



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:13 am GMT

PDB ID : 2CH2
Title : Structure of the Anopheles gambiae 3-hydroxykynurenine transaminase in complex with inhibitor
Authors : Rossi, F.; Garavaglia, S.; Giovenzana, G.B.; Arca, B.; Li, J.; Rizzi, M.
Deposited on : 2006-03-10
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

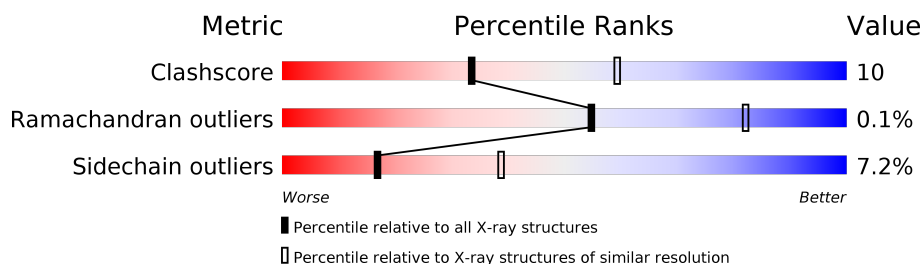
1 Overall quality at a glance

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	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	396	
1	B	396	
1	C	396	
1	D	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	KY1	D	1390	-	-	X	-

2 Entry composition [i](#)

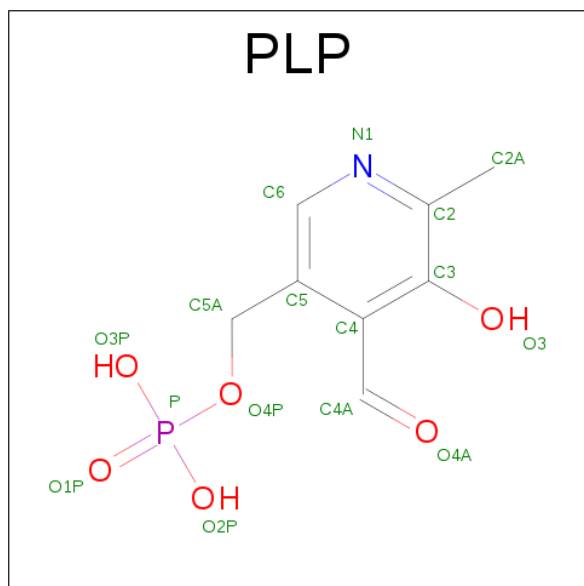
There are 4 unique types of molecules in this entry. The entry contains 12385 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 3-HYDROXYKYNURENINE TRANSAMINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	0	0
			3037	1943	522	550	22			
1	B	387	Total	C	N	O	S	0	0	0
			3037	1943	522	550	22			
1	C	387	Total	C	N	O	S	4	0	0
			3037	1943	522	550	22			
1	D	387	Total	C	N	O	S	6	0	0
			3032	1940	522	548	22			

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



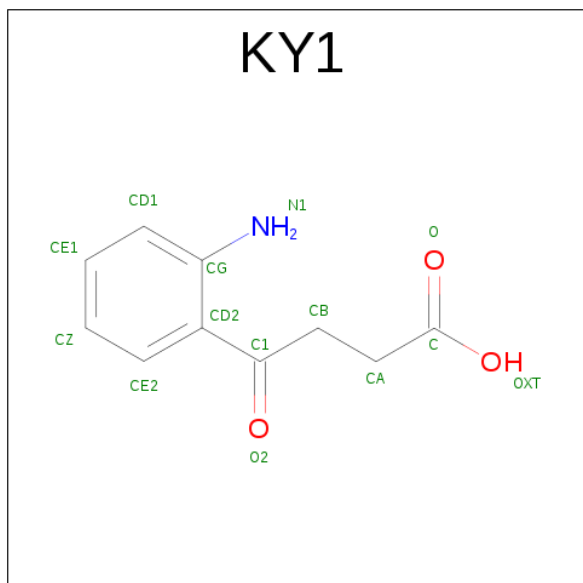
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

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

- Molecule 3 is 4-(2-AMINOPHENYL)-4-OXOBUTANOIC ACID (three-letter code: KY1) (formula: C₁₀H₁₁NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			14	10	1	3		
3	C	1	Total	C	N	O	0	0
			14	10	1	3		
3	D	1	Total	C	N	O	0	0
			14	10	1	3		
3	D	1	Total	C	N	O	0	0
			14	10	1	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	39	Total	O	0	0
			39	39		
4	B	43	Total	O	0	0
			43	43		
4	C	25	Total	O	0	0
			25	25		

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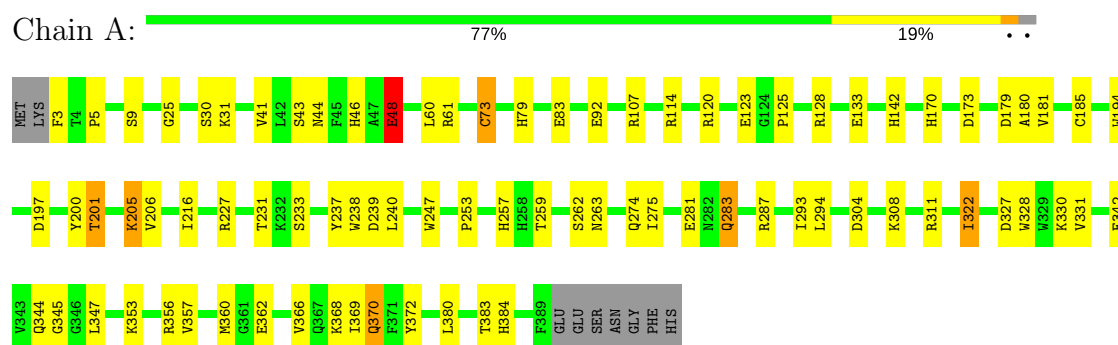
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	19	Total	O	0	0
			19	19		

3 Residue-property plots [i](#)

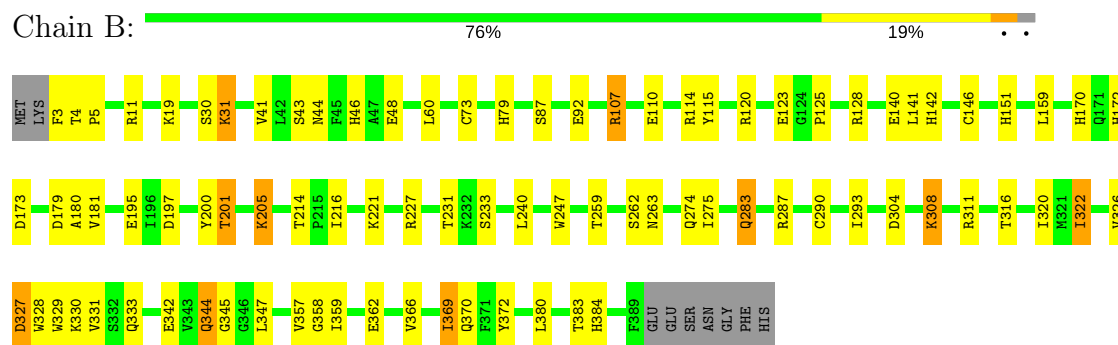
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

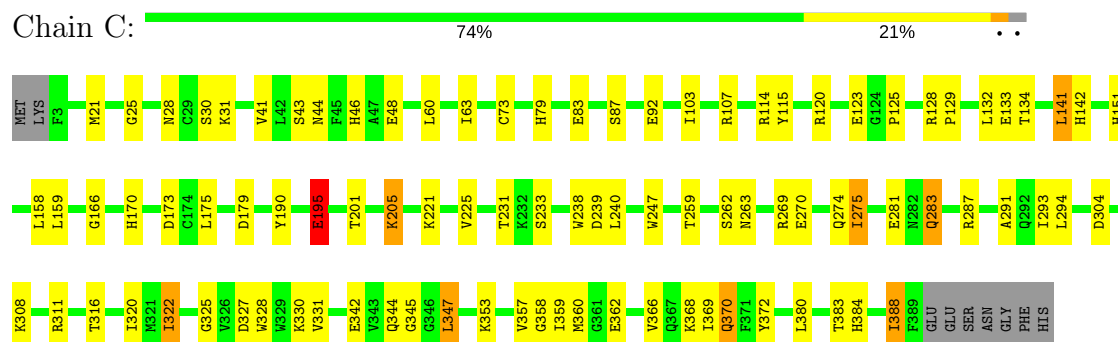
• Molecule 1: 3-HYDROXYKYNURENINE TRANSAMINASE



• Molecule 1: 3-HYDROXYKYNURENINE TRANSAMINASE



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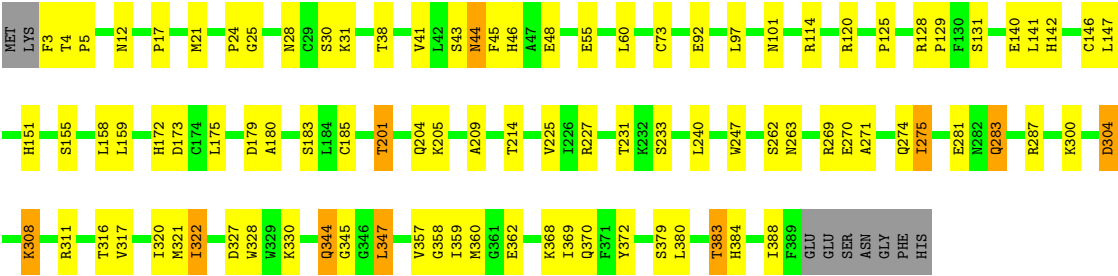


● Molecule 1: 3-HYDROXYKYNURENINE TRANSAMINASE

Chain D:

73%

22%



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	87.94Å 83.75Å 118.66Å 90.00° 100.09° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70	Depositor
% Data completeness (in resolution range)	100.0 (50.00-2.70)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.213 , 0.266	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12385	wwPDB-VP
Average B, all atoms (Å ²)	37.0	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: KY1, 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	0.83	4/3111 (0.1%)	0.78	4/4218 (0.1%)
1	B	0.83	2/3111 (0.1%)	0.78	2/4218 (0.0%)
1	C	0.87	4/3111 (0.1%)	0.80	3/4218 (0.1%)
1	D	1.02	6/3106 (0.2%)	0.83	4/4211 (0.1%)
All	All	0.89	16/12439 (0.1%)	0.80	13/16865 (0.1%)

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	C	0	1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	384	HIS	CA-CB	24.85	2.08	1.53
1	C	195	GLU	CG-CD	10.50	1.67	1.51
1	A	48	GLU	CD-OE2	-9.29	1.15	1.25
1	C	195	GLU	CB-CG	8.68	1.68	1.52
1	D	146	CYS	CB-SG	-8.30	1.68	1.82
1	D	48	GLU	CD-OE2	-7.91	1.17	1.25
1	A	185	CYS	CB-SG	-7.67	1.69	1.82
1	B	48	GLU	CD-OE2	-7.65	1.17	1.25
1	C	48	GLU	CD-OE2	-7.16	1.17	1.25
1	B	146	CYS	CB-SG	-6.48	1.71	1.82
1	D	44	ASN	CG-ND2	-5.66	1.18	1.32
1	C	388	ILE	CA-CB	5.47	1.67	1.54
1	A	133	GLU	CG-CD	5.47	1.60	1.51
1	D	185	CYS	CB-SG	-5.43	1.73	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	44	ASN	CG-OD1	-5.39	1.12	1.24
1	A	73	CYS	CB-SG	-5.37	1.73	1.81

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	388	ILE	N-CA-CB	7.15	127.24	110.80
1	D	48	GLU	CA-CB-CG	-6.76	98.53	113.40
1	D	384	HIS	CA-CB-CG	-6.55	102.47	113.60
1	D	48	GLU	OE1-CD-OE2	-6.39	115.63	123.30
1	A	48	GLU	OE1-CD-OE2	-6.31	115.73	123.30
1	C	388	ILE	CA-CB-CG1	6.07	122.54	111.00
1	B	48	GLU	OE1-CD-OE2	-5.70	116.46	123.30
1	D	227	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	B	327	ASP	CB-CG-OD1	5.16	122.94	118.30
1	A	369	ILE	CG1-CB-CG2	-5.14	100.08	111.40
1	C	388	ILE	CA-CB-CG2	5.04	120.99	110.90
1	A	239	ASP	CB-CG-OD2	-5.03	113.77	118.30
1	A	48	GLU	CA-CB-CG	-5.00	102.39	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	325	GLY	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3037	0	3037	61	0
1	B	3037	0	3037	62	1
1	C	3037	0	3037	64	0
1	D	3032	0	3032	65	1
2	A	15	0	6	2	0
2	B	15	0	6	3	0
2	C	15	0	6	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	15	0	6	1	0
3	B	14	0	10	0	0
3	C	14	0	10	3	0
3	D	28	0	20	8	0
4	A	39	0	0	6	0
4	B	43	0	0	2	0
4	C	25	0	0	1	0
4	D	19	0	0	3	0
All	All	12385	0	12207	236	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (236) 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:383:THR:HG23	1:B:384:HIS:CD2	1.51	1.41
1:A:383:THR:HG23	1:A:384:HIS:CD2	1.72	1.22
1:C:383:THR:HG23	1:C:384:HIS:CD2	1.75	1.19
1:B:383:THR:CG2	1:B:384:HIS:HD2	1.55	1.18
1:B:308:LYS:HD2	4:B:2034:HOH:O	1.52	1.10
1:A:383:THR:HG23	1:A:384:HIS:HD2	1.02	1.10
1:A:61:ARG:HD2	4:A:2012:HOH:O	1.48	1.09
1:C:283:GLN:NE2	1:C:287:ARG:HH12	1.55	1.05
1:C:383:THR:HG23	1:C:384:HIS:HD2	1.13	1.04
1:A:283:GLN:NE2	1:A:287:ARG:HH12	1.56	1.02
1:B:11:ARG:NH2	1:D:327:ASP:HB2	1.74	1.02
1:B:283:GLN:NE2	1:B:287:ARG:HH12	1.63	0.96
1:C:283:GLN:HE21	1:C:287:ARG:HH12	1.13	0.96
1:A:283:GLN:HE21	1:A:287:ARG:HH12	1.12	0.93
1:A:383:THR:CG2	1:A:384:HIS:HD2	1.80	0.93
1:B:283:GLN:HE21	1:B:287:ARG:HH12	1.19	0.88
1:D:283:GLN:HE21	1:D:287:ARG:HH12	1.20	0.88
1:D:283:GLN:NE2	1:D:287:ARG:HH12	1.71	0.88
1:C:21:MET:H	1:C:28:ASN:HD21	1.18	0.87
1:C:383:THR:CG2	1:C:384:HIS:HD2	1.88	0.86
1:A:370:GLN:HG3	4:A:2035:HOH:O	1.78	0.84
1:B:327:ASP:H	1:B:384:HIS:HE1	1.26	0.84
1:B:322:ILE:HD12	1:B:328:TRP:HB3	1.59	0.83
1:B:179:ASP:OD1	2:B:1390:PLP:H2A2	1.81	0.81
1:D:21:MET:H	1:D:28:ASN:HD21	1.27	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:179:ASP:OD1	2:D:1391:PLP:H2A2	1.83	0.78
3:D:1392:KY1:HAC2	3:D:1392:KY1:HE2	1.64	0.77
1:A:120:ARG:HH11	1:A:142:HIS:HD2	1.31	0.77
1:C:344:GLN:HE21	1:C:345:GLY:H	1.32	0.76
1:C:21:MET:H	1:C:28:ASN:ND2	1.84	0.75
1:A:322:ILE:HD12	1:A:328:TRP:HB3	1.68	0.75
1:B:327:ASP:H	1:B:384:HIS:CE1	2.06	0.74
1:D:344:GLN:HE21	1:D:345:GLY:H	1.32	0.73
1:C:120:ARG:HH11	1:C:142:HIS:HD2	1.36	0.72
1:A:179:ASP:OD1	2:A:1390:PLP:H2A2	1.89	0.72
1:A:194:TRP:O	4:A:2022:HOH:O	2.08	0.72
1:A:283:GLN:HE21	1:A:287:ARG:NH1	1.88	0.71
1:D:322:ILE:HD12	1:D:328:TRP:HB3	1.70	0.71
1:C:41:VAL:HG22	1:C:263:ASN:HD21	1.56	0.70
1:C:281:GLU:HB2	4:C:2016:HOH:O	1.91	0.69
1:A:43:SER:H	1:A:46:HIS:CD2	2.11	0.69
1:D:12:ASN:HB2	4:D:2001:HOH:O	1.93	0.69
1:D:120:ARG:HH11	1:D:142:HIS:HD2	1.38	0.69
1:C:322:ILE:HD12	1:C:328:TRP:HB3	1.76	0.68
1:B:383:THR:HG23	1:B:384:HIS:HD2	0.63	0.68
1:B:170:HIS:HD2	1:B:195:GLU:OE1	1.75	0.68
1:B:383:THR:CG2	1:B:384:HIS:CD2	2.45	0.68
1:C:283:GLN:HE21	1:C:287:ARG:NH1	1.88	0.68
1:A:253:PRO:CB	1:B:3:PHE:N	2.57	0.68
1:A:41:VAL:HG22	1:A:263:ASN:HD21	1.60	0.66
1:B:120:ARG:HH11	1:B:142:HIS:HD2	1.42	0.66
1:C:283:GLN:NE2	1:C:287:ARG:NH1	2.38	0.66
1:A:356:ARG:NH1	3:D:1390:KY1:OXT	2.26	0.65
1:D:41:VAL:HG22	1:D:263:ASN:HD21	1.62	0.64
1:B:11:ARG:HH22	1:D:327:ASP:HB2	1.62	0.62
1:A:253:PRO:HB3	1:B:3:PHE:N	2.14	0.62
1:A:3:PHE:CE1	1:D:281:GLU:HG3	2.35	0.62
1:C:327:ASP:H	1:C:384:HIS:CE1	2.17	0.62
1:D:344:GLN:HE21	1:D:345:GLY:N	1.97	0.61
1:D:25:GLY:N	1:D:360:MET:HE1	2.17	0.60
1:A:356:ARG:HH12	3:D:1390:KY1:C	2.14	0.59
1:D:24:PRO:C	1:D:360:MET:HE1	2.23	0.58
1:A:344:GLN:HE21	1:A:345:GLY:H	1.51	0.58
1:B:43:SER:H	1:B:46:HIS:CD2	2.21	0.58
1:A:180:ALA:O	1:A:201:THR:HG23	2.03	0.58
1:D:21:MET:H	1:D:28:ASN:ND2	1.99	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:VAL:HG13	1:B:384:HIS:CE1	2.39	0.57
1:C:179:ASP:OD1	2:C:1391:PLP:H2A2	2.03	0.56
1:B:180:ALA:O	1:B:201:THR:HG23	2.06	0.56
1:C:331:VAL:HG22	1:C:383:THR:HG21	1.88	0.56
1:D:311:ARG:HG2	1:D:311:ARG:O	2.05	0.56
1:A:331:VAL:HG22	1:A:383:THR:HG21	1.88	0.56
1:B:311:ARG:HG2	1:B:311:ARG:O	2.05	0.56
1:B:41:VAL:HG22	1:B:263:ASN:HD21	1.71	0.56
1:D:43:SER:H	1:D:46:HIS:CD2	2.23	0.56
1:A:170:HIS:HE1	1:A:197:ASP:OD2	1.89	0.55
1:A:253:PRO:HD3	1:C:190:TYR:CZ	2.41	0.55
1:C:205:LYS:NZ	2:C:1391:PLP:H5A1	2.22	0.55
1:D:125:PRO:HG2	1:D:128:ARG:HB3	1.89	0.55
2:B:1390:PLP:C4A	3:C:1390:KY1:HAC2	2.37	0.54
1:A:283:GLN:NE2	1:A:287:ARG:NH1	2.41	0.54
1:A:114:ARG:HD3	1:D:233:SER:O	2.08	0.54
2:A:1390:PLP:C4A	3:D:1390:KY1:HAC2	2.37	0.54
1:D:151:HIS:HD2	1:D:183:SER:OG	1.90	0.54
1:C:311:ARG:O	1:C:311:ARG:HG2	2.07	0.54
1:A:327:ASP:H	1:A:384:HIS:CE1	2.26	0.53
1:C:63:ILE:HG22	1:C:275:ILE:HD11	1.90	0.53
1:A:3:PHE:HE1	1:D:281:GLU:HG3	1.74	0.52
1:D:180:ALA:O	1:D:201:THR:HG23	2.09	0.52
1:A:357:VAL:HG22	1:A:372:TYR:OH	2.09	0.52
1:B:329:TRP:CH2	1:B:333:GLN:HG3	2.44	0.52
1:B:344:GLN:HE21	1:B:345:GLY:H	1.57	0.52
1:C:344:GLN:HE21	1:C:345:GLY:N	2.05	0.52
1:B:79:HIS:NE2	1:B:107:ARG:HD2	2.25	0.51
1:B:205:LYS:NZ	2:B:1390:PLP:H5A1	2.25	0.51
1:C:151:HIS:CE1	1:C:159:LEU:HD11	2.45	0.51
1:D:344:GLN:HA	1:D:344:GLN:HE21	1.76	0.51
1:B:283:GLN:HE21	1:B:287:ARG:NH1	1.98	0.51
1:D:201:THR:O	1:D:214:THR:HG23	2.11	0.51
1:C:322:ILE:HG12	1:C:353:LYS:O	2.11	0.51
1:D:45:PHE:CD1	3:D:1390:KY1:HE1	2.46	0.50
1:C:30:SER:CB	1:C:274:GLN:HE22	2.25	0.50
1:D:129:PRO:HD3	1:D:158:LEU:HD11	1.94	0.50
1:D:44:ASN:HB2	3:D:1390:KY1:CD1	2.41	0.50
1:A:253:PRO:HD3	1:C:190:TYR:CE2	2.47	0.49
3:D:1392:KY1:CA	3:D:1392:KY1:HE2	2.36	0.49
1:A:383:THR:CG2	1:A:384:HIS:CD2	2.64	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:HIS:ND1	1:C:221:LYS:HE3	2.27	0.49
1:C:43:SER:H	1:C:46:HIS:CD2	2.30	0.49
1:C:25:GLY:N	1:C:360:MET:HE1	2.27	0.49
1:A:5:PRO:HA	4:A:2001:HOH:O	2.12	0.49
1:B:320:ILE:HD11	1:B:357:VAL:CG2	2.43	0.49
1:D:357:VAL:HG22	1:D:372:TYR:OH	2.12	0.49
1:A:44:ASN:HD21	1:A:259:THR:HA	1.78	0.49
1:B:19:LYS:HE3	1:C:46:HIS:CD2	2.48	0.49
1:D:151:HIS:CD2	1:D:183:SER:OG	2.66	0.48
1:A:44:ASN:ND2	1:A:259:THR:HA	2.29	0.48
1:A:366:VAL:HB	4:A:2034:HOH:O	2.13	0.48
1:B:30:SER:CB	1:B:274:GLN:HE22	2.27	0.48
1:B:44:ASN:HD21	1:B:259:THR:HA	1.78	0.48
1:D:131:SER:HA	4:D:2013:HOH:O	2.14	0.48
1:D:344:GLN:HA	1:D:344:GLN:NE2	2.28	0.48
1:C:366:VAL:O	1:C:370:GLN:HG2	2.12	0.47
1:B:3:PHE:HE1	1:C:281:GLU:HG3	1.79	0.47
1:D:175:LEU:HD11	1:D:225:VAL:HG21	1.96	0.47
1:D:155:SER:HB2	1:D:347:LEU:O	2.15	0.47
1:B:114:ARG:HD3	1:C:233:SER:O	2.14	0.47
1:B:329:TRP:CH2	1:B:333:GLN:CG	2.97	0.47
1:C:368:LYS:HD3	1:C:368:LYS:HA	1.78	0.47
1:B:320:ILE:HD11	1:B:357:VAL:HG21	1.95	0.47
1:B:3:PHE:CE1	1:C:281:GLU:HG3	2.50	0.47
1:C:320:ILE:HD11	1:C:357:VAL:HG21	1.96	0.47
1:B:125:PRO:HG2	1:B:128:ARG:HB3	1.97	0.47
1:C:79:HIS:NE2	1:C:107:ARG:HD2	2.29	0.47
1:D:151:HIS:CE1	1:D:159:LEU:HD11	2.50	0.47
1:B:201:THR:O	1:B:214:THR:HG23	2.15	0.46
1:A:342:GLU:OE2	1:D:46:HIS:HE1	1.97	0.46
1:A:9:SER:HB2	1:D:55:GLU:HG2	1.98	0.46
1:C:83:GLU:HB3	1:C:238:TRP:CZ2	2.50	0.46
1:D:140:GLU:HG3	1:D:172:HIS:CE1	2.51	0.46
1:A:281:GLU:HG3	1:D:3:PHE:HE1	1.80	0.46
1:C:316:THR:O	1:C:358:GLY:HA2	2.16	0.46
1:A:366:VAL:O	1:A:370:GLN:HG2	2.16	0.46
1:A:79:HIS:NE2	1:A:107:ARG:HD2	2.31	0.46
1:D:101:ASN:C	4:D:2009:HOH:O	2.53	0.46
3:C:1390:KY1:O	3:C:1390:KY1:CE2	2.64	0.46
1:B:170:HIS:ND1	1:B:221:LYS:HE3	2.31	0.45
1:D:283:GLN:HE21	1:D:287:ARG:NH1	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:VAL:HA	1:B:201:THR:HG22	1.97	0.45
1:C:239:ASP:OD1	1:C:239:ASP:C	2.54	0.45
1:A:322:ILE:HD12	1:A:328:TRP:CB	2.42	0.45
3:D:1390:KY1:HBC1	3:D:1390:KY1:HE2	1.71	0.45
1:A:322:ILE:HG12	1:A:353:LYS:O	2.17	0.45
1:B:151:HIS:CE1	1:B:159:LEU:HD11	2.52	0.45
1:B:233:SER:O	1:C:114:ARG:HD3	2.16	0.45
1:B:290:CYS:HB3	1:B:369:ILE:HD13	1.99	0.45
1:D:322:ILE:HD12	1:D:328:TRP:CB	2.43	0.45
1:B:329:TRP:CZ3	1:B:333:GLN:HG3	2.51	0.45
1:A:200:TYR:HB3	1:A:216:ILE:HG22	1.99	0.44
1:B:357:VAL:HG22	1:B:372:TYR:OH	2.18	0.44
1:D:97:LEU:O	1:D:147:LEU:HD12	2.16	0.44
1:D:308:LYS:HA	1:D:308:LYS:HE3	1.99	0.44
1:B:331:VAL:HG22	1:B:383:THR:HG21	1.99	0.44
1:B:316:THR:O	1:B:358:GLY:HA2	2.17	0.44
1:C:125:PRO:HG2	1:C:128:ARG:HB3	2.00	0.44
1:C:73:CYS:HB2	1:C:247:TRP:CZ2	2.53	0.44
1:B:110:GLU:O	1:B:114:ARG:HG3	2.18	0.44
1:B:359:ILE:HG12	1:B:369:ILE:HD11	2.00	0.44
1:B:73:CYS:HB2	1:B:247:TRP:CZ2	2.53	0.44
1:D:316:THR:O	1:D:358:GLY:HA2	2.18	0.44
1:A:181:VAL:HA	1:A:201:THR:HG22	1.99	0.43
1:A:311:ARG:O	1:A:311:ARG:HG2	2.17	0.43
1:C:87:SER:HB3	1:C:115:TYR:CZ	2.53	0.43
1:C:175:LEU:HD11	1:C:225:VAL:HG21	2.01	0.43
1:C:357:VAL:HG22	1:C:372:TYR:OH	2.17	0.43
1:A:30:SER:CB	1:A:274:GLN:HE22	2.31	0.43
1:A:44:ASN:HD21	1:A:259:THR:HG23	1.84	0.43
1:B:4:THR:HA	1:B:5:PRO:HD3	1.92	0.43
1:B:322:ILE:HD12	1:B:328:TRP:CB	2.38	0.43
1:C:383:THR:CG2	1:C:384:HIS:CD2	2.66	0.43
1:D:320:ILE:HD11	1:D:357:VAL:HG21	2.00	0.43
1:B:326:VAL:HG13	1:B:384:HIS:ND1	2.34	0.43
1:B:293:ILE:HD13	1:B:366:VAL:HG13	1.99	0.42
1:C:293:ILE:HD13	1:C:366:VAL:HG13	2.01	0.42
1:D:322:ILE:H	1:D:322:ILE:HG12	1.50	0.42
1:D:304:ASP:O	1:D:321:MET:HG2	2.19	0.42
1:B:200:TYR:HB3	1:B:216:ILE:HG22	2.00	0.42
1:B:46:HIS:HE1	1:C:342:GLU:OE2	2.02	0.42
1:A:253:PRO:CD	1:C:190:TYR:CZ	3.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:362:GLU:HA	1:C:362:GLU:OE1	2.19	0.42
1:A:125:PRO:HG2	1:A:128:ARG:HB3	2.02	0.42
1:C:291:ALA:O	1:C:294:LEU:HB3	2.19	0.42
1:A:73:CYS:HB2	1:A:247:TRP:CZ2	2.55	0.42
1:D:344:GLN:NE2	1:D:345:GLY:H	2.10	0.42
1:B:344:GLN:HE21	1:B:344:GLN:HA	1.84	0.42
1:A:25:GLY:N	1:A:360:MET:HE1	2.35	0.42
1:B:366:VAL:HG23	4:B:2041:HOH:O	2.20	0.42
1:C:359:ILE:HG12	1:C:369:ILE:HD11	2.02	0.42
1:D:317:VAL:HA	1:D:357:VAL:O	2.20	0.42
1:D:204:GLN:HA	1:D:209:ALA:O	2.20	0.41
1:D:269:ARG:NH1	1:D:270:GLU:OE2	2.50	0.41
1:B:87:SER:HB3	1:B:115:TYR:CZ	2.55	0.41
1:C:179:ASP:OD1	1:C:179:ASP:C	2.58	0.41
1:A:3:PHE:CD1	1:D:281:GLU:HG3	2.55	0.41
1:C:322:ILE:HD12	1:C:328:TRP:CB	2.47	0.41
1:D:344:GLN:HE21	1:D:344:GLN:CA	2.32	0.41
1:D:4:THR:HA	1:D:5:PRO:HD3	1.90	0.41
1:A:205:LYS:HB3	1:A:206:VAL:H	1.73	0.41
1:A:237:TYR:O	1:A:257:HIS:HE1	2.03	0.41
1:A:48:GLU:HG2	1:A:48:GLU:H	1.09	0.41
1:B:342:GLU:OE2	1:C:46:HIS:HE1	2.02	0.41
1:C:129:PRO:HD3	1:C:158:LEU:HD11	2.02	0.41
1:A:283:GLN:HE21	1:A:283:GLN:HB3	1.68	0.41
1:C:141:LEU:HD13	1:C:142:HIS:CE1	2.56	0.41
1:C:166:GLY:HA3	1:C:195:GLU:HB2	2.02	0.41
1:D:379:SER:O	1:D:383:THR:HB	2.20	0.41
1:D:73:CYS:HB2	1:D:247:TRP:CZ2	2.55	0.41
1:A:83:GLU:HB3	1:A:238:TRP:CZ2	2.55	0.41
3:C:1390:KY1:HBC1	3:C:1390:KY1:HE2	1.77	0.41
1:C:44:ASN:HD21	1:C:259:THR:HA	1.85	0.41
1:D:30:SER:CB	1:D:274:GLN:HE22	2.34	0.41
1:D:368:LYS:HD3	1:D:368:LYS:HA	1.94	0.41
1:D:359:ILE:HG12	1:D:369:ILE:HD11	2.02	0.41
1:A:293:ILE:HD13	1:A:366:VAL:HG13	2.03	0.41
1:B:140:GLU:HG3	1:B:172:HIS:CE1	2.56	0.41
1:B:170:HIS:HE1	1:B:197:ASP:OD2	2.03	0.41
1:C:269:ARG:NH1	1:C:270:GLU:OE2	2.50	0.41
1:A:281:GLU:HG3	1:D:3:PHE:CE1	2.57	0.40
1:C:103:ILE:HG21	1:C:347:LEU:HD13	2.03	0.40
1:D:283:GLN:HB3	1:D:283:GLN:HE21	1.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:GLU:O	1:C:134:THR:C	2.58	0.40
1:D:271:ALA:O	1:D:275:ILE:HG23	2.21	0.40
1:A:233:SER:O	1:D:114:ARG:HD3	2.21	0.40
4:A:2010:HOH:O	1:D:17:PRO:HB3	2.20	0.40
1:A:368:LYS:HD3	1:A:368:LYS:HA	1.78	0.40
1:C:283:GLN:HE21	1:C:283:GLN:HB3	1.65	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:LYS:NZ	1:D:38:THR:OG1[2_545]	2.17	0.03

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	385/396 (97%)	373 (97%)	12 (3%)	0	100	100
1	B	385/396 (97%)	375 (97%)	10 (3%)	0	100	100
1	C	385/396 (97%)	373 (97%)	12 (3%)	0	100	100
1	D	385/396 (97%)	366 (95%)	18 (5%)	1 (0%)	44	73
All	All	1540/1584 (97%)	1487 (97%)	52 (3%)	1 (0%)	55	82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	300	LYS

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	327/335 (98%)	304 (93%)	23 (7%)	18	40
1	B	327/335 (98%)	302 (92%)	25 (8%)	15	35
1	C	327/335 (98%)	304 (93%)	23 (7%)	18	40
1	D	326/335 (97%)	303 (93%)	23 (7%)	17	39
All	All	1307/1340 (98%)	1213 (93%)	94 (7%)	17	39

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

Mol	Chain	Res	Type
1	A	31	LYS
1	A	48	GLU
1	A	60	LEU
1	A	92	GLU
1	A	123	GLU
1	A	173	ASP
1	A	201	THR
1	A	205	LYS
1	A	227	ARG
1	A	231	THR
1	A	240	LEU
1	A	262	SER
1	A	275	ILE
1	A	283	GLN
1	A	294	LEU
1	A	304	ASP
1	A	308	LYS
1	A	322	ILE
1	A	330	LYS
1	A	347	LEU
1	A	362	GLU
1	A	370	GLN
1	A	380	LEU
1	B	31	LYS

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Mol	Chain	Res	Type
1	B	60	LEU
1	B	92	GLU
1	B	107	ARG
1	B	123	GLU
1	B	141	LEU
1	B	173	ASP
1	B	201	THR
1	B	205	LYS
1	B	227	ARG
1	B	231	THR
1	B	240	LEU
1	B	262	SER
1	B	275	ILE
1	B	283	GLN
1	B	304	ASP
1	B	308	LYS
1	B	322	ILE
1	B	330	LYS
1	B	344	GLN
1	B	347	LEU
1	B	362	GLU
1	B	369	ILE
1	B	370	GLN
1	B	380	LEU
1	C	31	LYS
1	C	60	LEU
1	C	92	GLU
1	C	123	GLU
1	C	132	LEU
1	C	141	LEU
1	C	173	ASP
1	C	195	GLU
1	C	201	THR
1	C	205	LYS
1	C	231	THR
1	C	240	LEU
1	C	262	SER
1	C	275	ILE
1	C	283	GLN
1	C	304	ASP
1	C	308	LYS
1	C	322	ILE

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Mol	Chain	Res	Type
1	C	330	LYS
1	C	347	LEU
1	C	370	GLN
1	C	380	LEU
1	C	388	ILE
1	D	31	LYS
1	D	60	LEU
1	D	92	GLU
1	D	141	LEU
1	D	173	ASP
1	D	201	THR
1	D	205	LYS
1	D	231	THR
1	D	240	LEU
1	D	262	SER
1	D	275	ILE
1	D	283	GLN
1	D	304	ASP
1	D	308	LYS
1	D	322	ILE
1	D	330	LYS
1	D	344	GLN
1	D	347	LEU
1	D	362	GLU
1	D	370	GLN
1	D	380	LEU
1	D	383	THR
1	D	388	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	46	HIS
1	A	142	HIS
1	A	151	HIS
1	A	170	HIS
1	A	172	HIS
1	A	263	ASN
1	A	274	GLN
1	A	283	GLN
1	A	312	HIS

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Mol	Chain	Res	Type
1	A	333	GLN
1	A	344	GLN
1	A	384	HIS
1	B	44	ASN
1	B	46	HIS
1	B	142	HIS
1	B	151	HIS
1	B	170	HIS
1	B	172	HIS
1	B	263	ASN
1	B	274	GLN
1	B	283	GLN
1	B	333	GLN
1	B	344	GLN
1	B	370	GLN
1	B	384	HIS
1	C	28	ASN
1	C	44	ASN
1	C	46	HIS
1	C	142	HIS
1	C	151	HIS
1	C	172	HIS
1	C	263	ASN
1	C	274	GLN
1	C	283	GLN
1	C	344	GLN
1	C	370	GLN
1	C	384	HIS
1	D	28	ASN
1	D	46	HIS
1	D	142	HIS
1	D	151	HIS
1	D	172	HIS
1	D	263	ASN
1	D	274	GLN
1	D	283	GLN
1	D	312	HIS
1	D	344	GLN
1	D	370	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	PLP	A	1390	1	15,15,16	1.79	2 (13%)	20,22,23	2.11	6 (30%)
2	PLP	B	1390	1	15,15,16	2.00	2 (13%)	20,22,23	2.40	9 (45%)
3	KY1	B	1391	-	11,14,14	0.67	0	14,18,18	1.04	1 (7%)
3	KY1	C	1390	-	11,14,14	0.71	0	14,18,18	1.58	3 (21%)
2	PLP	C	1391	1	15,15,16	1.75	2 (13%)	20,22,23	2.15	6 (30%)
3	KY1	D	1390	-	11,14,14	0.61	0	14,18,18	1.57	1 (7%)
2	PLP	D	1391	1	15,15,16	1.94	3 (20%)	20,22,23	2.02	9 (45%)
3	KY1	D	1392	-	11,14,14	0.74	0	14,18,18	1.44	3 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	A	1390	1	-	0/6/6/8	0/1/1/1
2	PLP	B	1390	1	-	0/6/6/8	0/1/1/1
3	KY1	B	1391	-	-	0/7/9/9	0/1/1/1
3	KY1	C	1390	-	-	0/7/9/9	0/1/1/1
2	PLP	C	1391	1	-	0/6/6/8	0/1/1/1
3	KY1	D	1390	-	-	0/7/9/9	0/1/1/1
2	PLP	D	1391	1	-	0/6/6/8	0/1/1/1
3	KY1	D	1392	-	-	0/7/9/9	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1390	PLP	O3-C3	-5.76	1.23	1.37
2	D	1391	PLP	O3-C3	-5.57	1.24	1.37
2	C	1391	PLP	O3-C3	-5.37	1.24	1.37
2	A	1390	PLP	O3-C3	-5.21	1.25	1.37
2	C	1391	PLP	C6-N1	2.00	1.38	1.34
2	A	1390	PLP	C2-N1	2.28	1.38	1.33
2	B	1390	PLP	C2-N1	2.67	1.39	1.33
2	D	1391	PLP	C6-N1	2.96	1.40	1.34
2	D	1391	PLP	C2-N1	3.31	1.40	1.33

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1390	KY1	CB-CA-C	-5.01	104.11	112.66
2	B	1390	PLP	C2A-C2-C3	-3.73	116.51	120.96
3	C	1390	KY1	CB-CA-C	-3.42	106.82	112.66
2	B	1390	PLP	C4A-C4-C3	-3.41	114.65	120.54
2	D	1391	PLP	O3P-P-O4P	-3.07	98.57	106.73
3	D	1392	KY1	O2-C1-CB	-2.87	115.20	120.32
2	D	1391	PLP	O2P-P-O4P	-2.84	99.17	106.73
3	C	1390	KY1	CA-CB-C1	-2.74	106.71	113.04
2	A	1390	PLP	C2A-C2-C3	-2.69	117.76	120.96
2	C	1391	PLP	C2A-C2-C3	-2.67	117.78	120.96
2	C	1391	PLP	C4A-C4-C3	-2.65	115.96	120.54
2	B	1390	PLP	O3P-P-O4P	-2.63	99.73	106.73
2	D	1391	PLP	C4A-C4-C3	-2.54	116.16	120.54
2	A	1390	PLP	C5-C6-N1	-2.53	119.58	123.87
2	C	1391	PLP	O2P-P-O4P	-2.41	100.31	106.73
3	C	1390	KY1	O2-C1-CB	-2.28	116.26	120.32
2	B	1390	PLP	C5-C6-N1	-2.21	120.13	123.87
3	B	1391	KY1	CB-CA-C	-2.20	108.90	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1391	PLP	C5-C6-N1	-2.18	120.18	123.87
2	A	1390	PLP	C4A-C4-C3	-2.12	116.88	120.54
2	D	1391	PLP	C2A-C2-C3	-2.11	118.45	120.96
3	D	1392	KY1	CD1-CG-CD2	2.16	120.29	118.06
2	B	1390	PLP	C6-C5-C4	2.27	120.08	118.18
2	D	1391	PLP	C6-C5-C4	2.49	120.26	118.18
2	B	1390	PLP	O3-C3-C2	2.50	123.02	117.78
2	B	1390	PLP	C2A-C2-N1	2.56	123.02	117.89
2	C	1391	PLP	C6-C5-C4	2.67	120.41	118.18
3	D	1392	KY1	CB-C1-CD2	2.86	125.07	119.80
2	D	1391	PLP	O3P-P-O2P	2.91	119.34	107.61
2	D	1391	PLP	O4P-C5A-C5	3.46	116.28	109.32
2	D	1391	PLP	C4A-C4-C5	3.60	124.49	120.86
2	A	1390	PLP	C6-C5-C4	3.63	121.21	118.18
2	A	1390	PLP	C4A-C4-C5	3.65	124.55	120.86
2	C	1391	PLP	O4P-C5A-C5	4.63	118.64	109.32
2	B	1390	PLP	C4A-C4-C5	4.94	125.85	120.86
2	C	1391	PLP	C4A-C4-C5	5.03	125.94	120.86
2	A	1390	PLP	O4P-C5A-C5	5.18	119.73	109.32
2	B	1390	PLP	O4P-C5A-C5	5.20	119.78	109.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1390	PLP	2	0
2	B	1390	PLP	3	0
3	C	1390	KY1	3	0
2	C	1391	PLP	2	0
3	D	1390	KY1	6	0
2	D	1391	PLP	1	0
3	D	1392	KY1	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

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.