



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:36 PM UTC

PDB ID : 1QJ3 / pdb_00001qj3
Title : Crystal structure of 7,8-diaminopelargonic acid synthase in complex with 7-keto-8-aminopelargonic acid
Authors : Kaeck, H.; Sandmark, J.; Gibson, K.J.; Lindqvist, Y.; Schneider, G.
Deposited on : 1999-06-21
Resolution : 2.70 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

<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

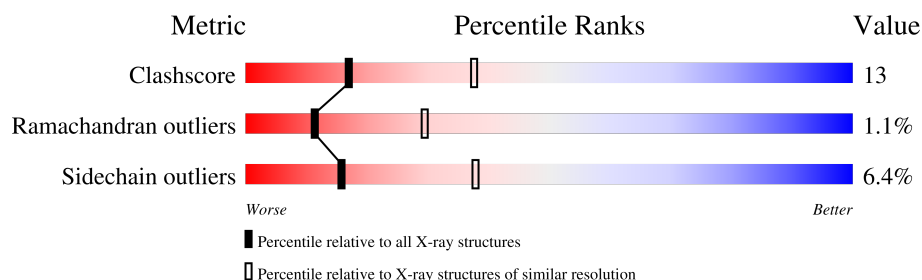
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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	429	
1	B	429	

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.

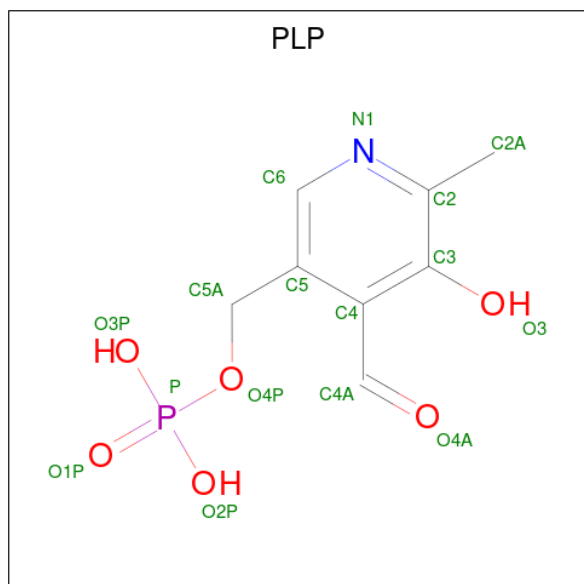
- Molecule 1 is a protein called 7,8-DIAMINOPELARGONIC ACID SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total 3201	C 2030	N 558	O 582	S 31	0	0	0
1	B	415	Total 3197	C 2028	N 557	O 581	S 31	4	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	LEU	TRP	conflict	UNP P12995
B	14	LEU	TRP	conflict	UNP P12995

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



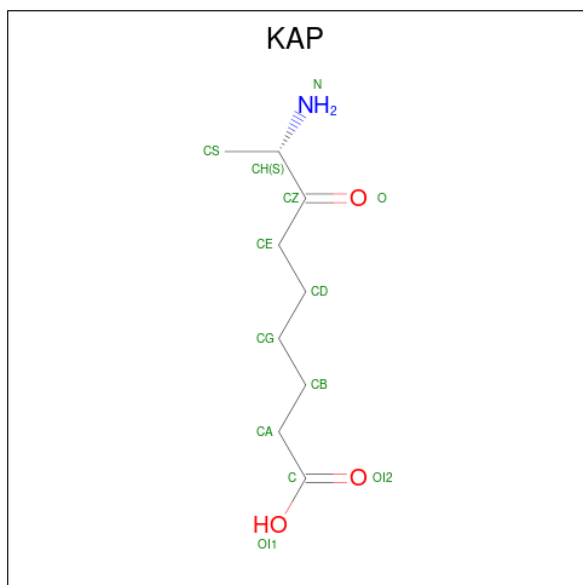
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

Continued on next page...

Continued from previous page...

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

- Molecule 3 is 7-KETO-8-AMINOPELARGONIC ACID (CCD ID: KAP) (formula: $C_9H_{17}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			13	9	1	3		
3	B	1	Total	C	N	O	0	0
			13	9	1	3		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		
4	B	1	Total	Na	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	55	Total	O	0	0
			55	55		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	39	Total	O	0	0
			39	39		

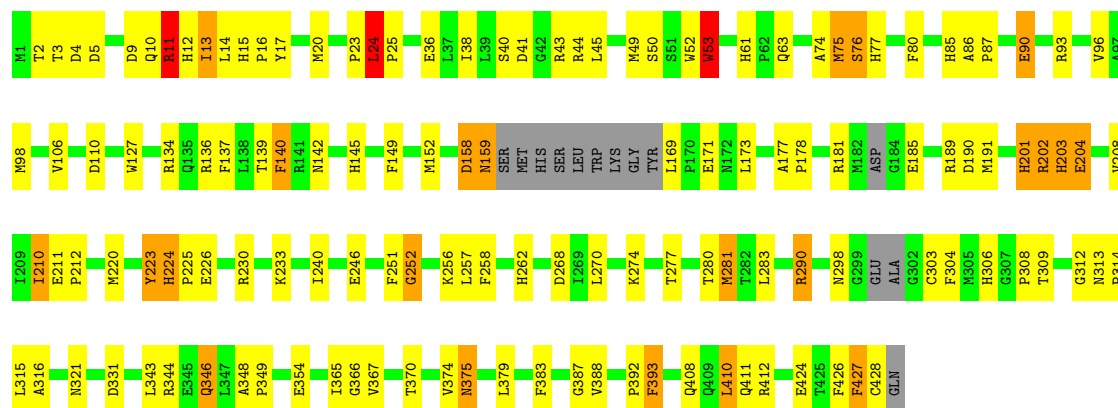
3 Residue-property plots

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: 7,8-DIAMINOPELARGONIC ACID SYNTHASE

Chain A: 



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	57.97Å 55.94Å 120.84Å 90.00° 95.69° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70	Depositor
% Data completeness (in resolution range)	99.9 (20.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.225 , 0.279	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6550	wwPDB-VP
Average B, all atoms (Å ²)	51.0	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: KAP, NA, PLP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.68	3/3272 (0.1%)	1.80	71/4438 (1.6%)
1	B	0.65	3/3268 (0.1%)	1.78	60/4433 (1.4%)
All	All	0.66	6/6540 (0.1%)	1.79	131/8871 (1.5%)

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	85	HIS	CE1-NE2	-8.90	1.23	1.32
1	B	85	HIS	CE1-NE2	-8.73	1.23	1.32
1	B	145	HIS	CE1-NE2	-7.74	1.24	1.32
1	A	145	HIS	CE1-NE2	-7.41	1.25	1.32
1	B	85	HIS	CG-ND1	-6.13	1.31	1.38
1	A	85	HIS	CG-ND1	-5.12	1.32	1.38

All (131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	346	GLN	OE1-CD-NE2	-22.07	100.53	122.60
1	A	346	GLN	OE1-CD-NE2	-20.36	102.24	122.60
1	A	11	ARG	NE-CZ-NH2	18.08	135.47	119.20
1	B	11	ARG	NE-CZ-NH2	16.98	134.48	119.20
1	B	145	HIS	ND1-CG-CD2	-14.80	91.30	106.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	HIS	ND1-CG-CD2	-14.77	91.33	106.10
1	B	85	HIS	ND1-CG-CD2	-14.74	91.36	106.10
1	B	145	HIS	CG-CD2-NE2	14.11	121.31	107.20
1	A	145	HIS	ND1-CG-CD2	-13.65	92.45	106.10
1	B	85	HIS	CG-CD2-NE2	13.46	120.66	107.20
1	A	149	PHE	CA-CB-CG	-12.32	101.47	113.80
1	A	85	HIS	CG-CD2-NE2	12.02	119.22	107.20
1	B	149	PHE	CA-CB-CG	-11.38	102.42	113.80
1	A	145	HIS	CG-CD2-NE2	10.83	118.03	107.20
1	B	12	HIS	CA-CB-CG	-10.39	103.41	113.80
1	A	346	GLN	CG-CD-OE1	10.27	141.34	120.80
1	A	201	HIS	CG-CD2-NE2	9.98	117.18	107.20
1	A	224	HIS	CA-CB-CG	-9.74	104.06	113.80
1	B	191	MET	N-CA-C	9.54	122.68	111.71
1	B	224	HIS	CA-CB-CG	-9.38	104.42	113.80
1	B	346	GLN	CG-CD-OE1	9.38	139.56	120.80
1	A	152	MET	CA-C-O	-9.33	110.66	120.55
1	A	201	HIS	ND1-CG-CD2	-9.32	96.78	106.10
1	B	145	HIS	CB-CG-ND1	9.10	136.35	122.70
1	A	375	ASN	CA-CB-CG	8.99	121.59	112.60
1	A	190	ASP	CA-CB-CG	8.90	121.50	112.60
1	B	11	ARG	NE-CZ-NH1	-8.89	112.61	121.50
1	A	12	HIS	CA-CB-CG	-8.83	104.97	113.80
1	B	158	ASP	CA-CB-CG	-8.34	104.26	112.60
1	B	201	HIS	ND1-CG-CD2	-8.26	97.84	106.10
1	A	145	HIS	CB-CG-CD2	8.15	141.79	131.20
1	A	11	ARG	NE-CZ-NH1	-8.11	113.39	121.50
1	A	304	PHE	CA-C-O	7.92	129.39	120.84
1	B	375	ASN	CA-CB-CG	7.72	120.33	112.60
1	A	149	PHE	N-CA-C	7.71	120.36	111.11
1	A	258	PHE	CA-CB-CG	-7.57	106.23	113.80
1	B	145	HIS	CE1-NE2-CD2	-7.54	101.46	109.00
1	B	85	HIS	CE1-NE2-CD2	-7.52	101.48	109.00
1	A	140	PHE	CA-CB-CG	7.51	121.31	113.80
1	B	258	PHE	CA-CB-CG	-7.37	106.43	113.80
1	A	427	PHE	CA-C-O	7.24	129.82	121.28
1	B	190	ASP	CA-C-N	7.18	130.62	120.28
1	B	190	ASP	C-N-CA	7.18	130.62	120.28
1	A	85	HIS	CG-ND1-CE1	7.13	121.42	109.30
1	A	145	HIS	CG-ND1-CE1	7.12	121.41	109.30
1	A	158	ASP	CA-CB-CG	-7.01	105.59	112.60
1	B	140	PHE	CA-CB-CG	6.93	120.73	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	149	PHE	N-CA-C	6.92	119.41	111.11
1	B	354	GLU	CA-CB-CG	6.90	127.90	114.10
1	A	190	ASP	CA-C-N	6.75	130.57	120.31
1	A	190	ASP	C-N-CA	6.75	130.57	120.31
1	B	201	HIS	CG-CD2-NE2	6.74	113.94	107.20
1	B	298	ASN	N-CA-C	6.73	121.34	113.20
1	A	171	GLU	N-CA-C	6.58	119.27	109.59
1	A	354	GLU	CA-CB-CG	6.54	127.19	114.10
1	A	93	ARG	CD-NE-CZ	6.53	133.54	124.40
1	B	107	PHE	CA-CB-CG	6.45	120.25	113.80
1	B	85	HIS	CG-ND1-CE1	6.44	120.25	109.30
1	A	298	ASN	N-CA-C	6.40	120.95	113.20
1	A	290	ARG	CD-NE-CZ	6.34	133.27	124.40
1	A	303	CYS	N-CA-C	6.32	117.45	108.74
1	A	11	ARG	NH1-CZ-NH2	-6.29	111.13	119.30
1	A	208	VAL	CA-C-O	-6.22	113.91	120.57
1	A	106	VAL	N-CA-C	6.20	116.79	107.80
1	B	427	PHE	CA-C-O	6.18	128.15	121.16
1	A	159	ASN	CA-CB-CG	-6.15	106.45	112.60
1	B	106	VAL	N-CA-C	6.12	116.73	108.17
1	A	201	HIS	CE1-NE2-CD2	-6.09	102.91	109.00
1	B	145	HIS	CG-ND1-CE1	6.09	119.65	109.30
1	A	252	GLY	N-CA-C	6.06	123.09	115.21
1	A	427	PHE	CA-CB-CG	-6.04	107.76	113.80
1	B	188	GLU	N-CA-C	6.03	120.11	112.87
1	A	12	HIS	N-CA-C	6.03	121.68	113.97
1	B	304	PHE	CA-C-O	5.96	126.74	120.54
1	A	191	MET	N-CA-C	5.93	118.70	111.82
1	A	13	ILE	N-CA-C	5.85	116.53	107.99
1	B	24	LEU	CB-CA-C	5.83	117.61	108.63
1	B	252	GLY	N-CA-C	5.83	122.78	115.21
1	B	208	VAL	CA-C-O	-5.81	114.33	120.48
1	B	426	PHE	CA-CB-CG	-5.80	108.00	113.80
1	B	13	ILE	N-CA-C	5.74	116.13	107.80
1	A	53	TRP	N-CA-CB	-5.71	104.04	112.78
1	B	61	HIS	CA-CB-CG	-5.66	108.14	113.80
1	A	426	PHE	CA-CB-CG	-5.66	108.14	113.80
1	A	181	ARG	CD-NE-CZ	5.65	132.30	124.40
1	B	12	HIS	N-CA-C	5.64	121.18	113.97
1	B	356	VAL	N-CA-C	5.63	116.86	109.21
1	B	304	PHE	CA-CB-CG	-5.62	108.18	113.80
1	B	251	PHE	CA-CB-CG	-5.61	108.19	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	PHE	CA-CB-CG	5.52	119.32	113.80
1	A	145	HIS	ND1-CE1-NE2	-5.50	102.90	108.40
1	A	204	GLU	CA-CB-CG	5.47	125.04	114.10
1	B	93	ARG	CD-NE-CZ	5.45	132.03	124.40
1	A	85	HIS	CB-CG-CD2	5.44	138.28	131.20
1	A	61	HIS	CA-CB-CG	-5.43	108.37	113.80
1	A	171	GLU	CB-CA-C	-5.43	102.11	110.26
1	B	346	GLN	N-CA-C	5.42	119.16	112.54
1	B	211	GLU	N-CA-C	-5.36	103.02	109.72
1	B	85	HIS	CB-CG-ND1	5.34	130.71	122.70
1	A	251	PHE	CA-CB-CG	-5.33	108.47	113.80
1	A	201	HIS	CB-CG-CD2	5.31	138.10	131.20
1	B	427	PHE	CA-CB-CG	-5.30	108.50	113.80
1	A	268	ASP	CA-CB-CG	-5.30	107.30	112.60
1	B	14	LEU	CB-CA-C	-5.28	101.23	109.84
1	B	137	PHE	CA-CB-CG	-5.28	108.52	113.80
1	B	342	GLN	CB-CG-CD	5.28	121.57	112.60
1	B	367	VAL	N-CA-C	5.28	115.56	108.17
1	A	223	TYR	CA-C-N	5.27	127.82	120.65
1	A	223	TYR	C-N-CA	5.27	127.82	120.65
1	B	427	PHE	N-CA-C	5.25	118.29	109.95
1	B	204	GLU	CA-CB-CG	5.24	124.58	114.10
1	A	189	ARG	CD-NE-CZ	5.23	131.73	124.40
1	A	85	HIS	CE1-NE2-CD2	-5.23	103.77	109.00
1	A	24	LEU	CA-CB-CG	5.21	134.54	116.30
1	A	96	VAL	CA-C-N	5.19	128.20	120.31
1	A	96	VAL	C-N-CA	5.19	128.20	120.31
1	A	270	LEU	CA-C-O	-5.18	114.75	120.30
1	B	24	LEU	CA-CB-CG	5.18	134.44	116.30
1	A	53	TRP	CA-CB-CG	5.18	123.44	113.60
1	A	304	PHE	CA-CB-CG	-5.17	108.63	113.80
1	B	85	HIS	CB-CG-CD2	5.17	137.92	131.20
1	B	345	GLU	CA-CB-CG	5.16	124.42	114.10
1	A	211	GLU	N-CA-C	-5.13	103.30	109.72
1	A	85	HIS	CB-CG-ND1	5.11	130.37	122.70
1	B	150	GLY	N-CA-C	-5.09	106.59	112.50
1	B	78	VAL	CA-C-O	-5.09	115.95	121.19
1	A	331	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	427	PHE	N-CA-C	5.06	118.31	110.17
1	A	24	LEU	N-CA-CB	5.02	121.95	110.56
1	A	137	PHE	CA-CB-CG	-5.01	108.79	113.80
1	B	290	ARG	CD-NE-CZ	5.01	131.41	124.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	52	TRP	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	3201	0	3165	88	0
1	B	3197	0	3163	89	0
2	A	15	0	6	1	0
2	B	15	0	6	0	0
3	A	13	0	16	3	0
3	B	13	0	16	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	55	0	0	1	0
5	B	39	0	0	2	0
All	All	6550	0	6372	163	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 (163) 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:140:PHE:HD2	1:B:178:PRO:HD3	1.45	0.81
1:B:140:PHE:CD2	1:B:178:PRO:HD3	2.20	0.77
1:B:77:HIS:HA	1:B:314:PRO:HD2	1.66	0.76
1:B:342:GLN:HG2	1:B:346:GLN:OE1	1.84	0.76
1:A:77:HIS:HA	1:A:314:PRO:HD2	1.66	0.75
1:A:315:LEU:HD23	1:B:281:MET:CE	2.20	0.72
1:B:136:ARG:HD3	1:B:204:GLU:OE1	1.89	0.72
1:A:136:ARG:HD3	1:A:204:GLU:OE1	1.91	0.71
1:A:281:MET:CE	1:B:315:LEU:HD23	2.20	0.70
1:A:313:ASN:ND2	1:A:316:ALA:H	1.90	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:ARG:HD3	1:B:11:ARG:HH21	1.57	0.69
1:A:127:TRP:CD2	1:A:134:ARG:HD2	2.28	0.68
1:B:313:ASN:ND2	1:B:316:ALA:H	1.91	0.68
1:B:127:TRP:CD2	1:B:134:ARG:HD2	2.29	0.67
1:A:142:ASN:HD22	1:A:177:ALA:HB2	1.59	0.66
1:A:178:PRO:HG2	1:A:223:TYR:CD2	2.31	0.66
1:A:290:ARG:CD	1:B:11:ARG:HH21	2.09	0.65
1:B:190:ASP:HB3	1:B:227:TRP:CZ2	2.35	0.62
3:B:1430:KAP:HS1	3:B:1430:KAP:HD1	1.83	0.60
1:A:86:ALA:HB3	1:A:87:PRO:HD3	1.84	0.60
1:B:348:ALA:HB3	1:B:349:PRO:HD3	1.82	0.60
1:B:188:GLU:OE2	1:B:230:ARG:NH2	2.32	0.59
1:A:274:LYS:HG2	1:B:309:THR:HG21	1.84	0.59
1:A:226:GLU:OE2	1:A:230:ARG:NH1	2.35	0.59
1:B:180:SER:HB2	1:B:190:ASP:OD2	2.03	0.59
1:A:43:ARG:HD2	5:A:2050:HOH:O	2.01	0.59
1:A:140:PHE:CD2	1:A:178:PRO:HD3	2.38	0.58
1:A:220:MET:HE2	1:A:365:ILE:HG21	1.85	0.57
1:A:392:PRO:O	1:A:393:PHE:CB	2.53	0.57
1:A:140:PHE:CE2	1:A:178:PRO:HG3	2.41	0.56
1:A:173:LEU:HD13	1:A:201:HIS:HD2	1.70	0.56
1:B:226:GLU:OE2	1:B:230:ARG:NH1	2.39	0.56
1:B:220:MET:HE2	1:B:365:ILE:HG21	1.88	0.56
1:A:15:HIS:HB3	1:A:16:PRO:CD	2.36	0.55
1:B:212:PRO:HG2	1:B:246:GLU:HG2	1.87	0.54
1:A:11:ARG:HH21	1:B:290:ARG:HD3	1.72	0.54
1:A:309:THR:HG21	1:B:274:LYS:HG2	1.90	0.54
1:B:86:ALA:HB3	1:B:87:PRO:HD3	1.90	0.53
1:B:178:PRO:HG2	1:B:223:TYR:CD2	2.44	0.53
1:A:281:MET:HE3	1:B:315:LEU:HD23	1.89	0.53
1:A:346:GLN:NE2	1:A:411:GLN:HG2	2.24	0.53
1:B:145:HIS:HD2	1:B:245:ASP:OD2	1.92	0.53
1:B:17:TYR:OH	3:B:1430:KAP:N	2.42	0.52
2:A:1429:PLP:C4A	3:A:1430:KAP:O	2.58	0.52
1:A:392:PRO:O	1:A:393:PHE:HB3	2.09	0.52
1:A:348:ALA:HB3	1:A:349:PRO:HD3	1.92	0.51
1:A:173:LEU:HD13	1:A:201:HIS:CD2	2.46	0.51
1:A:290:ARG:CZ	1:B:11:ARG:HE	2.24	0.51
1:A:140:PHE:CE1	1:A:210:ILE:HG21	2.45	0.51
1:B:2:THR:H	1:B:5:ASP:HB2	1.76	0.51
1:B:392:PRO:O	1:B:393:PHE:CB	2.57	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ALA:O	1:A:75:MET:HB3	2.12	0.50
1:A:212:PRO:HG2	1:A:246:GLU:HG2	1.92	0.50
1:A:15:HIS:HB3	1:A:16:PRO:HD2	1.93	0.49
1:B:220:MET:HE2	1:B:365:ILE:CG2	2.41	0.49
1:A:379:LEU:HG	1:A:383:PHE:CE2	2.47	0.49
1:B:379:LEU:HG	1:B:383:PHE:CE2	2.48	0.49
1:A:50:SER:HB2	1:A:53:TRP:HA	1.94	0.49
1:B:157:PRO:HD3	1:B:174:PHE:CE2	2.47	0.49
1:B:189:ARG:O	1:B:190:ASP:C	2.54	0.49
1:B:306:HIS:HD2	1:B:308:PRO:HD3	1.78	0.48
1:B:313:ASN:HD22	1:B:316:ALA:H	1.61	0.48
1:A:90:GLU:HB3	1:A:321:ASN:ND2	2.28	0.48
3:A:1430:KAP:HS1	3:A:1430:KAP:HD1	1.94	0.48
1:B:202:ARG:O	1:B:240:ILE:HD11	2.14	0.48
1:A:274:LYS:HE3	1:B:309:THR:OG1	2.13	0.48
1:B:277:THR:CG2	1:B:283:LEU:HB3	2.43	0.48
1:B:180:SER:HB3	1:B:224:HIS:HB2	1.95	0.48
1:B:343:LEU:HD13	1:B:366:GLY:HA3	1.97	0.47
1:A:203:HIS:ND1	1:A:203:HIS:N	2.54	0.47
1:B:374:VAL:HG21	1:B:392:PRO:HB2	1.97	0.47
1:B:173:LEU:HD11	1:B:201:HIS:CD2	2.50	0.47
1:A:20:MET:HE2	1:B:105:CYS:SG	2.55	0.47
1:B:383:PHE:HB3	1:B:388:VAL:HG23	1.96	0.47
1:B:140:PHE:CE2	1:B:178:PRO:HG3	2.50	0.46
1:B:50:SER:HB2	1:B:53:TRP:HA	1.98	0.46
1:B:186:TRP:HZ3	1:B:227:TRP:CD1	2.32	0.46
1:A:173:LEU:CD1	1:A:201:HIS:CD2	2.99	0.46
1:A:11:ARG:NH2	1:B:290:ARG:HD3	2.31	0.46
1:A:277:THR:CG2	1:A:283:LEU:HB3	2.45	0.46
1:A:309:THR:OG1	1:B:274:LYS:HE3	2.15	0.46
1:B:427:PHE:O	1:B:428:CYS:HB2	2.16	0.46
1:A:140:PHE:HD1	1:A:210:ILE:HG22	1.80	0.45
1:B:41:ASP:OD2	1:B:43:ARG:NE	2.47	0.45
1:A:140:PHE:HE1	1:A:210:ILE:HG21	1.81	0.45
1:A:220:MET:HE2	1:A:365:ILE:CG2	2.46	0.45
1:A:24:LEU:HB2	1:A:25:PRO:HD2	1.98	0.45
1:A:41:ASP:OD2	1:A:43:ARG:NE	2.47	0.45
1:B:140:PHE:CE1	1:B:210:ILE:HG21	2.51	0.45
1:A:14:LEU:CD1	1:A:20:MET:HG3	2.47	0.45
1:A:140:PHE:HD2	1:A:178:PRO:HD3	1.81	0.45
1:A:212:PRO:HG2	1:A:246:GLU:CG	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:VAL:O	1:B:120:MET:HG3	2.17	0.45
1:A:374:VAL:HG21	1:A:392:PRO:HB2	1.99	0.45
1:A:427:PHE:O	1:A:428:CYS:HB2	2.16	0.45
1:B:140:PHE:CD1	1:B:210:ILE:HG22	2.52	0.45
1:B:175:ALA:HA	1:B:197:LEU:HD12	1.99	0.45
1:A:306:HIS:HD2	1:A:308:PRO:HD3	1.82	0.44
1:A:312:GLY:O	1:A:313:ASN:C	2.60	0.44
1:B:10:GLN:HG3	1:B:23:PRO:HG2	2.00	0.44
1:B:127:TRP:CE3	1:B:134:ARG:HD2	2.52	0.44
1:A:76:SER:HB2	1:B:280:THR:O	2.17	0.44
1:B:74:ALA:O	1:B:75:MET:HB3	2.17	0.44
1:B:212:PRO:HG2	1:B:246:GLU:CG	2.47	0.44
1:A:173:LEU:HD22	1:A:201:HIS:CD2	2.53	0.44
1:A:220:MET:HB3	1:A:367:VAL:HG21	2.00	0.44
1:B:145:HIS:HE1	5:B:2020:HOH:O	2.00	0.44
1:B:192:VAL:O	1:B:196:ARG:N	2.38	0.44
1:B:134:ARG:NH1	1:B:202:ARG:O	2.45	0.43
1:A:220:MET:HE3	1:A:220:MET:HA	2.00	0.43
1:B:98:MET:HE3	1:B:257:LEU:HD21	2.00	0.43
1:A:49:MET:O	1:A:50:SER:HB2	2.18	0.43
1:A:139:THR:OG1	1:A:140:PHE:N	2.49	0.43
1:A:2:THR:H	1:A:5:ASP:HB2	1.83	0.43
1:A:14:LEU:HG	1:A:20:MET:CG	2.49	0.43
1:B:152:MET:HE2	1:B:169:LEU:HD11	2.01	0.43
1:B:392:PRO:O	1:B:393:PHE:HB3	2.19	0.43
1:A:98:MET:HE3	1:A:257:LEU:HD21	2.01	0.43
1:A:315:LEU:HD23	1:B:281:MET:HE2	1.99	0.42
1:B:14:LEU:CD1	1:B:20:MET:HG3	2.49	0.42
1:B:24:LEU:O	1:B:25:PRO:C	2.62	0.42
1:B:180:SER:HB3	1:B:224:HIS:CB	2.49	0.42
1:A:10:GLN:HG3	1:A:23:PRO:HG2	2.01	0.42
1:A:343:LEU:HD13	1:A:366:GLY:HA3	2.00	0.42
1:A:173:LEU:CD1	1:A:201:HIS:HD2	2.31	0.42
1:A:202:ARG:O	1:A:240:ILE:HD11	2.20	0.42
1:B:212:PRO:O	1:B:214:VAL:N	2.52	0.42
1:A:387:GLY:HA3	1:A:412:ARG:NH2	2.34	0.42
1:B:187:ASP:O	1:B:190:ASP:HB2	2.20	0.42
1:B:220:MET:HB3	1:B:367:VAL:HG21	2.01	0.42
1:B:382:PHE:O	1:B:386:GLN:HG2	2.19	0.42
1:A:173:LEU:CD2	1:A:201:HIS:CD2	3.03	0.42
1:A:9:ASP:HA	1:A:13:ILE:HD12	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ARG:NH1	1:A:202:ARG:O	2.46	0.41
1:B:343:LEU:CD2	1:B:410:LEU:HD11	2.50	0.41
1:A:158:ASP:O	1:A:159:ASN:C	2.63	0.41
1:A:20:MET:HE3	1:A:20:MET:HB3	1.84	0.41
1:B:233:LYS:N	1:B:233:LYS:HD2	2.34	0.41
1:B:339:ILE:HG23	1:B:410:LEU:HD21	2.02	0.41
1:A:343:LEU:CD2	1:A:410:LEU:HD11	2.50	0.41
1:B:18:THR:OG1	1:B:19:SER:N	2.52	0.41
1:B:186:TRP:HE1	1:B:230:ARG:NH2	2.18	0.41
1:B:343:LEU:HD13	1:B:366:GLY:CA	2.51	0.41
1:A:36:GLU:HA	1:A:45:LEU:O	2.21	0.41
1:A:280:THR:O	1:B:76:SER:HB2	2.21	0.41
1:A:17:TYR:OH	3:A:1430:KAP:N	2.54	0.41
1:B:23:PRO:HB2	5:B:2011:HOH:O	2.19	0.41
1:B:110:ASP:OD2	1:B:308:PRO:HB3	2.21	0.41
1:A:233:LYS:HD2	1:A:233:LYS:N	2.35	0.41
1:A:256:LYS:HD2	1:A:262:HIS:ND1	2.36	0.41
1:B:90:GLU:HB3	1:B:321:ASN:ND2	2.36	0.41
1:B:312:GLY:O	1:B:313:ASN:C	2.63	0.41
1:A:306:HIS:CE1	1:B:147:ASP:HB2	2.56	0.41
1:A:370:THR:HG21	1:A:427:PHE:CE1	2.56	0.41
1:A:383:PHE:HB3	1:A:388:VAL:HG23	2.03	0.41
1:A:24:LEU:O	1:A:25:PRO:C	2.64	0.40
1:A:38:ILE:HG12	1:A:44:ARG:HG2	2.03	0.40
1:B:391:ARG:HE	3:B:1430:KAP:C	2.35	0.40
1:A:224:HIS:HA	1:A:225:PRO:HD3	1.91	0.40
1:B:20:MET:HB3	1:B:20:MET:HE3	1.88	0.40
1:A:281:MET:HE1	1:A:315:LEU:CD2	2.52	0.40
1:A:252:GLY:HA2	1:A:256:LYS:O	2.21	0.40
1:B:424:GLU:O	1:B:425:THR:C	2.64	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	100/429 (23%)	97 (97%)	2 (2%)	1 (1%)	12	32
1	B	88/429 (20%)	82 (93%)	5 (6%)	1 (1%)	11	29
All	All	188/858 (22%)	179 (95%)	7 (4%)	2 (1%)	11	29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	MET
1	B	393	PHE

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	334/345 (97%)	312 (93%)	22 (7%)	15	36
1	B	334/345 (97%)	313 (94%)	21 (6%)	16	39
All	All	668/690 (97%)	625 (94%)	43 (6%)	16	38

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	4	ASP
1	A	11	ARG
1	A	24	LEU
1	A	40	SER
1	A	53	TRP
1	A	63	GLN
1	A	76	SER
1	A	90	GLU
1	A	110	ASP
1	A	169	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	185	GLU
1	A	202	ARG
1	A	203	HIS
1	A	210	ILE
1	A	281	MET
1	A	344	ARG
1	A	375	ASN
1	A	393	PHE
1	A	408	GLN
1	A	410	LEU
1	A	424	GLU
1	B	3	THR
1	B	4	ASP
1	B	24	LEU
1	B	40	SER
1	B	53	TRP
1	B	63	GLN
1	B	76	SER
1	B	90	GLU
1	B	110	ASP
1	B	180	SER
1	B	182	MET
1	B	191	MET
1	B	202	ARG
1	B	203	HIS
1	B	210	ILE
1	B	344	ARG
1	B	375	ASN
1	B	393	PHE
1	B	408	GLN
1	B	410	LEU
1	B	424	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	142	ASN
1	A	201	HIS
1	A	215	GLN
1	A	313	ASN
1	A	334	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	335	GLN
1	A	342	GLN
1	A	346	GLN
1	A	386	GLN
1	B	85	HIS
1	B	142	ASN
1	B	145	HIS
1	B	215	GLN
1	B	313	ASN
1	B	334	GLN
1	B	335	GLN
1	B	386	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PLP	B	1429	1	15,15,16	1.43	2 (13%)	21,22,23	2.76	9 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	KAP	A	1430	-	11,12,12	0.99	1 (9%)	11,14,14	2.46	3 (27%)
3	KAP	B	1430	-	11,12,12	1.18	2 (18%)	11,14,14	1.56	2 (18%)
2	PLP	A	1429	1	15,15,16	1.44	3 (20%)	21,22,23	2.74	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	B	1429	1	-	2/6/6/8	0/1/1/1
3	KAP	A	1430	-	-	5/10/12/12	-
3	KAP	B	1430	-	-	6/10/12/12	-
2	PLP	A	1429	1	-	2/6/6/8	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1429	PLP	O4P-C5A	-3.09	1.33	1.44
2	A	1429	PLP	O4P-C5A	-3.09	1.33	1.44
2	B	1429	PLP	O3-C3	-2.90	1.30	1.36
2	A	1429	PLP	O3-C3	-2.47	1.31	1.36
3	B	1430	KAP	CE-CZ	-2.28	1.48	1.51
3	B	1430	KAP	O-CZ	2.26	1.25	1.21
3	A	1430	KAP	CE-CZ	-2.15	1.48	1.51
2	A	1429	PLP	C5-C4	-2.13	1.38	1.40

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1429	PLP	O4P-C5A-C5	6.61	121.75	109.36
2	A	1429	PLP	O4P-C5A-C5	6.44	121.44	109.36
2	A	1429	PLP	C5A-C5-C6	-6.08	109.44	119.36
2	B	1429	PLP	C5A-C5-C6	-5.62	110.21	119.36
2	A	1429	PLP	C5A-C5-C4	5.04	132.58	122.64
3	A	1430	KAP	O-CZ-CE	-4.53	114.01	121.68
2	B	1429	PLP	C5A-C5-C4	4.52	131.55	122.64
3	A	1430	KAP	CS-CH-CZ	4.37	115.97	109.67
2	B	1429	PLP	C2A-C2-C3	3.87	125.33	120.80
2	A	1429	PLP	C2A-C2-C3	3.50	124.90	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1429	PLP	C6-N1-C2	3.28	125.15	119.20
3	A	1430	KAP	CG-CD-CE	-3.23	101.26	113.13
2	B	1429	PLP	O2P-P-O4P	3.04	114.60	106.67
2	B	1429	PLP	C3-C2-N1	-2.96	117.22	120.96
2	A	1429	PLP	C6-N1-C2	2.89	124.44	119.20
3	B	1430	KAP	OI1-C-CA	2.74	122.65	114.00
2	A	1429	PLP	C3-C2-N1	-2.57	117.71	120.96
3	B	1430	KAP	OI2-C-CA	-2.50	115.16	123.09
2	A	1429	PLP	O2P-P-O4P	2.42	112.99	106.67
2	A	1429	PLP	C4A-C4-C5	2.38	123.39	120.94
2	B	1429	PLP	C4A-C4-C5	2.06	123.06	120.94
2	B	1429	PLP	C5-C6-N1	-2.06	120.48	123.83
2	A	1429	PLP	O3-C3-C4	2.02	123.37	118.10

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1429	PLP	C4-C5-C5A-O4P
2	A	1429	PLP	C6-C5-C5A-O4P
2	B	1429	PLP	C4-C5-C5A-O4P
2	B	1429	PLP	C6-C5-C5A-O4P
3	B	1430	KAP	CD-CE-CZ-CH
3	B	1430	KAP	CD-CE-CZ-O
3	A	1430	KAP	C-CA-CB-CG
3	B	1430	KAP	C-CA-CB-CG
3	A	1430	KAP	CG-CD-CE-CZ
3	B	1430	KAP	CA-CB-CG-CD
3	B	1430	KAP	CG-CD-CE-CZ
3	B	1430	KAP	CE-CD-CG-CB
3	A	1430	KAP	CD-CE-CZ-O
3	A	1430	KAP	CD-CE-CZ-CH
3	A	1430	KAP	CA-CB-CG-CD

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1430	KAP	3	0
3	B	1430	KAP	3	0
2	A	1429	PLP	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.