



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:21 AM UTC

PDB ID : 1L6G / pdb_00001l6g
Title : Alanine racemase bound with N-(5'-phosphopyridoxyl)-D-alanine
Authors : Watanabe, A.; Yoshimura, T.; Mikami, B.; Hayashi, H.; Kagamiyama, H.; Esaki, N.
Deposited on : 2002-03-10
Resolution : 2.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

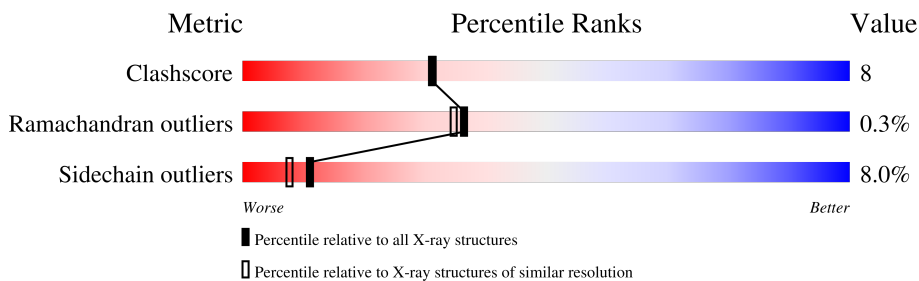
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	388	 76% 19% . .
1	B	388	 75% 21% . .

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.

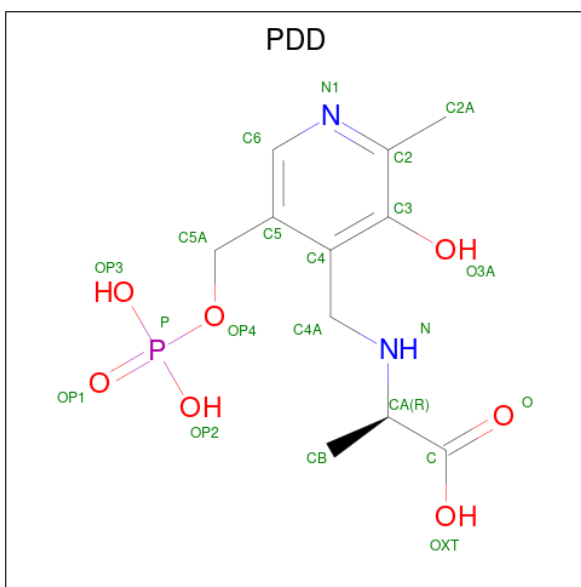
- Molecule 1 is a protein called alanine racemase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	382	Total 3033	C 1941	N 538	O 541	S 13	0	0	0
1	B	382	Total 3033	C 1941	N 538	O 541	S 13	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	129	KCX	LYS	modified residue	UNP P10724
B	129	KCX	LYS	modified residue	UNP P10724

- Molecule 2 is N-(5'-PHOSPHOPYRIDOXYL)-D-ALANINE (CCD ID: PDD) (formula: $C_{11}H_{17}N_2O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			21	11	2	7	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
			21	11	2	7	1		

- Molecule 3 is water.

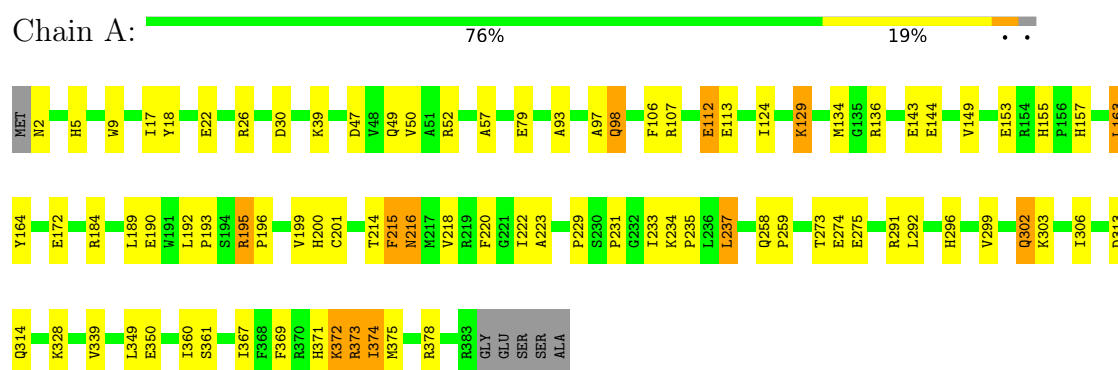
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	119	Total	O	0	0
			119	119		
3	B	128	Total	O	0	0
			128	128		

3 Residue-property plots

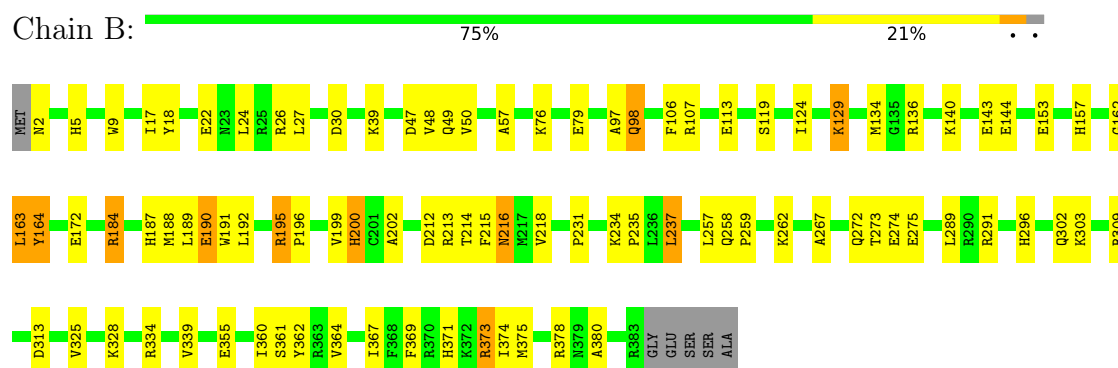
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



- Molecule 1: alanine racemase



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.79Å 90.71Å 85.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.99 – 2.00	Depositor
% Data completeness (in resolution range)	75.9 (7.99-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.169 , 0.216	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6355	wwPDB-VP
Average B, all atoms (Å ²)	22.0	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: KCX, PDD

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	0.44	0/3098	0.89	6/4211 (0.1%)
1	B	0.44	0/3098	0.90	9/4211 (0.2%)
All	All	0.44	0/6196	0.90	15/8422 (0.2%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	361	SER	N-CA-C	10.45	123.26	110.41
1	A	361	SER	N-CA-C	10.39	123.19	110.41
1	A	47	ASP	N-CA-C	6.55	119.02	111.02
1	B	360	ILE	N-CA-C	-6.49	100.27	108.84
1	B	47	ASP	N-CA-C	6.38	118.81	111.02
1	A	360	ILE	N-CA-C	-6.23	99.77	108.12
1	A	306	ILE	N-CA-C	-5.91	101.96	109.58
1	B	364	VAL	N-CA-C	5.81	113.30	107.55
1	B	355	GLU	N-CA-C	5.75	118.49	111.82
1	B	5	HIS	N-CA-C	5.72	119.94	111.87
1	A	5	HIS	N-CA-C	5.66	119.85	111.87
1	A	112	GLU	N-CA-C	-5.38	105.32	111.07
1	B	164	TYR	N-CA-C	5.22	115.43	108.38
1	B	289	LEU	N-CA-C	5.16	116.94	110.24
1	B	202	ALA	N-CA-C	5.13	118.31	110.20

There are no chirality outliers.

There are no planarity outliers.

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	3033	0	3017	51	0
1	B	3033	0	3017	49	0
2	A	21	0	14	3	0
2	B	21	0	14	3	0
3	A	119	0	0	3	0
3	B	128	0	0	2	0
All	All	6355	0	6062	100	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 8.

All (100) 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:39:LYS:NZ	2:A:390:PDD:H	1.69	0.90
1:A:39:LYS:HZ1	2:A:390:PDD:H	1.17	0.88
1:A:231:PRO:HA	1:A:234:LYS:HG3	1.60	0.83
1:B:39:LYS:NZ	2:B:1390:PDD:H	1.83	0.76
1:B:212:ASP:OD2	1:B:213:ARG:HD3	1.89	0.73
1:B:184:ARG:HD2	3:B:575:HOH:O	1.87	0.73
1:A:97:ALA:HB2	1:A:124:ILE:HG12	1.71	0.72
1:A:371:HIS:O	1:A:373:ARG:HD3	1.92	0.70
1:A:163:LEU:HD21	1:A:189:LEU:HD21	1.72	0.70
1:B:291:ARG:HB2	1:B:291:ARG:HH11	1.59	0.67
1:A:369:PHE:CE2	1:A:374:ILE:HG13	2.29	0.67
1:A:163:LEU:HD13	1:A:163:LEU:O	1.95	0.67
1:B:163:LEU:O	1:B:163:LEU:HD13	1.95	0.66
1:B:163:LEU:HD21	1:B:189:LEU:HD21	1.77	0.65
1:A:259:PRO:HG3	1:A:273:THR:HA	1.77	0.64
1:B:231:PRO:HA	1:B:234:LYS:HG3	1.80	0.64
1:A:17:ILE:HD13	1:A:50:VAL:HG22	1.80	0.63
1:B:163:LEU:HD21	1:B:189:LEU:CD2	2.28	0.63
1:B:195:ARG:HH22	1:B:216:ASN:HD21	1.45	0.62
1:A:163:LEU:HD21	1:A:189:LEU:CD2	2.31	0.61
1:B:296:HIS:CD2	1:B:303:LYS:HD2	2.37	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:ARG:HB2	1:B:291:ARG:NH1	2.19	0.57
1:A:220:PHE:CE1	1:A:223:ALA:HB3	2.40	0.56
1:A:163:LEU:HG	1:A:192:LEU:HD11	1.87	0.56
1:B:97:ALA:HB2	1:B:124:ILE:HG12	1.85	0.56
1:A:129:KCX:OQ2	1:A:136:ARG:HB3	2.05	0.56
1:B:258:GLN:OE1	1:B:274:GLU:HG2	2.05	0.56
1:B:106:PHE:CD1	1:B:107:ARG:HG3	2.42	0.55
1:B:39:LYS:HZ1	2:B:1390:PDD:H	1.54	0.55
1:A:155:HIS:CE1	1:A:157:HIS:HB2	2.43	0.54
1:B:163:LEU:CD1	1:B:199:VAL:HG22	2.38	0.54
1:A:22:GLU:HG2	1:A:26:ARG:NH2	2.23	0.53
1:B:129:KCX:OQ2	1:B:136:ARG:HB3	2.08	0.52
1:A:234:LYS:N	1:A:235:PRO:HD2	2.25	0.52
1:B:22:GLU:HG2	1:B:26:ARG:NH2	2.24	0.52
1:A:258:GLN:OE1	1:A:274:GLU:HG2	2.11	0.51
1:B:259:PRO:HG3	1:B:273:THR:HA	1.91	0.51
1:A:134:MET:HB3	3:A:430:HOH:O	2.10	0.51
1:A:39:LYS:NZ	2:A:390:PDD:N	2.51	0.50
1:B:134:MET:HB3	3:B:529:HOH:O	2.10	0.50
1:B:17:ILE:HD13	1:B:50:VAL:HG22	1.92	0.50
1:B:163:LEU:HG	1:B:192:LEU:HD11	1.94	0.50
1:B:371:HIS:O	1:B:373:ARG:HD3	2.11	0.50
1:A:291:ARG:HH11	1:A:291:ARG:HB2	1.77	0.49
1:A:163:LEU:C	1:A:163:LEU:HD22	2.36	0.49
1:A:214:THR:O	1:A:215:PHE:HB2	2.11	0.49
1:A:371:HIS:C	1:A:372:LYS:HG2	2.36	0.49
1:A:106:PHE:CD1	1:A:107:ARG:HG3	2.48	0.48
1:A:18:TYR:CD1	1:A:57:ALA:HB2	2.49	0.48
1:B:369:PHE:CE2	1:B:374:ILE:HG13	2.48	0.48
1:A:49:GLN:OE1	1:A:378:ARG:NH1	2.47	0.48
1:B:214:THR:HB	1:B:218:VAL:HG12	1.96	0.47
1:B:234:LYS:N	1:B:235:PRO:HD2	2.29	0.47
1:B:24:LEU:HD12	1:B:27:LEU:HD23	1.96	0.47
1:B:187:HIS:O	1:B:190:GLU:HB2	2.15	0.47
1:B:234:LYS:HA	1:B:237:LEU:HD22	1.96	0.47
1:A:144:GLU:HA	1:A:144:GLU:OE2	2.15	0.46
1:B:164:TYR:HB2	1:B:200:HIS:O	2.15	0.46
1:A:222:ILE:HG23	1:A:223:ALA:N	2.31	0.45
1:A:299:VAL:O	1:A:299:VAL:HG13	2.16	0.45
1:B:49:GLN:OE1	1:B:378:ARG:NH1	2.49	0.45
1:A:214:THR:HB	1:A:218:VAL:HG12	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:MET:HG2	1:B:191:TRP:CZ3	2.52	0.45
1:A:302:GLN:HE21	1:A:302:GLN:HB3	1.57	0.45
1:A:234:LYS:HA	1:A:237:LEU:HD22	1.98	0.44
1:A:195:ARG:HH22	1:A:216:ASN:HD21	1.64	0.44
1:A:163:LEU:CD1	1:A:199:VAL:HG22	2.48	0.44
1:A:52:ARG:HD3	3:A:626:HOH:O	2.17	0.43
1:B:9:TRP:CD1	1:B:367:ILE:HD12	2.53	0.43
1:A:155:HIS:HE1	1:A:157:HIS:HB2	1.83	0.43
1:B:163:LEU:HD13	1:B:163:LEU:C	2.43	0.43
1:A:164:TYR:HB2	1:A:200:HIS:O	2.19	0.43
1:A:273:THR:O	1:A:275:GLU:HG2	2.19	0.43
1:B:262:LYS:HG2	1:B:267:ALA:HB1	2.01	0.43
1:A:98:GLN:HE21	1:A:98:GLN:HB3	1.61	0.43
1:A:149:VAL:HG11	1:A:193:PRO:HG3	2.01	0.42
1:A:163:LEU:HD11	1:A:189:LEU:HD21	2.01	0.42
1:B:39:LYS:HZ3	2:B:1390:PDD:H	1.63	0.42
1:B:162:GLY:HA2	1:B:196:PRO:HB2	2.01	0.42
1:B:144:GLU:OE2	1:B:144:GLU:HA	2.20	0.42
1:B:98:GLN:HE21	1:B:98:GLN:HB3	1.60	0.41
1:B:119:SER:O	1:B:157:HIS:CD2	2.73	0.41
1:B:234:LYS:N	1:B:235:PRO:CD	2.82	0.41
1:B:18:TYR:CD1	1:B:57:ALA:HB2	2.54	0.41
1:B:214:THR:O	1:B:215:PHE:HB2	2.20	0.41
1:A:93:ALA:HB1	1:A:124:ILE:CD1	2.49	0.41
1:A:234:LYS:HB2	1:A:235:PRO:HD3	2.01	0.41
1:A:303:LYS:HD3	3:A:448:HOH:O	2.20	0.41
1:A:229:PRO:HB2	1:A:233:ILE:HD11	2.01	0.41
1:A:296:HIS:CD2	1:A:303:LYS:HD2	2.56	0.41
1:A:195:ARG:HA	1:A:196:PRO:HD3	1.94	0.41
1:B:140:LYS:HB3	1:B:140:LYS:HE2	1.90	0.41
1:B:273:THR:O	1:B:275:GLU:HG2	2.20	0.41
1:B:362:TYR:O	1:B:380:ALA:HB3	2.20	0.41
1:B:163:LEU:HD11	1:B:189:LEU:HD21	2.02	0.40
1:B:291:ARG:O	1:B:291:ARG:HG2	2.20	0.40
1:A:234:LYS:N	1:A:235:PRO:CD	2.84	0.40
1:A:9:TRP:CD1	1:A:367:ILE:HD12	2.57	0.40
1:A:292:LEU:HG	1:A:349:LEU:HD21	2.04	0.40
1:B:48:VAL:HB	1:B:76:LYS:HD3	2.04	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	379/388 (98%)	369 (97%)	8 (2%)	2 (0%)	24	21
1	B	379/388 (98%)	366 (97%)	13 (3%)	0	100	100
All	All	758/776 (98%)	735 (97%)	21 (3%)	2 (0%)	36	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	215	PHE
1	A	201	CYS

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	317/322 (98%)	292 (92%)	25 (8%)	11	8
1	B	317/322 (98%)	291 (92%)	26 (8%)	10	7
All	All	634/644 (98%)	583 (92%)	51 (8%)	11	8

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	30	ASP
1	A	79	GLU
1	A	98	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	112	GLU
1	A	113	GLU
1	A	143	GLU
1	A	153	GLU
1	A	163	LEU
1	A	172	GLU
1	A	184	ARG
1	A	190	GLU
1	A	195	ARG
1	A	216	ASN
1	A	237	LEU
1	A	302	GLN
1	A	313	ASP
1	A	314	GLN
1	A	328	LYS
1	A	339	VAL
1	A	350	GLU
1	A	372	LYS
1	A	373	ARG
1	A	374	ILE
1	A	375	MET
1	B	2	ASN
1	B	30	ASP
1	B	79	GLU
1	B	98	GLN
1	B	113	GLU
1	B	143	GLU
1	B	153	GLU
1	B	163	LEU
1	B	172	GLU
1	B	184	ARG
1	B	190	GLU
1	B	195	ARG
1	B	200	HIS
1	B	216	ASN
1	B	237	LEU
1	B	257	LEU
1	B	272	GLN
1	B	302	GLN
1	B	309	ARG
1	B	313	ASP
1	B	325	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	328	LYS
1	B	334	ARG
1	B	339	VAL
1	B	373	ARG
1	B	375	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	GLN
1	A	157	HIS
1	A	296	HIS
1	A	302	GLN
1	A	314	GLN
1	B	98	GLN
1	B	157	HIS
1	B	302	GLN
1	B	314	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	KCX	B	129	1	10,11,12	1.06	1 (10%)	6,12,14	1.24	1 (16%)
1	KCX	A	129	1	10,11,12	0.99	0	6,12,14	1.26	1 (16%)

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
1	KCX	B	129	1	-	1/9/10/12	-
1	KCX	A	129	1	-	1/9/10/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	129	KCX	OQ1-CX	2.19	1.25	1.21

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	129	KCX	OQ1-CX-NZ	-2.14	121.68	124.92
1	A	129	KCX	OQ1-CX-NZ	-2.10	121.73	124.92

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	129	KCX	CG-CD-CE-NZ
1	B	129	KCX	CG-CD-CE-NZ

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	129	KCX	1	0
1	A	129	KCX	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PDD	A	390	-	20,21,21	2.11	7 (35%)	26,30,30	1.52	4 (15%)
2	PDD	B	1390	-	20,21,21	2.11	5 (25%)	26,30,30	1.51	4 (15%)

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	PDD	A	390	-	-	5/15/15/15	0/1/1/1
2	PDD	B	1390	-	-	5/15/15/15	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1390	PDD	O-C	4.64	1.35	1.22
2	A	390	PDD	O-C	4.31	1.34	1.22
2	A	390	PDD	C5-C4	3.97	1.46	1.40
2	B	1390	PDD	CA-C	3.96	1.58	1.52
2	A	390	PDD	OXT-C	-3.83	1.18	1.30
2	B	1390	PDD	OXT-C	-3.58	1.19	1.30
2	B	1390	PDD	C5-C4	3.44	1.45	1.40
2	A	390	PDD	C3-C4	3.02	1.44	1.40
2	A	390	PDD	CA-C	2.71	1.56	1.52
2	B	1390	PDD	C3-C4	2.63	1.43	1.40
2	A	390	PDD	C6-N1	2.18	1.38	1.34
2	A	390	PDD	C6-C5	2.16	1.42	1.37

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	390	PDD	C4A-C4-C5	4.59	124.74	119.75
2	B	1390	PDD	C4A-C4-C5	4.49	124.63	119.75
2	B	1390	PDD	OXT-C-CA	3.57	125.61	113.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	390	PDD	OXT-C-CA	3.49	125.33	113.84
2	A	390	PDD	O-C-CA	-2.95	113.20	122.14
2	B	1390	PDD	O-C-CA	-2.90	113.35	122.14
2	A	390	PDD	C4A-C4-C3	-2.58	116.56	119.98
2	B	1390	PDD	C4A-C4-C3	-2.53	116.62	119.98

There are no chirality outliers.

All (10) torsion outliers are listed below:

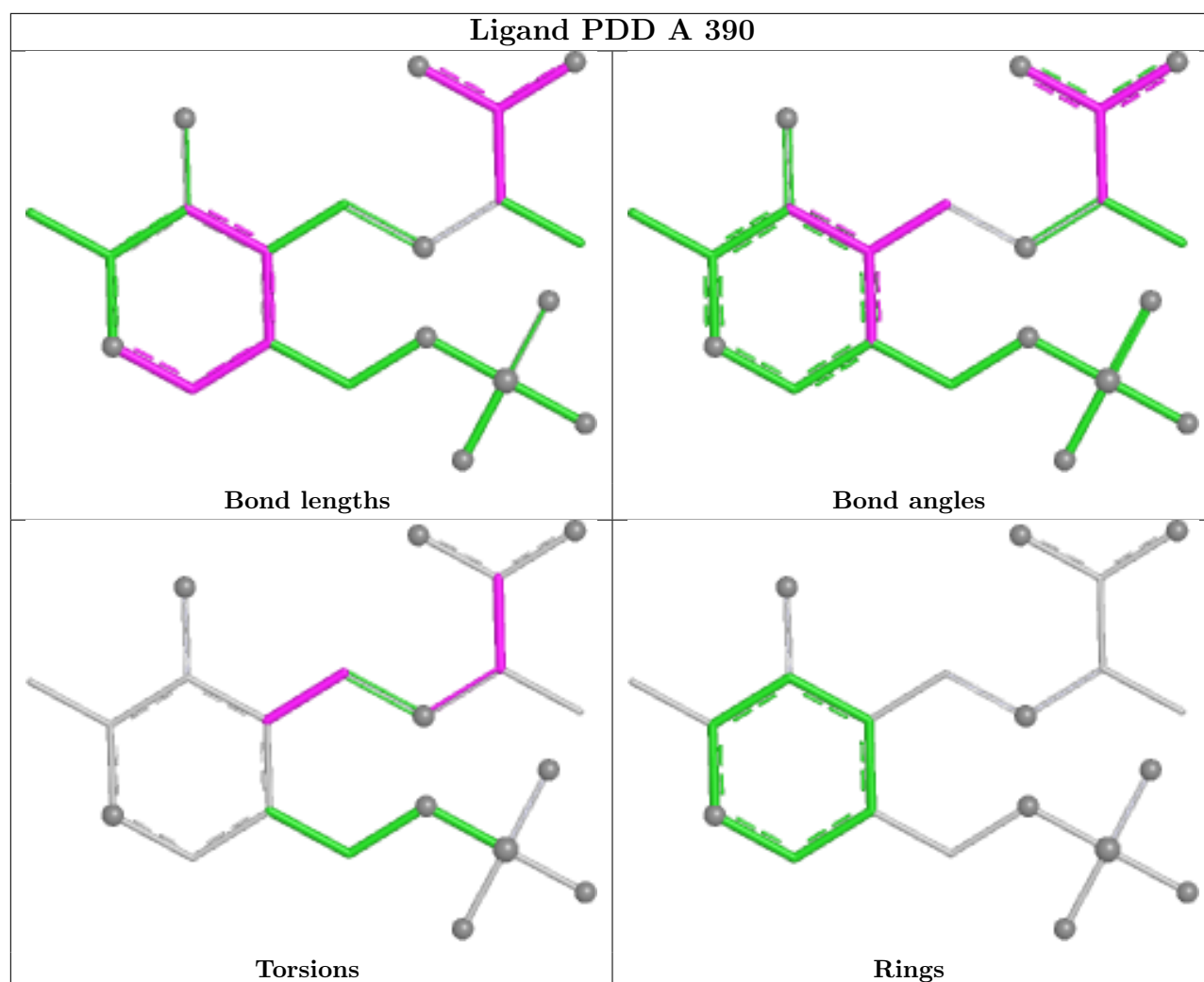
Mol	Chain	Res	Type	Atoms
2	A	390	PDD	CB-CA-N-C4A
2	B	1390	PDD	CB-CA-N-C4A
2	A	390	PDD	C5-C4-C4A-N
2	A	390	PDD	O-C-CA-CB
2	B	1390	PDD	C5-C4-C4A-N
2	A	390	PDD	OXT-C-CA-CB
2	B	1390	PDD	O-C-CA-CB
2	B	1390	PDD	OXT-C-CA-CB
2	A	390	PDD	C3-C4-C4A-N
2	B	1390	PDD	C3-C4-C4A-N

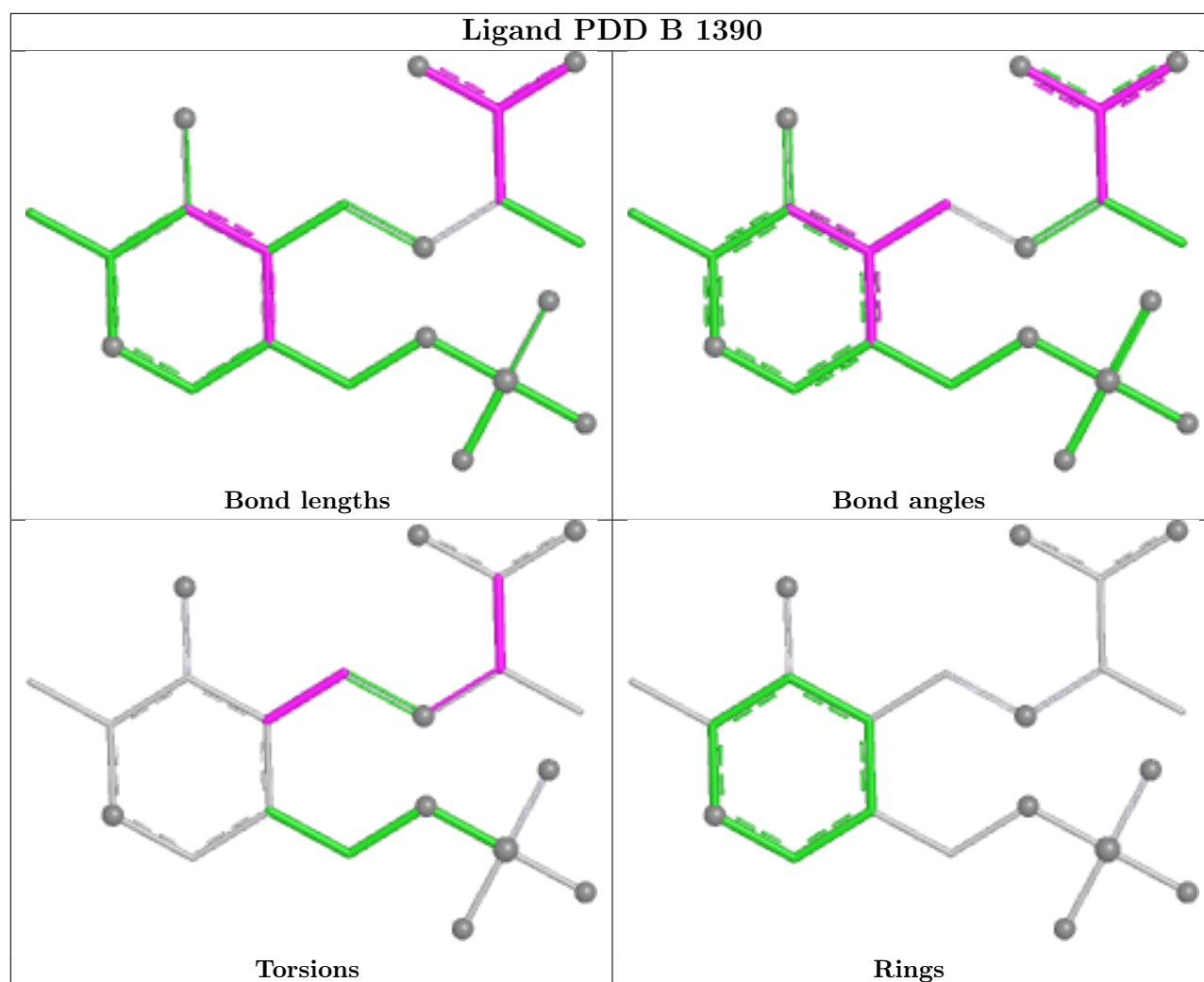
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	390	PDD	3	0
2	B	1390	PDD	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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.