



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:51 AM UTC

PDB ID : 1AIB / pdb_00001aib
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 : 2.80 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

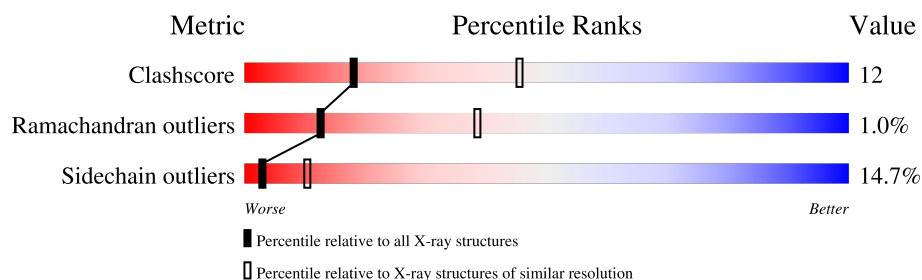
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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	
1	B	396	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	AKG	B	412	-	X	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6192 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.

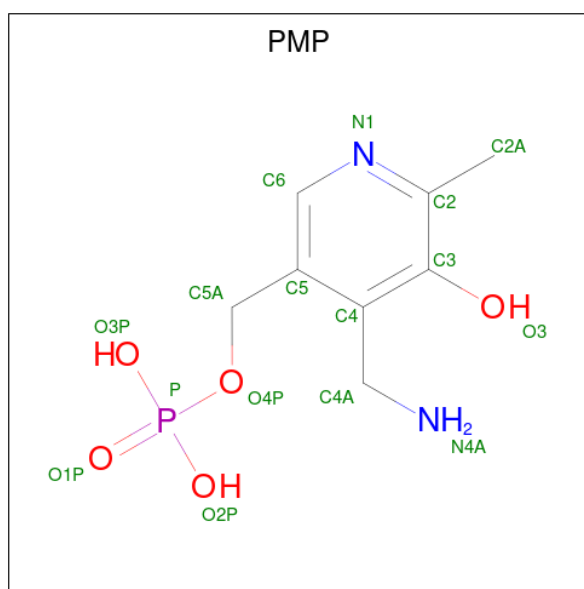
- Molecule 1 is a protein called ASPARTATE AMINOTRANSFERASE.

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 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (CCD ID: PMP) (formula: C₈H₁₃N₂O₅P).



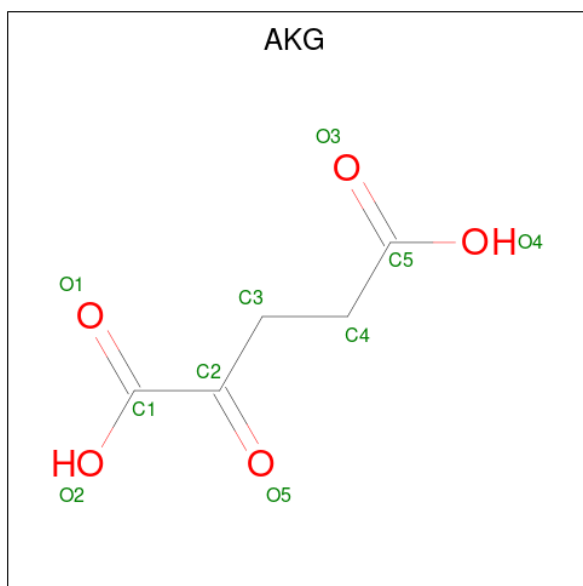
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			16	8	2	5	1		

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

- Molecule 3 is 2-OXOGLUTARIC ACID (CCD ID: AKG) (formula: $C_5H_6O_5$).



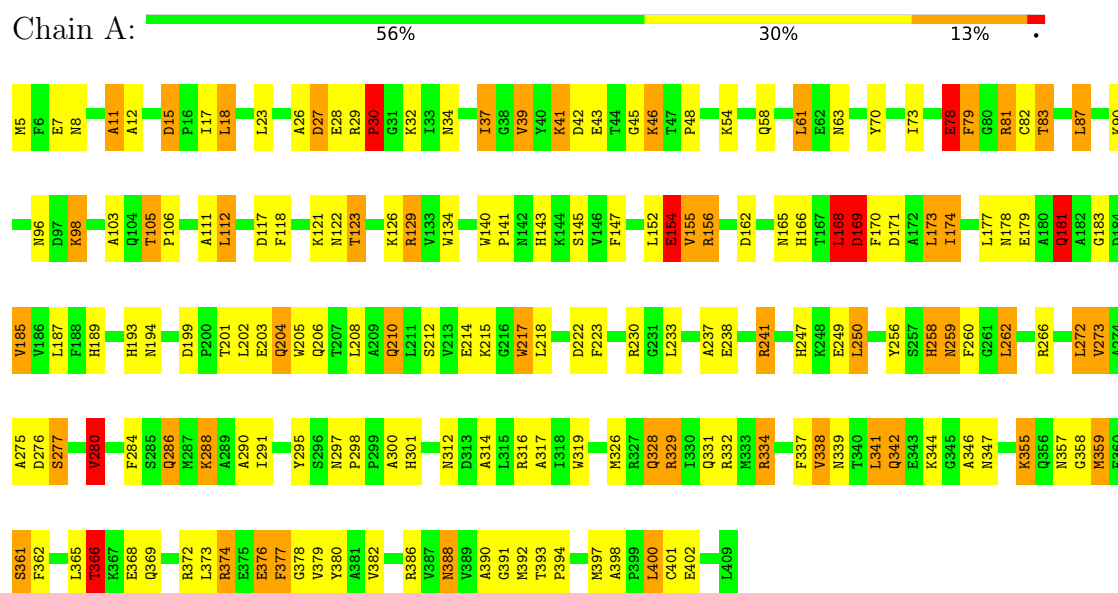
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	5	5		
3	B	1	Total	C	O	0	0
			10	5	5		

3 Residue-property plots

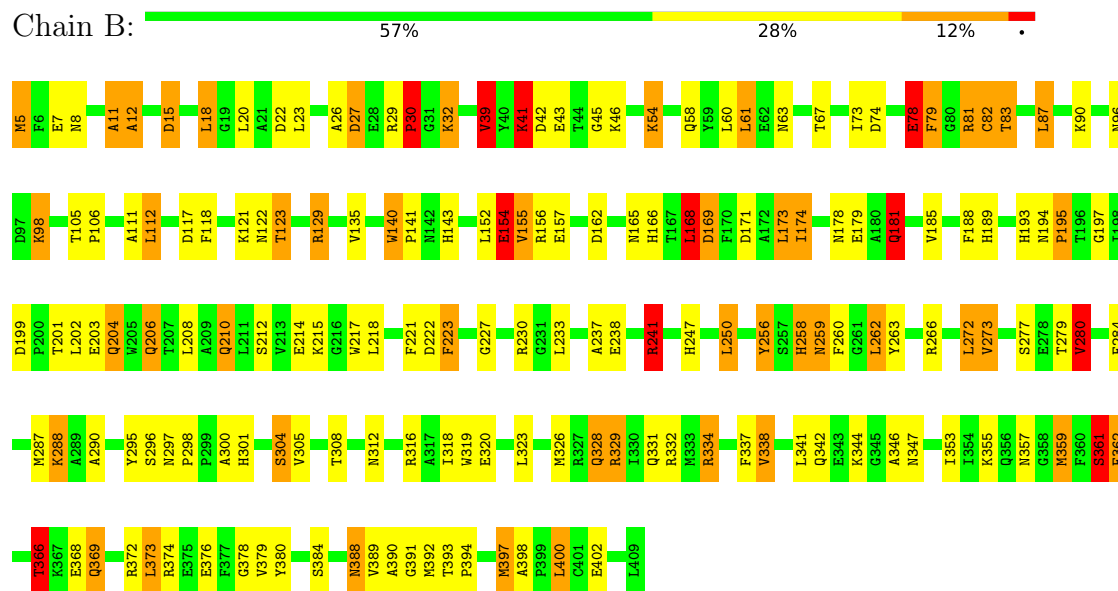
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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	86.60Å 79.80Å 89.80Å 90.00° 119.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.219 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6192	wwPDB-VP
Average B, all atoms (Å ²)	25.0	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: AKG, PMP

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	1.19	11/3132 (0.4%)	2.07	126/4244 (3.0%)
1	B	1.19	10/3132 (0.3%)	2.11	131/4244 (3.1%)
All	All	1.19	21/6264 (0.3%)	2.09	257/8488 (3.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	155	VAL	CA-CB	8.96	1.65	1.54
1	B	155	VAL	CA-CB	7.61	1.63	1.54
1	B	105	THR	CA-CB	7.06	1.62	1.54
1	B	193	HIS	CD2-NE2	-6.92	1.30	1.37
1	A	143	HIS	CD2-NE2	-6.88	1.30	1.37
1	A	258	HIS	CD2-NE2	-6.72	1.30	1.37
1	A	189	HIS	CG-ND1	-6.65	1.30	1.38
1	B	143	HIS	CD2-NE2	-6.65	1.30	1.37
1	A	166	HIS	CD2-NE2	-6.36	1.30	1.37
1	B	166	HIS	CD2-NE2	-6.34	1.30	1.37
1	A	189	HIS	CD2-NE2	-6.34	1.30	1.37
1	A	193	HIS	CD2-NE2	-6.25	1.30	1.37
1	B	189	HIS	CG-ND1	-6.21	1.31	1.38
1	B	258	HIS	CD2-NE2	-6.18	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	189	HIS	CD2-NE2	-6.17	1.31	1.37
1	A	301	HIS	CD2-NE2	-6.06	1.31	1.37
1	A	388	ASN	CA-CB	-5.42	1.46	1.53
1	A	247	HIS	CD2-NE2	-5.40	1.31	1.37
1	B	301	HIS	CD2-NE2	-5.33	1.31	1.37
1	A	338	VAL	CA-CB	5.33	1.61	1.54
1	B	247	HIS	CD2-NE2	-5.30	1.32	1.37

All (257) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	8	ASN	CA-CB-CG	12.40	125.00	112.60
1	A	81	ARG	CA-CB-CG	11.54	137.17	114.10
1	B	169	ASP	CA-CB-CG	11.49	124.09	112.60
1	B	81	ARG	CA-CB-CG	11.04	136.18	114.10
1	A	8	ASN	CA-CB-CG	10.77	123.37	112.60
1	A	347	ASN	CA-CB-CG	10.42	123.02	112.60
1	B	199	ASP	CA-CB-CG	10.19	122.79	112.60
1	B	347	ASN	CA-CB-CG	9.67	122.27	112.60
1	A	169	ASP	CA-CB-CG	9.57	122.17	112.60
1	A	280	VAL	CB-CA-C	-9.42	97.00	112.26
1	B	230	ARG	N-CA-CB	-9.38	98.60	110.98
1	B	280	VAL	CB-CA-C	-9.26	97.80	112.16
1	B	90	LYS	N-CA-C	9.21	121.32	111.28
1	B	168	LEU	CA-C-O	-8.99	110.96	120.58
1	A	230	ARG	N-CA-CB	-8.91	99.21	110.98
1	B	169	ASP	CA-C-O	8.74	129.63	120.54
1	B	11	ALA	N-CA-C	8.54	129.00	110.80
1	B	258	HIS	CA-CB-CG	-8.54	105.26	113.80
1	A	79	PHE	N-CA-C	-8.52	101.94	111.14
1	B	300	ALA	N-CA-C	8.49	120.53	111.28
1	A	168	LEU	CA-C-O	-8.44	111.56	120.58
1	A	11	ALA	N-CA-C	8.27	128.41	110.80
1	A	18	LEU	N-CA-C	8.12	120.14	111.28
1	B	30	PRO	N-CA-C	7.99	128.92	112.47
1	B	82	CYS	N-CA-C	-7.90	102.75	111.36
1	A	169	ASP	CA-C-O	7.78	128.63	120.54
1	A	42	ASP	CA-CB-CG	7.77	120.37	112.60
1	B	178	ASN	CA-CB-CG	-7.77	104.83	112.60
1	A	90	LYS	N-CA-C	7.76	119.74	111.28
1	B	366	THR	N-CA-CB	-7.75	98.51	110.29
1	B	8	ASN	N-CA-CB	-7.74	99.32	111.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	301	HIS	CB-CG-CD2	-7.72	121.16	131.20
1	B	388	ASN	CB-CG-ND2	7.68	127.92	116.40
1	B	82	CYS	CA-C-O	-7.68	112.28	120.42
1	A	30	PRO	N-CA-C	7.66	128.25	112.47
1	A	359	MET	N-CA-C	7.56	122.26	112.89
1	A	366	THR	N-CA-CB	-7.55	98.98	110.45
1	B	18	LEU	N-CA-C	7.51	119.47	111.28
1	A	8	ASN	N-CA-CB	-7.50	100.42	111.51
1	A	300	ALA	N-CA-C	7.41	120.30	111.33
1	B	204	GLN	OE1-CD-NE2	-7.32	115.28	122.60
1	A	129	ARG	CB-CG-CD	-7.29	94.54	111.30
1	A	298	PRO	N-CA-C	7.28	119.58	110.70
1	A	388	ASN	CB-CG-ND2	7.23	127.24	116.40
1	A	7	GLU	N-CA-C	7.19	120.03	111.33
1	B	79	PHE	N-CA-C	-7.19	103.38	111.14
1	B	174	ILE	CB-CG1-CD1	-7.16	98.77	113.80
1	B	168	LEU	CA-C-N	-7.16	113.54	122.84
1	B	168	LEU	C-N-CA	-7.16	113.54	122.84
1	A	174	ILE	CB-CG1-CD1	-7.12	98.85	113.80
1	B	374	ARG	CB-CA-C	-7.07	100.07	110.96
1	B	42	ASP	CA-CB-CG	7.04	119.64	112.60
1	A	366	THR	CA-CB-OG1	-7.01	99.08	109.60
1	A	301	HIS	CB-CG-CD2	-7.00	122.11	131.20
1	B	39	VAL	N-CA-CB	-6.99	100.69	112.44
1	A	194	ASN	CA-CB-CG	6.99	119.59	112.60
1	B	366	THR	CA-CB-OG1	-6.99	99.11	109.60
1	B	280	VAL	N-CA-CB	6.97	122.56	110.65
1	A	162	ASP	CA-CB-CG	6.95	119.55	112.60
1	A	280	VAL	N-CA-CB	6.95	123.35	110.77
1	A	203	GLU	CA-CB-CG	-6.93	100.25	114.10
1	A	377	PHE	CA-CB-CG	-6.86	106.94	113.80
1	B	162	ASP	CA-CB-CG	6.86	119.46	112.60
1	B	359	MET	N-CA-C	6.86	121.74	113.23
1	A	286	GLN	OE1-CD-NE2	-6.85	115.75	122.60
1	A	63	ASN	N-CA-C	6.79	121.86	113.50
1	B	366	THR	CA-CB-CG2	6.67	121.85	110.50
1	B	74	ASP	CA-CB-CG	6.67	119.27	112.60
1	A	290	ALA	CA-C-N	6.64	129.06	120.56
1	A	290	ALA	C-N-CA	6.64	129.06	120.56
1	B	279	THR	CA-C-O	-6.63	113.87	120.70
1	B	388	ASN	OD1-CG-ND2	-6.63	115.97	122.60
1	B	287	MET	CA-CB-CG	-6.62	100.86	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	HIS	CB-CG-CD2	-6.60	122.61	131.20
1	B	154	GLU	CA-C-N	-6.56	115.05	123.19
1	B	154	GLU	C-N-CA	-6.56	115.05	123.19
1	B	331	GLN	OE1-CD-NE2	-6.54	116.06	122.60
1	A	204	GLN	OE1-CD-NE2	-6.51	116.09	122.60
1	B	334	ARG	N-CA-C	-6.48	104.13	111.07
1	B	81	ARG	CB-CA-C	-6.47	100.73	110.88
1	B	346	ALA	CA-C-O	6.41	129.68	120.51
1	B	123	THR	N-CA-CB	-6.41	101.24	111.62
1	B	238	GLU	CA-CB-CG	6.41	126.92	114.10
1	B	250	LEU	N-CA-CB	-6.41	101.82	111.56
1	B	41	LYS	N-CA-CB	-6.39	100.09	110.71
1	B	165	ASN	N-CA-C	6.39	121.08	113.28
1	A	123	THR	N-CA-CB	-6.38	101.47	111.56
1	A	168	LEU	CA-C-N	-6.37	114.55	122.84
1	A	168	LEU	C-N-CA	-6.37	114.55	122.84
1	B	112	LEU	N-CA-C	-6.37	103.96	111.03
1	B	129	ARG	CB-CG-CD	-6.35	96.69	111.30
1	A	328	GLN	CA-CB-CG	-6.35	101.40	114.10
1	A	331	GLN	OE1-CD-NE2	-6.34	116.26	122.60
1	A	366	THR	CA-CB-CG2	6.34	121.28	110.50
1	A	41	LYS	N-CA-CB	-6.33	100.21	110.71
1	B	204	GLN	CG-CD-NE2	6.27	125.80	116.40
1	B	397	MET	CA-C-O	-6.26	113.91	120.92
1	A	165	ASN	N-CA-C	6.24	121.03	113.17
1	B	288	LYS	CA-CB-CG	-6.24	101.63	114.10
1	B	301	HIS	N-CA-C	6.22	117.75	110.97
1	A	199	ASP	CA-CB-CG	6.22	118.82	112.60
1	A	210	GLN	OE1-CD-NE2	-6.22	116.38	122.60
1	A	288	LYS	CA-CB-CG	-6.20	101.70	114.10
1	A	329	ARG	CG-CD-NE	-6.13	98.52	112.00
1	A	43	GLU	N-CA-C	6.12	119.59	111.75
1	A	359	MET	CG-SD-CE	-6.12	87.44	100.90
1	B	301	HIS	CB-CG-ND1	6.09	131.84	122.70
1	A	277	SER	N-CA-C	6.06	118.41	111.02
1	B	78	GLU	N-CA-CB	6.05	120.58	110.41
1	A	179	GLU	N-CA-C	-6.04	97.93	110.80
1	B	247	HIS	CB-CG-CD2	-6.04	123.35	131.20
1	A	145	SER	CA-C-O	-6.02	114.04	120.42
1	A	258	HIS	CA-CB-CG	-6.02	107.78	113.80
1	A	346	ALA	O-C-N	6.02	130.59	122.59
1	B	320	GLU	CA-CB-CG	-6.01	102.09	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	346	ALA	CA-C-O	6.00	129.09	120.51
1	B	290	ALA	CA-C-N	5.97	128.08	120.56
1	B	290	ALA	C-N-CA	5.97	128.08	120.56
1	B	346	ALA	CA-C-N	5.97	129.09	120.38
1	B	346	ALA	C-N-CA	5.97	129.09	120.38
1	A	81	ARG	CB-CA-C	-5.96	100.89	110.79
1	A	250	LEU	N-CA-CB	-5.96	101.76	111.24
1	A	275	ALA	N-CA-C	5.94	119.63	112.38
1	B	43	GLU	N-CA-C	5.92	119.33	111.75
1	B	359	MET	CG-SD-CE	-5.92	87.88	100.90
1	B	27	ASP	CA-CB-CG	5.91	118.51	112.60
1	B	179	GLU	N-CA-C	-5.91	98.21	110.80
1	B	298	PRO	N-CA-C	5.91	117.91	110.70
1	B	58	GLN	CB-CG-CD	5.91	122.64	112.60
1	A	82	CYS	CA-C-O	-5.90	114.17	120.42
1	A	374	ARG	CB-CA-C	-5.89	101.89	110.96
1	B	230	ARG	CB-CA-C	5.88	118.92	109.27
1	B	347	ASN	N-CA-CB	-5.88	100.85	110.14
1	B	143	HIS	CB-CG-CD2	-5.86	123.58	131.20
1	B	319	TRP	CG-CD1-NE1	-5.85	102.59	110.20
1	B	328	GLN	CA-CB-CG	-5.85	102.41	114.10
1	B	63	ASN	N-CA-C	5.82	120.66	113.50
1	A	346	ALA	CA-C-N	5.82	129.99	120.63
1	A	346	ALA	C-N-CA	5.82	129.99	120.63
1	B	210	GLN	OE1-CD-NE2	-5.82	116.78	122.60
1	A	41	LYS	CA-CB-CG	5.78	125.65	114.10
1	B	15	ASP	CA-C-N	5.77	125.24	119.24
1	B	15	ASP	C-N-CA	5.77	125.24	119.24
1	A	154	GLU	CA-C-N	-5.77	116.03	123.19
1	A	154	GLU	C-N-CA	-5.77	116.03	123.19
1	A	179	GLU	CA-C-O	-5.77	112.26	120.51
1	A	301	HIS	CB-CG-ND1	5.77	131.35	122.70
1	A	58	GLN	CB-CG-CD	5.76	122.39	112.60
1	B	357	ASN	N-CA-C	5.76	119.07	110.14
1	A	98	LYS	N-CA-CB	-5.75	103.17	111.91
1	B	241	ARG	N-CA-C	5.73	118.47	111.82
1	A	112	LEU	N-CA-C	-5.71	104.69	111.03
1	A	34	ASN	OD1-CG-ND2	-5.69	116.91	122.60
1	B	272	LEU	CA-C-N	-5.69	115.76	123.10
1	B	272	LEU	C-N-CA	-5.69	115.76	123.10
1	B	215	LYS	N-CA-C	5.67	118.40	111.82
1	A	230	ARG	CB-CA-C	5.67	118.57	109.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	98	LYS	N-CA-CB	-5.67	103.29	111.91
1	B	189	HIS	CB-CG-CD2	-5.66	123.84	131.20
1	B	308	THR	CA-CB-OG1	-5.66	101.11	109.60
1	B	223	PHE	CA-CB-CG	-5.64	108.16	113.80
1	B	384	SER	CA-CB-OG	5.63	122.37	111.10
1	A	342	GLN	CB-CG-CD	5.62	122.16	112.60
1	A	316	ARG	CG-CD-NE	-5.62	99.64	112.00
1	B	361	SER	CA-CB-OG	-5.61	99.87	111.10
1	A	206	GLN	OE1-CD-NE2	-5.60	117.00	122.60
1	B	22	ASP	CA-CB-CG	-5.59	107.01	112.60
1	B	199	ASP	CA-C-N	5.59	125.53	119.78
1	B	199	ASP	C-N-CA	5.59	125.53	119.78
1	A	347	ASN	N-CA-CB	-5.58	100.14	110.18
1	A	28	GLU	CA-C-O	5.56	128.46	120.51
1	B	166	HIS	CB-CG-CD2	-5.56	123.97	131.20
1	A	276	ASP	CA-CB-CG	5.55	118.15	112.60
1	A	178	ASN	CA-CB-CG	-5.53	107.07	112.60
1	A	204	GLN	CG-CD-NE2	5.53	124.70	116.40
1	B	206	GLN	CG-CD-NE2	5.53	124.69	116.40
1	B	256	TYR	N-CA-C	-5.51	106.41	113.02
1	B	206	GLN	OE1-CD-NE2	-5.50	117.09	122.60
1	A	233	LEU	N-CA-C	5.49	117.97	111.33
1	B	179	GLU	CA-C-O	-5.47	112.69	120.51
1	B	54	LYS	CA-CB-CG	-5.46	103.17	114.10
1	B	58	GLN	OE1-CD-NE2	-5.46	117.14	122.60
1	A	238	GLU	CB-CA-C	-5.46	101.73	110.79
1	A	206	GLN	CG-CD-NE2	5.45	124.57	116.40
1	A	319	TRP	CG-CD1-NE1	-5.44	103.13	110.20
1	B	32	LYS	N-CA-C	5.44	117.96	110.35
1	A	382	VAL	CA-C-O	-5.44	115.41	121.23
1	A	259	ASN	CA-CB-CG	5.43	118.03	112.60
1	A	334	ARG	N-CA-C	-5.43	105.28	111.14
1	A	185	VAL	CG1-CB-CG2	-5.42	98.87	110.80
1	A	41	LYS	N-CA-C	-5.42	98.72	108.48
1	A	78	GLU	N-CA-CB	5.42	119.51	110.41
1	A	215	LYS	N-CA-C	5.41	119.14	112.54
1	A	105	THR	CA-C-N	5.39	126.58	119.84
1	A	105	THR	C-N-CA	5.39	126.58	119.84
1	A	39	VAL	N-CA-CB	-5.38	100.77	111.91
1	A	166	HIS	CB-CG-CD2	-5.38	124.20	131.20
1	B	373	LEU	CA-C-O	-5.38	115.17	120.82
1	A	189	HIS	CB-CG-CD2	-5.37	124.23	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	HIS	CB-CG-CD2	-5.36	124.23	131.20
1	B	272	LEU	CA-C-O	-5.35	114.78	120.40
1	A	355	LYS	CA-CB-CG	5.35	124.80	114.10
1	B	305	VAL	N-CA-C	-5.34	105.30	110.42
1	B	193	HIS	CB-CG-CD2	-5.33	124.28	131.20
1	B	203	GLU	CA-CB-CG	-5.32	103.47	114.10
1	A	29	ARG	CA-C-N	5.29	126.46	119.84
1	A	29	ARG	C-N-CA	5.29	126.46	119.84
1	B	337	PHE	CA-CB-CG	5.29	119.09	113.80
1	A	15	ASP	CA-C-N	5.29	125.35	119.32
1	A	15	ASP	C-N-CA	5.29	125.35	119.32
1	A	70	TYR	N-CA-C	5.28	117.73	110.35
1	A	147	PHE	CA-CB-CG	-5.28	108.53	113.80
1	B	316	ARG	CG-CD-NE	-5.28	100.39	112.00
1	A	326	MET	N-CA-C	-5.27	105.62	111.36
1	B	8	ASN	CB-CA-C	5.27	119.60	111.28
1	B	67	THR	CA-C-N	-5.26	114.81	122.86
1	B	67	THR	C-N-CA	-5.26	114.81	122.86
1	A	26	ALA	N-CA-C	5.26	119.44	113.19
1	B	181	GLN	N-CA-C	5.26	122.00	110.80
1	A	96	ASN	N-CA-C	5.25	117.00	111.28
1	B	111	ALA	CA-C-N	5.25	127.78	120.63
1	B	111	ALA	C-N-CA	5.25	127.78	120.63
1	A	217	TRP	CE2-CD2-CG	-5.25	100.90	107.20
1	B	7	GLU	N-CA-C	5.25	117.68	111.33
1	A	372	ARG	CA-CB-CG	-5.23	103.64	114.10
1	B	329	ARG	CG-CD-NE	-5.20	100.56	112.00
1	A	338	VAL	CA-C-O	-5.20	115.34	120.85
1	B	389	VAL	N-CA-CB	-5.19	101.78	110.65
1	B	366	THR	CB-CA-C	5.18	118.99	109.46
1	A	82	CYS	N-CA-C	-5.18	105.72	111.36
1	B	338	VAL	CA-C-O	-5.18	115.57	120.95
1	B	318	ILE	N-CA-C	-5.17	105.67	110.53
1	B	26	ALA	N-CA-C	5.17	119.21	113.01
1	B	217	TRP	CE2-CD2-CG	-5.16	101.01	107.20
1	A	170	PHE	O-C-N	5.15	128.03	122.15
1	A	58	GLN	OE1-CD-NE2	-5.15	117.45	122.60
1	B	230	ARG	CA-CB-CG	5.15	124.39	114.10
1	B	346	ALA	O-C-N	5.14	129.42	122.59
1	B	96	ASN	OD1-CG-ND2	-5.13	117.47	122.60
1	A	357	ASN	N-CA-C	5.12	117.45	109.52
1	B	41	LYS	N-CA-C	-5.11	99.29	108.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	339	ASN	CB-CA-C	-5.10	103.11	110.96
1	A	155	VAL	CA-C-O	5.10	125.88	120.48
1	B	374	ARG	N-CA-CB	5.10	117.35	109.91
1	A	111	ALA	CA-C-N	5.09	127.56	120.63
1	A	111	ALA	C-N-CA	5.09	127.56	120.63
1	A	272	LEU	O-C-N	-5.07	116.43	123.12
1	A	27	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	37	ILE	CB-CA-C	-5.06	106.02	111.59
1	A	169	ASP	O-C-N	5.05	129.06	123.05
1	B	197	GLY	N-CA-C	-5.05	108.03	115.30
1	B	369	GLN	OE1-CD-NE2	-5.05	117.55	122.60
1	A	105	THR	CA-C-O	-5.04	115.65	120.64
1	B	140	TRP	CG-CD2-CE3	5.04	138.94	133.90
1	B	168	LEU	N-CA-C	-5.04	100.30	108.41
1	A	272	LEU	CA-CB-CG	5.02	133.88	116.30
1	A	205	TRP	CE2-CD2-CG	-5.00	101.20	107.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	169	ASP	Mainchain
1	B	169	ASP	Mainchain

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	80	0
1	B	3070	0	3012	73	0
2	A	16	0	10	4	0
2	B	16	0	6	1	0
3	A	10	0	4	2	0
3	B	10	0	4	0	0
All	All	6192	0	6048	149	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 12.

All (149) 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:A:17:ILE:HG21	3:A:412:AKG:O5	1.57	1.02
2:A:411:PMP:H5A1	2:A:411:PMP:N4A	1.81	0.93
2:A:411:PMP:H5A1	2:A:411:PMP:HNA1	1.35	0.92
1:A:386:ARG:NH1	3:A:412:AKG:O1	2.13	0.79
1:B:397:MET:HE3	1:B:397:MET:HA	1.66	0.77
1:A:266:ARG:HD2	1:B:297:ASN:O	1.87	0.75
1:B:41:LYS:HE2	1:B:391:GLY:HA2	1.71	0.73
1:A:258:HIS:CD2	1:A:359:MET:HE1	2.25	0.72
1:B:201:THR:H	1:B:204:GLN:HE21	1.39	0.69
1:A:41:LYS:HE2	1:A:391:GLY:HA2	1.74	0.69
1:A:297:ASN:O	1:B:266:ARG:HD2	1.93	0.69
1:A:201:THR:H	1:A:204:GLN:HE21	1.41	0.68
1:B:366:THR:HG22	1:B:369:GLN:H	1.57	0.68
1:A:258:HIS:HD2	1:A:359:MET:HE1	1.59	0.68
1:A:208:LEU:O	1:A:212:SER:HB2	2.01	0.61
1:A:222:ASP:OD2	2:A:411:PMP:N1	2.34	0.61
1:B:258:HIS:CD2	1:B:359:MET:HE1	2.35	0.60
1:A:41:LYS:HZ1	1:A:393:THR:HG23	1.67	0.60
1:B:373:LEU:HB3	1:B:379:VAL:HB	1.83	0.59
1:A:397:MET:HE3	1:A:397:MET:HA	1.83	0.59
1:A:201:THR:HG23	1:A:204:GLN:HE21	1.68	0.59
1:B:284:PHE:O	1:B:288:LYS:HG3	2.03	0.59
1:A:397:MET:HE2	1:A:401:CYS:SG	2.43	0.59
1:B:258:HIS:HD2	1:B:359:MET:HE1	1.68	0.58
1:B:41:LYS:CD	1:B:45:GLY:HA2	2.34	0.58
1:A:32:LYS:HA	1:A:378:GLY:HA3	1.86	0.57
1:B:41:LYS:HD2	1:B:45:GLY:HA2	1.85	0.57
1:A:366:THR:HG22	1:A:369:GLN:H	1.69	0.57
1:B:32:LYS:HA	1:B:378:GLY:HA3	1.87	0.57
1:A:61:LEU:HD12	1:B:61:LEU:HD12	1.87	0.56
1:A:187:LEU:HD21	1:A:222:ASP:HB2	1.86	0.56
1:B:15:ASP:HB3	1:B:18:LEU:HB2	1.87	0.56
1:B:366:THR:HG22	1:B:369:GLN:N	2.21	0.56
1:B:392:MET:HG2	1:B:400:LEU:HD21	1.87	0.56
2:A:411:PMP:N4A	2:A:411:PMP:C5A	2.62	0.56
1:A:277:SER:O	1:A:280:VAL:HG23	2.07	0.55
1:B:171:ASP:O	1:B:174:ILE:HG22	2.08	0.54
1:B:78:GLU:HA	1:B:81:ARG:HG3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:PHE:O	1:B:83:THR:HG23	2.08	0.53
1:A:250:LEU:HB3	1:A:273:VAL:HG13	1.89	0.53
1:B:250:LEU:HB3	1:B:273:VAL:HG13	1.89	0.53
1:A:46:LYS:O	1:A:48:PRO:HD3	2.08	0.53
1:B:29:ARG:HG3	1:B:30:PRO:HD2	1.91	0.53
1:A:260:PHE:HB3	1:A:262:LEU:HD22	1.91	0.52
1:B:237:ALA:O	1:B:241:ARG:HD3	2.08	0.52
1:B:260:PHE:HB3	1:B:262:LEU:HD22	1.92	0.52
1:A:284:PHE:O	1:A:288:LYS:HG3	2.09	0.52
1:A:359:MET:HB3	1:A:388:ASN:ND2	2.25	0.52
1:B:41:LYS:NZ	1:B:45:GLY:HA2	2.24	0.52
1:A:78:GLU:HA	1:A:81:ARG:HG3	1.92	0.51
1:A:171:ASP:O	1:A:174:ILE:HG22	2.10	0.51
1:A:129:ARG:HA	1:A:154:GLU:O	2.11	0.51
1:A:373:LEU:HB3	1:A:379:VAL:HB	1.90	0.51
1:A:366:THR:HG22	1:A:369:GLN:N	2.25	0.51
1:A:185:VAL:HG22	1:A:218:LEU:HD23	1.94	0.50
1:A:237:ALA:O	1:A:241:ARG:HD3	2.11	0.50
1:B:201:THR:OG1	1:B:204:GLN:HG3	2.11	0.50
1:B:328:GLN:O	1:B:332:ARG:HD3	2.12	0.50
1:A:15:ASP:HB3	1:A:18:LEU:HB2	1.93	0.50
1:B:208:LEU:O	1:B:212:SER:HB2	2.11	0.50
1:A:41:LYS:CD	1:A:45:GLY:HA2	2.42	0.49
1:A:83:THR:O	1:A:87:LEU:HD22	2.13	0.49
1:A:376:GLU:HB2	1:A:377:PHE:CD2	2.48	0.49
1:B:227:GLY:HA3	1:B:323:LEU:HD21	1.94	0.49
1:B:359:MET:HB3	1:B:388:ASN:ND2	2.27	0.49
1:A:168:LEU:HD21	1:A:173:LEU:HD23	1.94	0.49
1:B:329:ARG:NH2	1:B:393:THR:HA	2.28	0.49
1:B:87:LEU:O	1:B:241:ARG:HD2	2.13	0.49
1:A:392:MET:HG2	1:A:400:LEU:HD21	1.95	0.48
1:A:366:THR:HG23	1:A:368:GLU:OE1	2.13	0.48
1:A:334:ARG:NH2	1:A:361:SER:OG	2.46	0.48
1:B:185:VAL:HG22	1:B:218:LEU:HD23	1.96	0.48
1:A:41:LYS:HD2	1:A:45:GLY:HA2	1.95	0.48
1:B:393:THR:HB	1:B:394:PRO:HD2	1.95	0.48
1:B:78:GLU:O	1:B:82:CYS:HB2	2.13	0.48
1:A:41:LYS:NZ	1:A:45:GLY:HA2	2.29	0.47
1:A:87:LEU:O	1:A:241:ARG:HD2	2.14	0.47
1:B:397:MET:HA	1:B:397:MET:CE	2.42	0.47
1:A:392:MET:HE2	1:A:400:LEU:HD21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:THR:HG23	1:A:204:GLN:NE2	2.29	0.46
1:B:277:SER:O	1:B:280:VAL:HG23	2.16	0.46
1:B:41:LYS:HE3	1:B:41:LYS:HB3	1.72	0.46
1:B:168:LEU:HD21	1:B:173:LEU:CD2	2.45	0.46
1:A:286:GLN:CD	1:B:12:ALA:HB2	2.41	0.46
1:B:366:THR:HG23	1:B:368:GLU:OE1	2.16	0.46
1:A:183:GLY:HA2	1:B:5:MET:HE1	1.99	0.45
1:A:378:GLY:O	1:A:380:TYR:HD1	1.99	0.45
1:B:5:MET:HB2	1:B:5:MET:HE2	1.61	0.45
1:B:106:PRO:HD2	1:B:295:TYR:CZ	2.52	0.45
1:A:134:TRP:HA	1:A:156:ARG:O	2.17	0.45
1:B:41:LYS:HZ3	1:B:45:GLY:HA2	1.82	0.45
1:B:73:ILE:HG12	1:B:296:SER:O	2.17	0.44
1:B:78:GLU:H	1:B:78:GLU:CD	2.25	0.44
1:B:378:GLY:O	1:B:380:TYR:HD1	2.00	0.44
1:A:41:LYS:HZ1	1:A:393:THR:CG2	2.30	0.44
1:A:79:PHE:O	1:A:83:THR:HG23	2.16	0.44
1:A:106:PRO:HD2	1:A:295:TYR:CZ	2.52	0.44
1:A:73:ILE:HD11	1:B:18:LEU:HD21	2.00	0.44
1:A:168:LEU:HD21	1:A:173:LEU:CD2	2.48	0.44
1:A:177:LEU:O	1:A:217:TRP:HZ2	2.00	0.44
1:B:118:PHE:O	1:B:122:ASN:HB2	2.18	0.43
1:B:201:THR:HG23	1:B:204:GLN:HE21	1.82	0.43
1:A:329:ARG:NH2	1:A:392:MET:O	2.49	0.43
1:B:188:PHE:O	1:B:221:PHE:HA	2.18	0.43
1:A:388:ASN:ND2	1:A:390:ALA:H	2.17	0.43
1:B:222:ASP:OD2	2:B:411:PMP:N1	2.51	0.43
1:B:201:THR:H	1:B:204:GLN:NE2	2.11	0.43
1:B:334:ARG:NH2	1:B:361:SER:OG	2.51	0.43
1:A:314:ALA:O	1:A:317:ALA:HB3	2.19	0.43
1:B:117:ASP:O	1:B:121:LYS:HG2	2.19	0.43
1:A:328:GLN:O	1:A:332:ARG:HD3	2.19	0.42
1:B:168:LEU:HD21	1:B:173:LEU:HD22	2.00	0.42
1:B:353:ILE:HD13	1:B:353:ILE:HA	1.74	0.42
1:A:118:PHE:O	1:A:122:ASN:HB2	2.18	0.42
1:A:393:THR:HB	1:A:394:PRO:HD2	2.01	0.42
1:A:341:LEU:HD12	1:A:341:LEU:HA	1.90	0.42
1:B:323:LEU:HD12	1:B:326:MET:HE3	2.02	0.42
1:A:46:LYS:HG3	1:A:48:PRO:HG3	2.02	0.42
1:B:83:THR:O	1:B:87:LEU:HD22	2.20	0.42
1:A:103:ALA:O	1:A:105:THR:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:PHE:HD1	1:B:362:PHE:HA	1.75	0.42
1:A:249:GLU:HA	1:A:273:VAL:O	2.20	0.41
1:A:329:ARG:NH2	1:A:393:THR:HA	2.35	0.41
1:B:60:LEU:HD11	1:B:304:SER:HB3	2.02	0.41
1:A:337:PHE:O	1:A:341:LEU:HB2	2.20	0.41
1:B:256:TYR:HA	1:B:259:ASN:HD21	1.85	0.41
1:A:78:GLU:H	1:A:78:GLU:CD	2.29	0.41
1:A:334:ARG:NH1	1:A:358:GLY:O	2.52	0.41
1:B:129:ARG:HA	1:B:154:GLU:O	2.20	0.41
1:B:135:VAL:O	1:B:157:GLU:HA	2.19	0.41
1:A:218:LEU:HB2	1:B:5:MET:HE3	2.03	0.41
1:B:39:VAL:HG22	1:B:263:TYR:CZ	2.55	0.41
1:B:329:ARG:NH2	1:B:393:THR:HG22	2.35	0.41
1:B:140:TRP:HA	1:B:141:PRO:HD2	1.82	0.41
1:A:117:ASP:O	1:A:121:LYS:HG2	2.20	0.41
1:B:388:ASN:ND2	1:B:390:ALA:H	2.19	0.41
1:B:398:ALA:O	1:B:402:GLU:HG3	2.20	0.41
1:A:374:ARG:HH11	1:A:374:ARG:HD3	1.74	0.41
1:B:233:LEU:HD13	1:B:323:LEU:CD2	2.51	0.41
1:A:181:GLN:H	1:A:181:GLN:HG2	1.54	0.40
1:A:280:VAL:O	1:A:284:PHE:HB2	2.21	0.40
1:A:291:ILE:HG23	1:A:295:TYR:CZ	2.56	0.40
1:A:41:LYS:CE	1:A:391:GLY:HA2	2.49	0.40
1:A:83:THR:HB	1:A:256:TYR:OH	2.21	0.40
1:A:337:PHE:HD1	1:A:397:MET:HE1	1.86	0.40
1:A:388:ASN:HD22	1:A:390:ALA:H	1.70	0.40
1:A:398:ALA:O	1:A:402:GLU:HG3	2.20	0.40
1:B:194:ASN:HA	1:B:195:PRO:HA	1.84	0.40
1:A:140:TRP:HA	1:A:141:PRO:HD2	1.79	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	371 (94%)	19 (5%)	4 (1%)	12	38
1	B	394/396 (100%)	371 (94%)	19 (5%)	4 (1%)	12	38
All	All	788/792 (100%)	742 (94%)	38 (5%)	8 (1%)	12	38

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	PRO
1	A	181	GLN
1	B	12	ALA
1	B	30	PRO
1	B	181	GLN
1	A	11	ALA
1	B	11	ALA
1	A	12	ALA

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%)	274 (86%)	46 (14%)	3	11
1	B	320/320 (100%)	272 (85%)	48 (15%)	3	10
All	All	640/640 (100%)	546 (85%)	94 (15%)	3	10

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	MET
1	A	23	LEU
1	A	27	ASP
1	A	30	PRO
1	A	37	ILE
1	A	39	VAL
1	A	46	LYS
1	A	54	LYS

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Mol	Chain	Res	Type
1	A	61	LEU
1	A	78	GLU
1	A	83	THR
1	A	87	LEU
1	A	98	LYS
1	A	112	LEU
1	A	123	THR
1	A	126	LYS
1	A	152	LEU
1	A	154	GLU
1	A	155	VAL
1	A	156	ARG
1	A	168	LEU
1	A	169	ASP
1	A	173	LEU
1	A	181	GLN
1	A	202	LEU
1	A	210	GLN
1	A	214	GLU
1	A	223	PHE
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	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	376	GLU
1	A	400	LEU
1	B	5	MET
1	B	20	LEU
1	B	23	LEU
1	B	27	ASP

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Mol	Chain	Res	Type
1	B	30	PRO
1	B	39	VAL
1	B	41	LYS
1	B	46	LYS
1	B	54	LYS
1	B	61	LEU
1	B	78	GLU
1	B	83	THR
1	B	87	LEU
1	B	98	LYS
1	B	112	LEU
1	B	123	THR
1	B	152	LEU
1	B	154	GLU
1	B	155	VAL
1	B	156	ARG
1	B	168	LEU
1	B	173	LEU
1	B	181	GLN
1	B	195	PRO
1	B	202	LEU
1	B	206	GLN
1	B	210	GLN
1	B	214	GLU
1	B	223	PHE
1	B	241	ARG
1	B	259	ASN
1	B	262	LEU
1	B	272	LEU
1	B	273	VAL
1	B	280	VAL
1	B	304	SER
1	B	312	ASN
1	B	338	VAL
1	B	341	LEU
1	B	342	GLN
1	B	344	LYS
1	B	355	LYS
1	B	361	SER
1	B	362	PHE
1	B	366	THR
1	B	372	ARG

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Mol	Chain	Res	Type
1	B	376	GLU
1	B	400	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	166	HIS
1	A	189	HIS
1	A	204	GLN
1	A	210	GLN
1	A	226	GLN
1	A	247	HIS
1	A	259	ASN
1	A	297	ASN
1	A	312	ASN
1	A	339	ASN
1	A	388	ASN
1	B	58	GLN
1	B	63	ASN
1	B	96	ASN
1	B	166	HIS
1	B	189	HIS
1	B	204	GLN
1	B	210	GLN
1	B	247	HIS
1	B	259	ASN
1	B	297	ASN
1	B	312	ASN
1	B	339	ASN
1	B	342	GLN
1	B	357	ASN
1	B	388	ASN

5.3.3 RNA ⓘ

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](#)

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$
3	AKG	A	412	-	9,9,9	3.77	3 (33%)	11,11,11	2.84	4 (36%)
2	PMP	A	411	-	16,16,16	2.02	7 (43%)	22,23,23	1.88	4 (18%)
2	PMP	B	411	-	16,16,16	3.57	7 (43%)	22,23,23	2.17	3 (13%)
3	AKG	B	412	-	9,9,9	4.13	4 (44%)	11,11,11	2.25	4 (36%)

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	AKG	A	412	-	-	0/9/9/9	-
2	PMP	A	411	-	-	4/8/8/8	0/1/1/1
2	PMP	B	411	-	-	1/8/8/8	0/1/1/1
3	AKG	B	412	-	-	4/9/9/9	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	412	AKG	C2-C1	-10.19	1.38	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	411	PMP	O4P-C5A	-9.48	1.09	1.44
3	B	412	AKG	C2-C1	-9.32	1.39	1.53
3	B	412	AKG	O5-C2	7.16	1.37	1.23
2	B	411	PMP	P-O4P	-6.22	1.40	1.60
2	B	411	PMP	C5A-C5	4.56	1.62	1.50
2	B	411	PMP	C5-C4	-3.61	1.35	1.40
3	A	412	AKG	O5-C2	3.26	1.29	1.23
2	A	411	PMP	C3-C2	-3.11	1.37	1.41
2	A	411	PMP	P-O4P	2.98	1.69	1.60
2	A	411	PMP	C5A-C5	-2.94	1.43	1.50
2	B	411	PMP	C3-C2	-2.94	1.37	1.41
3	A	412	AKG	O2-C1	-2.60	1.23	1.30
2	A	411	PMP	C4A-C4	-2.60	1.42	1.51
2	B	411	PMP	P-O2P	-2.46	1.45	1.54
2	A	411	PMP	C5-C4	-2.43	1.37	1.40
2	A	411	PMP	C2-N1	2.38	1.38	1.33
2	B	411	PMP	C2-N1	2.34	1.38	1.33
3	B	412	AKG	C4-C5	2.26	1.55	1.50
3	B	412	AKG	O2-C1	-2.20	1.24	1.30
2	A	411	PMP	O4P-C5A	-2.14	1.37	1.44

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	411	PMP	O4P-C5A-C5	7.45	123.33	109.36
3	A	412	AKG	C3-C2-C1	7.13	127.97	115.86
2	A	411	PMP	O4P-C5A-C5	5.99	120.58	109.36
3	B	412	AKG	C3-C2-C1	5.76	125.65	115.86
3	A	412	AKG	O5-C2-C1	-4.12	113.78	119.67
2	A	411	PMP	C6-C5-C4	3.96	121.05	118.06
2	B	411	PMP	C6-C5-C4	3.83	120.96	118.06
2	A	411	PMP	C5-C6-N1	-2.86	119.18	123.83
2	B	411	PMP	C5-C6-N1	-2.60	119.61	123.83
3	B	412	AKG	O1-C1-C2	-2.39	118.83	121.81
3	A	412	AKG	O4-C5-C4	2.13	120.73	114.00
2	A	411	PMP	O3P-P-O4P	-2.12	101.13	106.67
3	B	412	AKG	O5-C2-C3	-2.08	116.71	121.17
3	B	412	AKG	O4-C5-C4	2.07	120.56	114.00
3	A	412	AKG	O3-C5-C4	-2.05	116.58	123.09

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	411	PMP	C5-C4-C4A-N4A
2	B	411	PMP	C5A-O4P-P-O2P
3	B	412	AKG	O2-C1-C2-C3
3	B	412	AKG	C2-C3-C4-C5
2	A	411	PMP	C3-C4-C4A-N4A
2	A	411	PMP	C4-C5-C5A-O4P
2	A	411	PMP	C6-C5-C5A-O4P
3	B	412	AKG	C3-C4-C5-O4
3	B	412	AKG	C3-C4-C5-O3

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	412	AKG	2	0
2	A	411	PMP	4	0
2	B	411	PMP	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

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.