



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:59 PM UTC

PDB ID : 1HNY / pdb_00001hny
Title : The structure of human pancreatic alpha-amylase at 1.8 angstroms resolution and comparisons with related enzymes
Authors : Luo, Y.; Brayer, G.D.
Deposited on : 1995-06-28
Resolution : 1.80 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

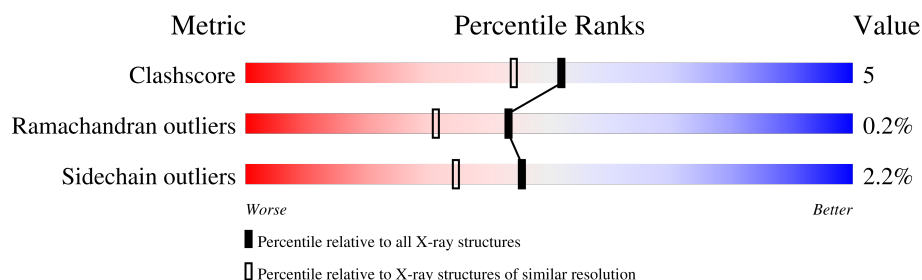
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)

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	496	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4307 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 HUMAN PANCREATIC ALPHA-AMYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	0	0
			3946	2497	696	733	20			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

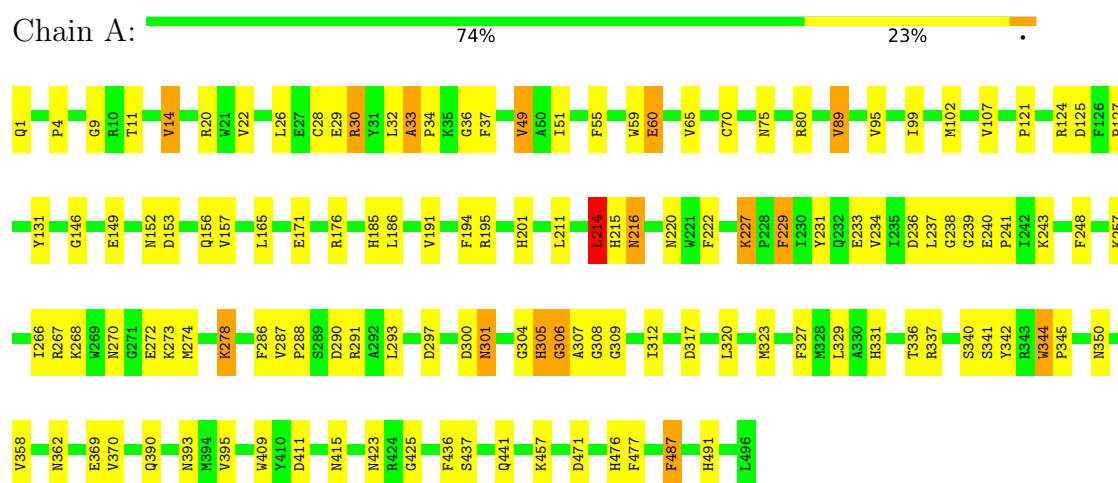
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	359	Total	O	0	0
			359	359		

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: HUMAN PANCREATIC ALPHA-AMYLASE



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	53.04Å 74.80Å 137.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 1.80	Depositor
% Data completeness (in resolution range)	81.9 (8.00-1.80)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR 2.1	Depositor
R, R_{free}	0.174 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4307	wwPDB-VP
Average B, all atoms (Å ²)	22.0	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: CA, PCA, CL

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	1.25	9/4053 (0.2%)	1.97	97/5506 (1.8%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	237	LEU	N-CA	7.10	1.54	1.45
1	A	238	GLY	N-CA	6.32	1.53	1.44
1	A	99	ILE	CA-CB	6.30	1.61	1.54
1	A	491	HIS	N-CA	6.01	1.53	1.45
1	A	237	LEU	C-O	5.87	1.30	1.23
1	A	344	TRP	CA-C	5.86	1.57	1.52
1	A	425	GLY	N-CA	5.76	1.52	1.45
1	A	11	THR	CA-CB	5.18	1.62	1.53
1	A	336	THR	CA-CB	5.03	1.60	1.53

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	350	ASN	CA-CB-CG	12.98	125.58	112.60
1	A	344	TRP	O-C-N	11.93	129.35	121.71
1	A	358	VAL	O-C-N	9.99	132.48	122.79
1	A	215	HIS	CA-CB-CG	9.94	123.74	113.80
1	A	305	HIS	CA-CB-CG	9.71	123.51	113.80
1	A	14	VAL	CB-CA-C	-9.66	96.22	110.62
1	A	487	PHE	CA-CB-CG	9.42	123.22	113.80
1	A	327	PHE	O-C-N	8.64	130.97	122.07
1	A	248	PHE	CA-CB-CG	8.58	122.38	113.80
1	A	201	HIS	CA-CB-CG	-8.51	105.29	113.80
1	A	239	GLY	N-CA-C	8.21	132.63	113.18
1	A	393	ASN	OD1-CG-ND2	-7.93	114.67	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	291	ARG	CD-NE-CZ	7.67	135.14	124.40
1	A	195	ARG	NE-CZ-NH2	-7.60	112.36	119.20
1	A	233	GLU	CB-CG-CD	7.58	125.49	112.60
1	A	80	ARG	CD-NE-CZ	7.43	134.80	124.40
1	A	185	HIS	CA-CB-CG	7.32	121.11	113.80
1	A	20	ARG	NE-CZ-NH1	7.17	128.67	121.50
1	A	290	ASP	CA-CB-CG	7.09	119.69	112.60
1	A	237	LEU	N-CA-C	-7.08	98.88	109.86
1	A	237	LEU	O-C-N	-6.89	113.01	121.83
1	A	317	ASP	CA-CB-CG	6.86	119.46	112.60
1	A	304	GLY	N-CA-C	-6.83	106.28	115.36
1	A	336	THR	N-CA-C	6.67	120.53	109.46
1	A	286	PHE	CA-CB-CG	6.66	120.46	113.80
1	A	20	ARG	CD-NE-CZ	6.65	133.71	124.40
1	A	171	GLU	CB-CG-CD	6.51	123.67	112.60
1	A	305	HIS	CA-C-N	6.48	134.12	121.41
1	A	305	HIS	C-N-CA	6.48	134.12	121.41
1	A	370	VAL	N-CA-CB	6.37	118.26	111.00
1	A	146	GLY	N-CA-C	-6.31	107.01	115.21
1	A	229	PHE	CA-CB-CG	6.26	120.06	113.80
1	A	149	GLU	CB-CG-CD	6.21	123.15	112.60
1	A	340	SER	CB-CA-C	6.20	120.06	110.14
1	A	309	GLY	N-CA-C	6.10	121.97	111.47
1	A	369	GLU	CA-CB-CG	6.10	126.30	114.10
1	A	341	SER	N-CA-C	6.08	118.71	109.95
1	A	327	PHE	CA-C-O	-6.04	114.48	120.82
1	A	441	GLN	N-CA-CB	6.01	120.26	110.17
1	A	390	GLN	O-C-N	5.98	129.22	122.22
1	A	214	LEU	N-CA-C	5.96	119.80	110.32
1	A	75	ASN	OD1-CG-ND2	-5.90	116.70	122.60
1	A	272	GLU	CB-CG-CD	5.83	122.51	112.60
1	A	36	GLY	N-CA-C	5.82	123.86	114.90
1	A	237	LEU	CB-CA-C	5.78	126.90	113.15
1	A	99	ILE	N-CA-CB	-5.75	104.89	112.36
1	A	395	VAL	N-CA-C	-5.74	104.92	110.72
1	A	30	ARG	CD-NE-CZ	5.71	132.40	124.40
1	A	102	MET	N-CA-CB	5.71	115.98	108.96
1	A	194	PHE	N-CA-C	5.68	118.03	109.23
1	A	70	CYS	N-CA-CB	-5.61	102.14	110.71
1	A	33	ALA	O-C-N	5.60	125.47	120.48
1	A	30	ARG	NE-CZ-NH2	5.58	124.22	119.20
1	A	342	TYR	N-CA-CB	5.54	120.56	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	268	LYS	CA-C-O	5.54	127.87	121.28
1	A	22	VAL	CB-CA-C	5.53	119.60	112.14
1	A	220	ASN	OD1-CG-ND2	5.52	128.12	122.60
1	A	37	PHE	O-C-N	5.52	129.53	123.01
1	A	216	ASN	N-CA-C	-5.52	103.10	110.55
1	A	231	TYR	CA-CB-CG	5.46	123.73	113.90
1	A	390	GLN	OE1-CD-NE2	-5.46	117.14	122.60
1	A	286	PHE	O-C-N	5.44	129.03	122.94
1	A	236	ASP	CA-C-N	-5.43	112.56	122.12
1	A	236	ASP	C-N-CA	-5.43	112.56	122.12
1	A	293	LEU	N-CA-C	-5.41	98.55	108.02
1	A	267	ARG	NE-CZ-NH2	5.41	124.07	119.20
1	A	195	ARG	N-CA-C	-5.38	99.96	108.73
1	A	152	ASN	N-CA-C	-5.37	106.73	113.28
1	A	390	GLN	CG-CD-OE1	5.36	131.52	120.80
1	A	222	PHE	O-C-N	5.36	125.90	121.35
1	A	471	ASP	O-C-N	5.35	128.47	122.22
1	A	331	HIS	CA-CB-CG	-5.34	108.46	113.80
1	A	231	TYR	N-CA-CB	5.33	120.01	110.80
1	A	270	ASN	N-CA-CB	-5.32	104.05	112.08
1	A	191	VAL	CB-CA-C	5.29	118.58	111.28
1	A	131	TYR	CA-CB-CG	5.28	123.40	113.90
1	A	176	ARG	CD-NE-CZ	5.28	131.79	124.40
1	A	423	ASN	OD1-CG-ND2	-5.26	117.34	122.60
1	A	257	LYS	CA-C-N	5.25	127.58	120.65
1	A	257	LYS	C-N-CA	5.25	127.58	120.65
1	A	341	SER	N-CA-CB	-5.24	102.63	110.60
1	A	362	ASN	O-C-N	5.22	129.10	123.10
1	A	278	LYS	CA-CB-CG	5.21	124.52	114.10
1	A	238	GLY	CA-C-N	5.14	131.48	121.41
1	A	238	GLY	C-N-CA	5.14	131.48	121.41
1	A	60	GLU	CB-CG-CD	5.14	121.33	112.60
1	A	29	GLU	N-CA-C	5.12	117.98	111.69
1	A	55	PHE	N-CA-C	5.12	116.81	108.63
1	A	124	ARG	CD-NE-CZ	5.12	131.56	124.40
1	A	99	ILE	N-CA-C	5.11	118.06	113.10
1	A	65	VAL	CA-CB-CG1	5.10	119.06	110.40
1	A	337	ARG	NH1-CZ-NH2	-5.09	112.69	119.30
1	A	306	GLY	N-CA-C	5.08	125.21	113.18
1	A	297	ASP	CA-CB-CG	5.05	117.65	112.60
1	A	14	VAL	N-CA-CB	5.01	120.11	111.39
1	A	301	ASN	CA-CB-CG	5.01	117.61	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	VAL	O-C-N	5.01	128.39	123.18

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	3946	0	3718	39	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	359	0	0	6	0
All	All	4307	0	3718	39	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 5.

All (39) 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:278:LYS:HD3	1:A:409:TRP:CD1	2.31	0.66
1:A:121:PRO:HB3	4:A:838:HOH:O	1.95	0.66
1:A:274:MET:H	1:A:415:ASN:HD22	1.47	0.62
1:A:51:ILE:HD12	1:A:60:GLU:HB3	1.82	0.61
1:A:308:GLY:HA3	1:A:312:ILE:HD11	1.82	0.60
1:A:278:LYS:HD3	1:A:409:TRP:CG	2.37	0.60
1:A:95:VAL:HG11	1:A:186:LEU:HD13	1.84	0.60
1:A:274:MET:H	1:A:415:ASN:ND2	2.00	0.59
1:A:227:LYS:HA	1:A:227:LYS:HE2	1.84	0.59
1:A:26:LEU:O	1:A:30:ARG:HG2	2.02	0.59
1:A:49:VAL:HG21	1:A:107:VAL:HG11	1.85	0.58
1:A:153:ASP:OD2	1:A:156:GLN:HB2	2.06	0.54
1:A:51:ILE:HD12	1:A:60:GLU:CB	2.39	0.53
1:A:9:GLY:HA2	4:A:669:HOH:O	2.08	0.53
1:A:300:ASP:O	1:A:305:HIS:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ASP:O	1:A:157:VAL:HG23	2.11	0.50
1:A:28:CYS:HA	1:A:32:LEU:HB2	1.95	0.48
1:A:227:LYS:HD2	4:A:823:HOH:O	2.13	0.48
1:A:4:PRO:HA	1:A:229:PHE:CG	2.50	0.47
1:A:266:ILE:HG22	1:A:320:LEU:HD22	1.97	0.47
1:A:216:ASN:ND2	1:A:227:LYS:HE3	2.30	0.47
1:A:476:HIS:HD2	4:A:833:HOH:O	1.97	0.46
1:A:240:GLU:HB3	1:A:241:PRO:HD2	1.99	0.45
1:A:33:ALA:HB1	1:A:89:VAL:HG12	1.99	0.44
1:A:51:ILE:HD13	1:A:59:TRP:CZ3	2.54	0.43
1:A:301:ASN:HB3	1:A:307:ALA:HB3	1.99	0.43
1:A:344:TRP:HB2	1:A:345:PRO:HD2	2.01	0.43
1:A:241:PRO:HD2	4:A:670:HOH:O	2.18	0.43
1:A:287:VAL:HB	1:A:288:PRO:HD2	2.02	0.42
1:A:273:LYS:HA	1:A:415:ASN:HD21	1.85	0.42
1:A:323:MET:HG2	1:A:487:PHE:CD1	2.54	0.42
1:A:216:ASN:HD22	1:A:227:LYS:CE	2.33	0.42
1:A:457:LYS:HE3	4:A:689:HOH:O	2.19	0.42
1:A:436:PHE:HE1	1:A:477:PHE:HB2	1.85	0.42
1:A:211:LEU:HA	1:A:214:LEU:HD22	2.02	0.41
1:A:33:ALA:HB3	1:A:34:PRO:HD3	2.03	0.41
1:A:51:ILE:HD13	1:A:59:TRP:HZ3	1.86	0.41
1:A:437:SER:HA	1:A:477:PHE:O	2.21	0.41
1:A:125:ASP:C	1:A:127:PRO:HD3	2.45	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	494/496 (100%)	477 (97%)	16 (3%)	1 (0%)	43 31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	306	GLY

5.3.2 Protein sidechains [i](#)

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	418/418 (100%)	409 (98%)	9 (2%)	45	34

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	49	VAL
1	A	89	VAL
1	A	165	LEU
1	A	214	LEU
1	A	227	LYS
1	A	243	LYS
1	A	329	LEU
1	A	411	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	216	ASN
1	A	347	GLN
1	A	363	ASN
1	A	415	ASN
1	A	459	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	PCA	A	1	1	7,8,9	2.56	3 (42%)	9,10,12	2.46	4 (44%)

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	PCA	A	1	1	-	0/0/11/13	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	PCA	CB-CG	-5.27	1.41	1.53
1	A	1	PCA	CD-N	2.65	1.40	1.34
1	A	1	PCA	OE-CD	2.49	1.28	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	PCA	CB-CG-CD	5.18	112.42	104.41
1	A	1	PCA	CB-CA-C	-3.23	108.22	112.66
1	A	1	PCA	CG-CD-N	-2.66	101.89	108.39
1	A	1	PCA	O-C-CA	-2.55	118.21	124.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.