1	A	342	GLN	CB-CG-CD	7.60	125.52	112.60
1	A	178	ASN	OD1-CG-ND2	-7.57	115.03	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	125	VAL	CB-CA-C	-7.57	99.02	111.51
1	B	376	GLU	CB-CG-CD	7.57	125.47	112.60
1	B	5	MET	O-C-N	-7.53	110.95	123.00
1	A	331	GLN	OE1-CD-NE2	-7.49	115.11	122.60
1	A	388	ASN	CB-CG-ND2	7.49	127.63	116.40
1	B	42	ASP	CA-CB-CG	7.37	119.97	112.60
1	B	377	PHE	N-CA-C	7.34	126.42	110.80
1	A	97	ASP	CA-CB-CG	7.30	119.90	112.60
1	B	105	THR	N-CA-CB	-7.30	98.05	111.18
1	A	42	ASP	CA-CB-CG	7.22	119.82	112.60
1	A	41	LYS	N-CA-CB	-7.22	98.21	111.13
1	B	15	ASP	N-CA-C	-7.21	95.11	109.60
1	B	301	HIS	N-CA-C	7.18	118.80	110.97
1	A	41	LYS	CB-CG-CD	-7.18	94.78	111.30
1	B	347	ASN	OD1-CG-ND2	-7.17	115.43	122.60
1	A	366	THR	N-CA-CB	-7.14	99.43	110.29
1	A	301	HIS	CB-CG-CD2	-7.11	121.95	131.20
1	B	39	VAL	CB-CA-C	7.10	120.92	111.19
1	B	165	ASN	OD1-CG-ND2	-7.10	115.50	122.60
1	B	298	PRO	CB-CA-C	7.08	119.56	110.92
1	B	387	VAL	N-CA-CB	-7.04	99.90	111.45
1	A	189	HIS	CB-CG-ND1	7.04	133.26	122.70
1	A	25	ARG	O-C-N	7.01	129.58	122.08
1	A	84	GLN	OE1-CD-NE2	-7.00	115.60	122.60
1	A	335	GLN	OE1-CD-NE2	-6.95	115.65	122.60
1	A	259	ASN	CA-CB-CG	6.92	119.52	112.60
1	A	7	GLU	N-CA-C	6.90	119.39	111.11
1	B	319	TRP	CG-CD2-CE3	6.90	140.80	133.90
1	A	388	ASN	OD1-CG-ND2	-6.88	115.72	122.60
1	B	238	GLU	CA-CB-CG	6.86	127.83	114.10
1	A	346	ALA	O-C-N	6.82	131.66	122.59
1	B	22	ASP	CA-CB-CG	-6.82	105.78	112.60
1	A	74	ASP	CA-CB-CG	6.81	119.41	112.60
1	A	215	LYS	N-CA-C	6.78	121.30	112.89
1	B	316	ARG	CG-CD-NE	-6.77	97.10	112.00
1	A	312	ASN	CB-CG-ND2	6.74	126.51	116.40
1	A	22	ASP	CA-CB-CG	-6.70	105.90	112.60
1	B	266	ARG	NE-CZ-NH2	-6.70	113.17	119.20
1	A	373	LEU	CA-C-O	-6.69	113.74	120.90
1	A	238	GLU	CA-CB-CG	6.68	127.47	114.10
1	A	257	SER	N-CA-C	6.68	118.56	111.28
1	B	356	GLN	OE1-CD-NE2	-6.66	115.94	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	194	ASN	O-C-N	-6.61	115.27	121.35
1	B	294	ASN	CB-CG-ND2	6.58	126.27	116.40
1	B	169	ASP	N-CA-C	-6.55	96.46	107.99
1	B	267	VAL	O-C-N	-6.54	116.69	123.03
1	A	266	ARG	NE-CZ-NH1	6.51	128.01	121.50
1	A	194	ASN	CA-CB-CG	6.51	119.11	112.60
1	A	313	ASP	N-CA-C	6.50	120.08	111.75
1	A	178	ASN	CA-C-O	6.50	128.51	121.16
1	A	105	THR	O-C-N	-6.50	116.48	121.55
1	A	96	ASN	CB-CG-ND2	6.49	126.14	116.40
1	B	30	PRO	N-CA-C	6.49	125.84	112.47
1	B	134	TRP	O-C-N	-6.49	115.82	123.22
1	A	204	GLN	OE1-CD-NE2	-6.47	116.13	122.60
1	B	360	PHE	N-CA-C	6.45	120.55	110.17
1	B	41	LYS	N-CA-C	-6.42	99.36	109.50
1	B	28	GLU	CA-C-O	6.41	129.68	120.51
1	B	258	HIS	CA-CB-CG	-6.41	107.39	113.80
1	A	179	GLU	N-CA-C	-6.41	97.16	110.80
1	A	41	LYS	N-CA-C	-6.40	98.18	109.06
1	B	105	THR	O-C-N	-6.37	117.63	121.71
1	B	168	LEU	N-CA-C	-6.35	99.53	109.25
1	B	41	LYS	CG-CD-CE	6.34	125.89	111.30
1	B	337	PHE	CA-CB-CG	6.33	120.13	113.80
1	B	344	LYS	N-CA-C	-6.33	105.54	113.20
1	A	280	VAL	N-CA-CB	6.32	122.21	110.77
1	B	272	LEU	CB-CA-C	-6.31	99.84	110.19
1	A	286	GLN	OE1-CD-NE2	-6.27	116.33	122.60
1	B	16	PRO	O-C-N	6.27	131.10	122.64
1	B	272	LEU	CA-C-O	-6.26	113.44	120.32
1	B	226	GLN	CG-CD-NE2	6.25	125.77	116.40
1	A	356	GLN	OE1-CD-NE2	-6.24	116.36	122.60
1	B	154	GLU	CA-CB-CG	6.24	126.57	114.10
1	A	374	ARG	N-CA-CB	6.22	118.99	109.98
1	B	376	GLU	CA-C-O	6.20	127.11	119.05
1	B	53	VAL	CA-C-O	-6.19	114.18	121.05
1	B	68	LYS	CA-CB-CG	-6.18	101.75	114.10
1	B	341	LEU	N-CA-C	-6.13	104.52	111.14
1	B	347	ASN	CB-CG-ND2	6.13	125.59	116.40
1	B	27	ASP	CA-CB-CG	6.10	118.70	112.60
1	B	259	ASN	CA-CB-CG	6.06	118.66	112.60
1	A	63	ASN	OD1-CG-ND2	-6.05	116.55	122.60
1	A	8	ASN	OD1-CG-ND2	-6.03	116.57	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	298	PRO	N-CA-CB	-6.03	97.23	103.08
1	B	217	TRP	CE2-CD2-CE3	6.02	124.82	118.80
1	A	319	TRP	CG-CD1-NE1	-6.01	102.38	110.20
1	A	210	GLN	OE1-CD-NE2	-6.01	116.59	122.60
1	A	41	LYS	CG-CD-CE	6.00	125.10	111.30
1	A	30	PRO	N-CA-C	6.00	124.82	112.47
1	A	343	GLU	CB-CA-C	-5.98	101.50	110.88
1	B	357	ASN	N-CA-C	5.98	119.14	109.40
1	A	187	LEU	CD1-CG-CD2	-5.98	97.65	110.80
1	A	199	ASP	O-C-N	-5.98	115.77	121.57
1	A	238	GLU	CB-CA-C	-5.97	100.87	110.79
1	B	196	THR	CA-C-O	5.95	126.57	119.60
1	A	380	TYR	CA-C-O	-5.95	114.35	120.54
1	B	105	THR	CB-CA-C	5.94	119.48	109.32
1	A	319	TRP	CG-CD2-CE3	5.94	139.84	133.90
1	A	369	GLN	OE1-CD-NE2	-5.93	116.67	122.60
1	B	50	LEU	CA-C-O	-5.92	115.28	121.55
1	B	301	HIS	CB-CG-ND1	5.91	131.57	122.70
1	A	248	LYS	N-CA-C	-5.90	104.44	111.69
1	B	58	GLN	CB-CG-CD	-5.88	102.60	112.60
1	B	217	TRP	CA-CB-CG	5.88	124.77	113.60
1	B	199	ASP	O-C-N	-5.88	116.75	121.80
1	B	154	GLU	N-CA-C	-5.87	100.14	109.76
1	A	236	ASP	O-C-N	-5.85	114.64	122.43
1	B	193	HIS	CB-CG-CD2	-5.85	123.59	131.20
1	A	78	GLU	N-CA-CB	5.85	119.23	110.22
1	B	194	ASN	OD1-CG-ND2	-5.85	116.75	122.60
1	B	129	ARG	O-C-N	5.84	129.90	123.25
1	A	342	GLN	CG-CD-NE2	5.83	125.14	116.40
1	A	39	VAL	CB-CA-C	5.81	119.38	110.55
1	B	396	ASN	CA-CB-CG	5.80	118.40	112.60
1	B	104	GLN	N-CA-C	-5.79	102.34	110.50
1	A	113	ARG	NE-CZ-NH2	-5.78	114.00	119.20
1	A	398	ALA	CA-C-O	-5.78	112.25	120.16
1	A	135	VAL	O-C-N	-5.77	116.97	123.03
1	A	82	CYS	CA-C-O	-5.76	114.45	120.55
1	B	348	ARG	N-CA-C	-5.73	100.64	109.52
1	A	218	LEU	CA-C-O	5.72	124.16	119.36
1	B	6	PHE	CB-CA-C	-5.71	99.05	110.42
1	B	229	ALA	CA-C-O	-5.70	113.99	120.32
1	B	229	ALA	N-CA-C	-5.69	99.15	108.76
1	A	301	HIS	N-CA-C	5.68	117.16	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	377	PHE	CA-C-O	5.68	128.64	120.51
1	A	166	HIS	CB-CG-CD2	-5.68	123.82	131.20
1	A	332	ARG	CB-CA-C	-5.67	101.97	110.88
1	B	308	THR	CA-CB-OG1	-5.67	101.09	109.60
1	A	154	GLU	CA-CB-CG	5.66	125.43	114.10
1	A	63	ASN	N-CA-C	5.66	120.31	113.41
1	A	359	MET	N-CA-C	5.65	120.18	113.28
1	B	78	GLU	CB-CG-CD	5.63	122.17	112.60
1	B	332	ARG	CB-CA-C	-5.58	101.53	110.79
1	B	262	LEU	N-CA-CB	-5.57	103.12	111.25
1	B	210	GLN	N-CA-CB	-5.54	101.96	110.16
1	A	258	HIS	CB-CG-CD2	-5.53	124.01	131.20
1	B	28	GLU	CB-CG-CD	5.52	121.98	112.60
1	A	68	LYS	CA-CB-CG	-5.51	103.08	114.10
1	B	316	ARG	NE-CZ-NH2	-5.51	114.24	119.20
1	B	366	THR	CA-CB-OG1	5.51	117.86	109.60
1	B	12	ALA	N-CA-C	-5.49	102.22	110.24
1	A	264	ASN	CA-CB-CG	5.47	118.07	112.60
1	A	346	ALA	CA-C-N	5.47	131.99	121.54
1	A	346	ALA	C-N-CA	5.47	131.99	121.54
1	A	194	ASN	CB-CA-C	5.47	116.08	109.85
1	B	28	GLU	N-CA-C	5.46	122.42	110.80
1	A	262	LEU	N-CA-CB	-5.45	102.89	111.39
1	B	215	LYS	CG-CD-CE	5.45	123.83	111.30
1	B	145	SER	CA-C-O	-5.44	113.71	119.97
1	A	32	LYS	N-CA-C	5.44	117.31	110.24
1	A	214	GLU	CB-CG-CD	5.43	121.83	112.60
1	B	228	PHE	N-CA-C	5.43	120.57	113.30
1	A	260	PHE	CA-CB-CG	5.43	119.23	113.80
1	A	316	ARG	CG-CD-NE	-5.42	100.08	112.00
1	B	97	ASP	CA-CB-CG	5.41	118.01	112.60
1	B	387	VAL	CB-CA-C	5.41	120.07	110.71
1	A	171	ASP	CA-C-O	-5.41	115.32	121.00
1	A	374	ARG	CA-CB-CG	5.41	124.91	114.10
1	A	15	ASP	CA-C-N	5.39	124.84	119.24
1	A	15	ASP	C-N-CA	5.39	124.84	119.24
1	A	301	HIS	CB-CG-ND1	5.38	130.78	122.70
1	B	247	HIS	CA-C-O	5.38	126.77	120.80
1	B	114	VAL	O-C-N	-5.37	116.44	121.87
1	B	103	ALA	N-CA-C	-5.36	100.44	109.07
1	B	328	GLN	OE1-CD-NE2	-5.36	117.24	122.60
1	A	366	THR	CB-CA-C	5.35	119.30	109.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	217	TRP	CG-CD1-NE1	-5.34	103.25	110.20
1	A	129	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	B	271	THR	CA-C-N	5.33	130.51	123.05
1	B	271	THR	C-N-CA	5.33	130.51	123.05
1	A	84	GLN	CA-C-O	-5.31	115.24	120.82
1	A	235	GLU	CB-CA-C	5.30	119.28	110.81
1	B	349	ASP	CA-CB-CG	-5.28	107.32	112.60
1	B	214	GLU	N-CA-C	5.28	118.88	112.23
1	A	319	TRP	CD1-CG-CD2	5.27	114.74	106.30
1	A	334	ARG	CB-CG-CD	5.27	123.42	111.30
1	A	389	VAL	N-CA-CB	-5.26	101.65	110.65
1	A	84	GLN	CG-CD-NE2	5.26	124.29	116.40
1	A	199	ASP	CA-C-N	5.25	125.23	120.03
1	A	199	ASP	C-N-CA	5.25	125.23	120.03
1	A	168	LEU	CA-C-O	-5.25	115.08	120.54
1	A	90	LYS	N-CA-C	5.24	117.73	111.71
1	B	326	MET	N-CA-C	-5.24	105.49	111.14
1	A	395	ASP	CA-CB-CG	5.23	117.83	112.60
1	B	23	LEU	N-CA-C	-5.23	105.64	112.23
1	B	291	ILE	CA-C-O	-5.22	115.63	121.17
1	B	347	ASN	CA-CB-CG	5.22	117.82	112.60
1	A	247	HIS	CA-CB-CG	-5.21	108.59	113.80
1	A	145	SER	CA-C-O	-5.21	114.90	120.42
1	B	319	TRP	CE2-CD2-CG	-5.18	100.99	107.20
1	B	12	ALA	CA-C-N	5.18	124.94	119.76
1	B	12	ALA	C-N-CA	5.18	124.94	119.76
1	A	28	GLU	CA-C-O	5.17	127.91	120.51
1	A	168	LEU	CA-C-N	-5.17	115.49	123.14
1	A	168	LEU	C-N-CA	-5.17	115.49	123.14
1	A	343	GLU	CA-C-O	-5.17	115.39	120.82
1	A	328	GLN	CG-CD-NE2	5.16	124.14	116.40
1	B	356	GLN	O-C-N	-5.16	117.20	123.03
1	A	343	GLU	O-C-N	-5.16	116.76	122.07
1	B	193	HIS	CB-CG-ND1	5.15	130.43	122.70
1	B	319	TRP	CB-CG-CD1	-5.15	119.17	126.90
1	A	369	GLN	CG-CD-NE2	5.14	124.11	116.40
1	B	32	LYS	CA-C-O	-5.14	115.06	120.92
1	B	400	LEU	N-CA-C	-5.13	105.14	111.40
1	A	98	LYS	N-CA-CB	-5.12	104.12	111.70
1	A	319	TRP	CE2-CD2-CG	-5.12	101.06	107.20
1	A	178	ASN	CB-CG-ND2	5.11	124.07	116.40
1	B	158	TYR	CA-CB-CG	5.11	123.11	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	LEU	N-CA-CB	-5.11	102.29	110.77
1	A	316	ARG	CA-CB-CG	-5.11	103.89	114.10
1	A	280	VAL	CA-CB-CG1	-5.09	101.74	110.40
1	B	319	TRP	CG-CD1-NE1	-5.09	103.58	110.20
1	A	210	GLN	CG-CD-NE2	5.09	124.04	116.40
1	B	148	ASN	CB-CG-ND2	5.09	124.03	116.40
1	A	375	GLU	CA-C-O	-5.08	115.48	120.82
1	B	272	LEU	CA-C-N	-5.07	114.15	122.67
1	B	272	LEU	C-N-CA	-5.07	114.15	122.67
1	A	205	TRP	N-CA-C	-5.07	105.66	111.14
1	B	184	ASP	CA-CB-CG	5.07	117.67	112.60
1	A	321	GLN	CB-CA-C	-5.06	102.24	110.85
1	A	347	ASN	N-CA-CB	-5.06	101.93	110.49
1	A	247	HIS	CB-CG-CD2	-5.06	124.62	131.20
1	A	115	ALA	N-CA-C	-5.05	105.85	111.36
1	B	88	PHE	CA-CB-CG	-5.03	108.77	113.80
1	B	59	TYR	O-C-N	-5.03	116.79	122.12
1	A	357	ASN	OD1-CG-ND2	-5.02	117.58	122.60
1	A	331	GLN	CA-C-O	-5.01	115.23	120.55
1	A	382	VAL	O-C-N	-5.00	117.22	122.57

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	231	GLY	Mainchain
1	A	329	ARG	Sidechain
1	B	134	TRP	Mainchain
1	B	15	ASP	Mainchain
1	B	376	GLU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3070	0	3012	84	0
1	B	3070	0	3011	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	10	0	0	1	0
3	A	16	0	10	1	0
3	B	16	0	11	0	0
All	All	6182	0	6044	156	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 13.

All (156) 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:16:PRO:C	1:B:17:ILE:N	1.71	1.48
1:B:19:GLY:N	1:B:19:GLY:CA	1.90	1.34
1:B:15:ASP:N	1:B:15:ASP:CA	1.89	1.33
1:B:123:THR:HG22	1:B:125:VAL:H	0.99	1.11
1:B:123:THR:CG2	1:B:125:VAL:H	1.66	1.07
1:B:123:THR:HG22	1:B:125:VAL:N	1.81	0.95
1:A:294:ASN:HD21	1:B:294:ASN:HD21	1.11	0.93
1:A:123:THR:HG22	1:A:125:VAL:H	1.36	0.88
1:A:201:THR:H	1:A:204:GLN:HE21	1.23	0.86
1:A:126:LYS:HG2	1:A:126:LYS:O	1.78	0.82
1:A:123:THR:CG2	1:A:125:VAL:H	1.92	0.82
1:B:123:THR:HG21	1:B:125:VAL:HG23	1.63	0.81
1:A:29:ARG:HH11	1:A:29:ARG:HG2	1.44	0.81
1:A:123:THR:HG23	1:A:124:SER:H	1.46	0.79
1:B:123:THR:CG2	1:B:124:SER:N	2.48	0.77
1:A:266:ARG:HD2	1:B:297:ASN:O	1.88	0.74
1:B:337:PHE:HB2	1:B:392:MET:HE1	1.70	0.73
1:A:258:HIS:CD2	1:A:359:MET:HE1	2.24	0.72
1:A:123:THR:CG2	1:A:124:SER:N	2.52	0.71
1:B:126:LYS:C	1:B:129:ARG:HG3	2.15	0.71
1:B:344:LYS:HD2	1:B:402:GLU:HA	1.73	0.71
1:A:15:ASP:HB3	1:A:18:LEU:HB2	1.73	0.70
1:A:168:LEU:HD21	1:A:173:LEU:HD23	1.71	0.70
1:A:39:VAL:HG21	1:B:69:ASN:ND2	2.06	0.70
1:B:397:MET:HE3	1:B:397:MET:HA	1.74	0.69
1:B:123:THR:HG23	1:B:124:SER:N	2.08	0.68
1:A:29:ARG:HG2	1:A:29:ARG:NH1	2.07	0.67
1:A:123:THR:HG23	1:A:124:SER:N	2.07	0.67
1:A:297:ASN:O	1:B:266:ARG:HD2	1.95	0.67
1:B:15:ASP:N	1:B:15:ASP:C	2.52	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:THR:HG22	1:B:168:LEU:H	1.59	0.66
1:B:126:LYS:C	1:B:129:ARG:CG	2.69	0.65
1:B:105:THR:HG21	1:B:111:ALA:HB2	1.79	0.65
1:A:328:GLN:O	1:A:332:ARG:HD3	1.97	0.65
1:B:260:PHE:HB3	1:B:262:LEU:HD22	1.78	0.64
1:B:123:THR:HG23	1:B:124:SER:H	1.62	0.64
1:B:15:ASP:HB3	1:B:18:LEU:HB2	1.79	0.64
1:A:230:ARG:CG	1:A:235:GLU:HB3	2.30	0.62
1:B:16:PRO:CA	1:B:17:ILE:N	2.60	0.62
1:B:123:THR:CG2	1:B:125:VAL:N	2.51	0.61
1:A:294:ASN:HD21	1:B:294:ASN:ND2	1.92	0.61
1:B:16:PRO:C	1:B:17:ILE:CA	2.71	0.60
1:A:260:PHE:HB3	1:A:262:LEU:HD22	1.83	0.60
1:A:41:LYS:HD3	1:A:45:GLY:HA2	1.82	0.60
1:A:366:THR:HG22	1:A:369:GLN:H	1.67	0.60
1:B:168:LEU:HD21	1:B:173:LEU:HD23	1.84	0.58
1:B:227:GLY:HA3	1:B:323:LEU:HD21	1.85	0.58
1:A:41:LYS:CD	1:A:45:GLY:HA2	2.33	0.57
1:B:99:ARG:HD3	1:B:275:ALA:O	2.03	0.57
1:B:397:MET:HE3	1:B:400:LEU:HD13	1.86	0.56
1:B:99:ARG:HD2	1:B:274:ALA:O	2.06	0.56
1:A:133:VAL:HB	1:A:185:VAL:HB	1.87	0.56
1:B:39:VAL:HG22	1:B:263:TYR:CE1	2.41	0.56
1:A:78:GLU:H	1:A:78:GLU:CD	2.14	0.55
1:B:126:LYS:CG	1:B:126:LYS:O	2.53	0.55
1:A:126:LYS:O	1:A:126:LYS:CG	2.53	0.55
1:A:124:SER:O	1:A:125:VAL:C	2.48	0.54
1:B:20:LEU:HD12	1:B:380:TYR:HD2	1.73	0.53
1:A:263:TYR:HB2	1:B:68:LYS:O	2.07	0.53
1:A:39:VAL:HG22	1:A:263:TYR:CZ	2.44	0.52
1:A:292:ARG:HA	1:A:296:SER:HA	1.91	0.52
1:A:334:ARG:NH2	1:A:361:SER:OG	2.41	0.52
1:A:258:HIS:HD2	1:A:359:MET:HE1	1.71	0.52
1:B:133:VAL:HB	1:B:185:VAL:HG22	1.92	0.52
1:A:78:GLU:HA	1:A:81:ARG:HG3	1.91	0.51
1:A:129:ARG:HD3	1:A:184:ASP:OD2	2.10	0.51
1:B:142:ASN:O	1:B:146:VAL:HG13	2.11	0.51
1:B:123:THR:CG2	1:B:125:VAL:HG23	2.38	0.51
1:B:187:LEU:HD12	1:B:220:LEU:HG	1.92	0.50
1:A:397:MET:HE2	1:A:401:CYS:SG	2.51	0.50
1:B:129:ARG:HA	1:B:154:GLU:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:VAL:HG21	1:B:383:ALA:HA	1.93	0.50
1:A:117:ASP:O	1:A:121:LYS:HG2	2.12	0.50
1:A:337:PHE:HD1	1:A:397:MET:HE1	1.75	0.50
1:A:230:ARG:HG2	1:A:235:GLU:HB3	1.95	0.49
1:B:196:THR:CG2	1:B:198:ILE:H	2.25	0.49
1:A:359:MET:HB3	1:A:388:ASN:ND2	2.27	0.49
1:B:196:THR:HG22	1:B:198:ILE:H	1.77	0.49
1:A:68:LYS:O	1:B:263:TYR:HB2	2.12	0.48
1:A:87:LEU:O	1:A:241:ARG:HD2	2.13	0.48
1:A:5:MET:HE1	1:B:183:GLY:HA2	1.95	0.48
1:B:133:VAL:O	1:B:155:VAL:HA	2.12	0.48
1:A:201:THR:N	1:A:204:GLN:HE21	2.02	0.48
1:B:129:ARG:NH2	1:B:154:GLU:OE2	2.46	0.47
1:A:41:LYS:HE3	1:A:41:LYS:HB3	1.86	0.47
1:A:337:PHE:HD1	1:A:397:MET:CE	2.26	0.47
1:A:372:ARG:HD2	1:A:376:GLU:HG3	1.95	0.47
1:B:126:LYS:O	1:B:126:LYS:HG2	2.14	0.47
1:B:258:HIS:HD2	1:B:359:MET:HE1	1.79	0.47
1:A:373:LEU:HB3	1:A:379:VAL:HB	1.96	0.47
1:A:133:VAL:HA	1:A:185:VAL:O	2.13	0.46
1:B:196:THR:HG23	1:B:198:ILE:HB	1.96	0.46
1:A:39:VAL:HG21	1:B:69:ASN:HD21	1.77	0.46
1:A:144:LYS:HG3	1:A:155:VAL:HG21	1.97	0.46
1:A:34:ASN:HA	1:A:380:TYR:HB2	1.98	0.46
1:B:322:GLU:O	1:B:326:MET:HG3	2.15	0.46
1:A:248:LYS:HD3	1:A:248:LYS:HA	1.81	0.46
1:B:37:ILE:HD12	1:B:41:LYS:HD2	1.97	0.46
1:A:41:LYS:NZ	1:A:45:GLY:HA2	2.31	0.46
1:A:352:PHE:HA	1:A:355:LYS:HD3	1.98	0.46
1:A:392:MET:HG2	1:A:400:LEU:HD21	1.98	0.46
1:A:330:ILE:O	1:A:334:ARG:HG3	2.17	0.45
1:B:373:LEU:HD13	1:B:408:VAL:HG21	1.96	0.45
1:A:344:LYS:NZ	1:A:402:GLU:CD	2.75	0.45
1:A:397:MET:HE3	1:A:397:MET:HA	1.97	0.45
1:B:98:LYS:HA	1:B:98:LYS:HE2	1.99	0.45
1:B:177:LEU:HD23	1:B:177:LEU:HA	1.76	0.45
1:A:235:GLU:O	1:A:238:GLU:HG3	2.17	0.45
1:B:126:LYS:O	1:B:129:ARG:HG2	2.18	0.44
1:B:397:MET:CE	1:B:400:LEU:HD13	2.47	0.44
1:A:129:ARG:HD3	1:A:134:TRP:HE1	1.82	0.44
1:A:124:SER:C	1:A:125:VAL:O	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:HIS:O	1:A:355:LYS:NZ	2.51	0.44
1:A:123:THR:CG2	1:A:124:SER:H	2.16	0.44
1:A:323:LEU:HA	1:A:326:MET:HE3	1.99	0.44
1:B:154:GLU:OE2	1:B:156:ARG:NH1	2.51	0.44
1:A:95:ILE:HD13	1:A:95:ILE:HG21	1.79	0.44
1:B:24:PHE:O	1:B:32:LYS:NZ	2.51	0.44
2:A:412:SO4:O4	3:A:411:PMP:N4A	2.47	0.44
1:A:27:ASP:OD2	1:A:29:ARG:HB2	2.18	0.43
1:A:340:THR:O	1:A:344:LYS:HG2	2.17	0.43
1:B:133:VAL:HA	1:B:185:VAL:O	2.18	0.43
1:B:18:LEU:C	1:B:19:GLY:CA	2.80	0.43
1:A:5:MET:HE2	1:A:5:MET:HB2	1.67	0.43
1:A:344:LYS:HZ1	1:A:402:GLU:CD	2.26	0.43
1:A:83:THR:HB	1:A:256:TYR:OH	2.19	0.43
1:A:181:GLN:H	1:A:181:GLN:HG2	1.66	0.43
1:B:110:GLY:O	1:B:114:VAL:HG13	2.19	0.42
1:B:258:HIS:CD2	1:B:359:MET:HE1	2.53	0.42
1:A:94:LEU:H	1:A:94:LEU:HD12	1.84	0.42
1:B:15:ASP:HA	1:B:16:PRO:HD3	1.65	0.42
1:B:292:ARG:HA	1:B:296:SER:HA	2.02	0.42
1:A:308:THR:O	1:A:312:ASN:ND2	2.52	0.42
1:B:267:VAL:HG11	1:B:306:VAL:HG21	2.01	0.42
1:A:237:ALA:O	1:A:241:ARG:HD3	2.20	0.42
1:B:404:ILE:O	1:B:409:LEU:HG	2.19	0.42
1:A:140:TRP:O	1:A:143:HIS:HB2	2.20	0.41
1:B:53:VAL:HG13	1:B:305:VAL:HG11	2.02	0.41
1:B:100:ALA:O	1:B:101:ARG:HD2	2.20	0.41
1:B:112:LEU:HB3	1:B:146:VAL:HG21	2.01	0.41
1:A:133:VAL:O	1:A:155:VAL:HA	2.21	0.41
1:B:115:ALA:O	1:B:119:LEU:HB2	2.20	0.41
1:B:39:VAL:HG22	1:B:263:TYR:CZ	2.55	0.41
1:A:177:LEU:O	1:A:217:TRP:HZ2	2.03	0.41
1:A:334:ARG:NH1	1:A:358:GLY:O	2.54	0.41
1:A:341:LEU:HD11	1:A:404:ILE:HG12	2.02	0.41
1:A:398:ALA:O	1:A:402:GLU:HG3	2.21	0.41
1:A:129:ARG:HE	1:A:156:ARG:HG3	1.86	0.41
1:B:37:ILE:O	1:B:37:ILE:HG12	2.21	0.40
1:A:237:ALA:HB3	1:A:241:ARG:NH1	2.36	0.40
1:A:133:VAL:CB	1:A:185:VAL:HB	2.51	0.40
1:A:139:SER:OG	1:A:189:HIS:HE1	2.05	0.40
1:B:28:GLU:OE1	1:B:32:LYS:NZ	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:ILE:HG21	1:B:95:ILE:HD13	1.84	0.40
1:B:98:LYS:HA	1:B:98:LYS:CE	2.51	0.40
1:B:344:LYS:HD3	1:B:344:LYS:O	2.21	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	394/396 (100%)	364 (92%)	24 (6%)	6 (2%)	8	12
1	B	394/396 (100%)	373 (95%)	16 (4%)	5 (1%)	9	14
All	All	788/792 (100%)	737 (94%)	40 (5%)	11 (1%)	9	13

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	PRO
1	A	181	GLN
1	A	347	ASN
1	B	30	PRO
1	A	11	ALA
1	B	26	ALA
1	B	28	GLU
1	B	230	ARG
1	B	377	PHE
1	A	12	ALA
1	A	179	GLU

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	320/320 (100%)	258 (81%)	62 (19%)	1	2
1	B	320/320 (100%)	266 (83%)	54 (17%)	2	3
All	All	640/640 (100%)	524 (82%)	116 (18%)	2	2

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	MET
1	A	20	LEU
1	A	23	LEU
1	A	27	ASP
1	A	28	GLU
1	A	30	PRO
1	A	39	VAL
1	A	46	LYS
1	A	54	LYS
1	A	61	LEU
1	A	78	GLU
1	A	83	THR
1	A	87	LEU
1	A	98	LYS
1	A	101	ARG
1	A	112	LEU
1	A	123	THR
1	A	143	HIS
1	A	152	LEU
1	A	154	GLU
1	A	155	VAL
1	A	156	ARG
1	A	167	THR
1	A	168	LEU
1	A	169	ASP
1	A	173	LEU
1	A	174	ILE

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Mol	Chain	Res	Type
1	A	181	GLN
1	A	195	PRO
1	A	202	LEU
1	A	206	GLN
1	A	210	GLN
1	A	214	GLU
1	A	215	LYS
1	A	220	LEU
1	A	223	PHE
1	A	230	ARG
1	A	233	LEU
1	A	235	GLU
1	A	241	ARG
1	A	259	ASN
1	A	262	LEU
1	A	272	LEU
1	A	273	VAL
1	A	280	VAL
1	A	312	ASN
1	A	321	GLN
1	A	338	VAL
1	A	341	LEU
1	A	342	GLN
1	A	344	LYS
1	A	355	LYS
1	A	361	SER
1	A	362	PHE
1	A	365	LEU
1	A	366	THR
1	A	372	ARG
1	A	376	GLU
1	A	379	VAL
1	A	388	ASN
1	A	400	LEU
1	A	404	ILE
1	B	5	MET
1	B	6	PHE
1	B	20	LEU
1	B	23	LEU
1	B	28	GLU
1	B	29	ARG
1	B	37	ILE

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Mol	Chain	Res	Type
1	B	39	VAL
1	B	50	LEU
1	B	51	THR
1	B	61	LEU
1	B	74	ASP
1	B	87	LEU
1	B	92	SER
1	B	94	LEU
1	B	98	LYS
1	B	105	THR
1	B	112	LEU
1	B	119	LEU
1	B	123	THR
1	B	133	VAL
1	B	146	VAL
1	B	148	ASN
1	B	152	LEU
1	B	155	VAL
1	B	168	LEU
1	B	173	LEU
1	B	181	GLN
1	B	185	VAL
1	B	196	THR
1	B	215	LYS
1	B	220	LEU
1	B	223	PHE
1	B	233	LEU
1	B	240	LEU
1	B	241	ARG
1	B	246	MET
1	B	262	LEU
1	B	272	LEU
1	B	273	VAL
1	B	278	GLU
1	B	338	VAL
1	B	341	LEU
1	B	347	ASN
1	B	348	ARG
1	B	362	PHE
1	B	365	LEU
1	B	370	VAL
1	B	372	ARG

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Mol	Chain	Res	Type
1	B	376	GLU
1	B	377	PHE
1	B	387	VAL
1	B	400	LEU
1	B	402	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	166	HIS
1	A	175	ASN
1	A	189	HIS
1	A	204	GLN
1	A	210	GLN
1	A	226	GLN
1	A	258	HIS
1	A	259	ASN
1	A	294	ASN
1	A	297	ASN
1	A	312	ASN
1	A	335	GLN
1	A	339	ASN
1	A	357	ASN
1	A	388	ASN
1	B	69	ASN
1	B	84	GLN
1	B	122	ASN
1	B	247	HIS
1	B	297	ASN
1	B	335	GLN
1	B	342	GLN
1	B	356	GLN
1	B	357	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	SO4	A	412	-	4,4,4	1.13	0	6,6,6	1.02	0
3	PMP	B	411	-	16,16,16	2.28	7 (43%)	22,23,23	1.49	3 (13%)
3	PMP	A	411	-	16,16,16	1.81	4 (25%)	22,23,23	1.64	5 (22%)
2	SO4	A	413	-	4,4,4	1.04	0	6,6,6	0.83	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
3	PMP	B	411	-	-	0/8/8/8	0/1/1/1
3	PMP	A	411	-	-	2/8/8/8	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	411	PMP	C3-C2	-4.99	1.35	1.41
3	B	411	PMP	C4A-C4	-4.92	1.34	1.51
3	A	411	PMP	C3-C2	-3.85	1.37	1.41
3	A	411	PMP	O4P-C5A	-3.51	1.31	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	411	PMP	C4A-C4	-3.30	1.40	1.51
3	B	411	PMP	O4P-C5A	-2.43	1.35	1.44
3	B	411	PMP	P-O2P	-2.38	1.45	1.54
3	B	411	PMP	C2-N1	2.17	1.37	1.33
3	B	411	PMP	C2A-C2	-2.09	1.47	1.50
3	A	411	PMP	C6-N1	2.06	1.38	1.34
3	B	411	PMP	C6-N1	2.03	1.38	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	411	PMP	O4P-C5A-C5	4.97	118.68	109.36
3	B	411	PMP	C6-C5-C4	3.94	121.04	118.06
3	B	411	PMP	C5-C6-N1	-3.21	118.60	123.83
3	B	411	PMP	O4P-P-O1P	2.52	113.24	106.44
3	A	411	PMP	O2P-P-O4P	2.50	113.20	106.67
3	A	411	PMP	C6-C5-C4	2.50	119.95	118.06
3	A	411	PMP	C5-C6-N1	-2.46	119.83	123.83
3	A	411	PMP	O2P-P-O1P	2.03	118.74	110.83

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	411	PMP	C5A-O4P-P-O3P
3	A	411	PMP	C5A-O4P-P-O1P

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	412	SO4	1	0
3	A	411	PMP	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	16:PRO	C	17:ILE	N	1.71
1	B	15:ASP	C	16:PRO	N	1.14

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.