



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:57 PM GMT

PDB ID : 6CPA
Title : CRYSTAL STRUCTURE OF THE COMPLEX OF CARBOXYPEPTIDASE A WITH A STRONGLY BOUND PHOSPHONATE IN A NEW CRYSTALLINE FORM: COMPARISON WITH STRUCTURES OF OTHER COMPLEXES
Authors : Kim, H.; Lipscomb, W.N.
Deposited on : 1990-02-15
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
<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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

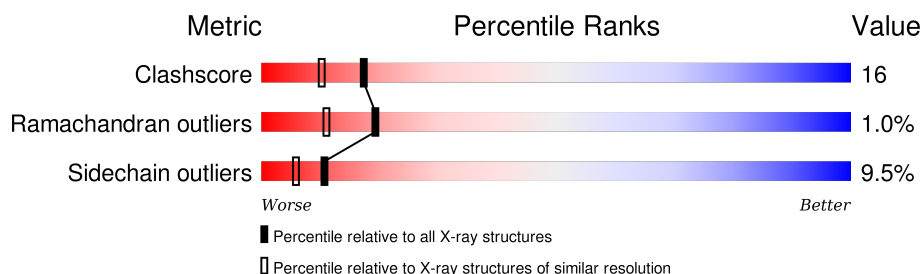
1 Overall quality at a glance

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	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (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 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	307	 70% 20% 8% •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2619 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 CARBOXYPEPTIDASE A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2437	1561	406	465	5			

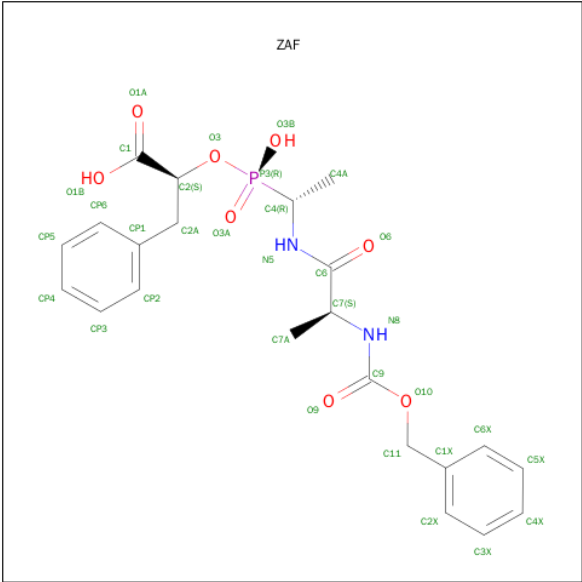
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	GLN	GLU	CONFLICT	UNP P00730
A	31	GLU	GLN	CONFLICT	UNP P00730
A	89	ASN	ASP	CONFLICT	UNP P00730
A	93	ASN	ASP	CONFLICT	UNP P00730
A	114	ASN	ASP	CONFLICT	UNP P00730
A	122	GLU	GLN	CONFLICT	UNP P00730
A	185	ASN	ASP	CONFLICT	UNP P00730
A	228	ALA	GLU	CONFLICT	UNP P00730
A	305	VAL	LEU	CONFLICT	UNP P00730

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is O-(((1R)-((N-PHENYLMETHOXYCARBONYL-L-ALANYL)AMINO)ETHYL)HYDROXYPHOSPHONO)-L-BENZYLACETIC ACID (three-letter code: ZAF) (formula: C₂₂H₂₇N₂O₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			33	22	2	8	1		

- Molecule 4 is water.

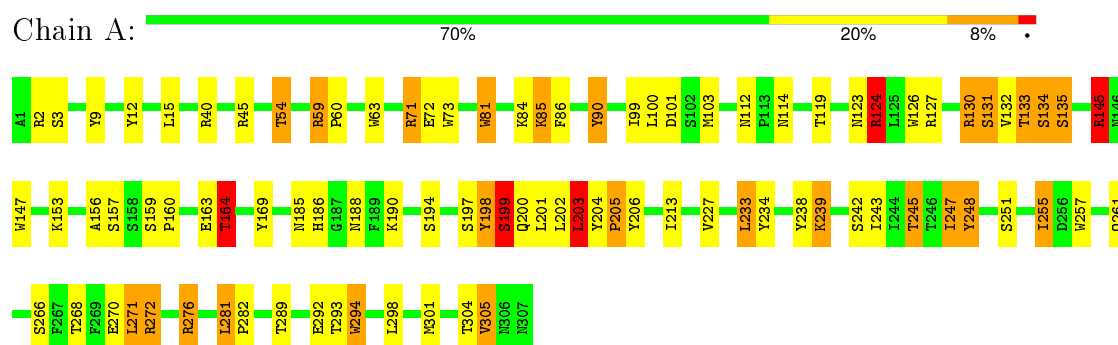
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	148	Total	O	0	0
			148	148		

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 errors 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: CARBOXYPEPTIDASE A



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.90 Å 67.20 Å 76.20 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.193 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2619	wwPDB-VP
Average B, all atoms (Å ²)	14.0	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: ZAF, ZN

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	0.77	0/2503	1.59	42/3402 (1.2%)

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	5

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	ARG	NE-CZ-NH1	-17.34	111.63	120.30
1	A	124	ARG	NE-CZ-NH2	15.69	128.14	120.30
1	A	130	ARG	NE-CZ-NH2	14.95	127.77	120.30
1	A	272	ARG	NE-CZ-NH2	10.93	125.76	120.30
1	A	145	ARG	NE-CZ-NH2	9.84	125.22	120.30
1	A	257	TRP	CD1-CG-CD2	9.26	113.71	106.30
1	A	145	ARG	NE-CZ-NH1	-8.82	115.89	120.30
1	A	63	TRP	CD1-CG-CD2	8.69	113.25	106.30
1	A	134	SER	CA-C-N	-7.73	100.20	117.20
1	A	257	TRP	CE2-CD2-CG	-7.67	101.16	107.30
1	A	81	TRP	CD1-CG-CD2	7.56	112.35	106.30
1	A	147	TRP	CD1-CG-CD2	7.52	112.32	106.30
1	A	238	TYR	CB-CG-CD2	-7.50	116.50	121.00
1	A	63	TRP	CE2-CD2-CG	-7.40	101.38	107.30
1	A	81	TRP	CE2-CD2-CG	-7.36	101.41	107.30
1	A	73	TRP	CD1-CG-CD2	7.07	111.95	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	ARG	NE-CZ-NH2	7.07	123.83	120.30
1	A	197	SER	O-C-N	-7.05	111.42	122.70
1	A	130	ARG	NE-CZ-NH1	-6.89	116.85	120.30
1	A	126	TRP	CE2-CD2-CG	-6.89	101.79	107.30
1	A	197	SER	CA-C-N	6.87	132.30	117.20
1	A	126	TRP	CD1-CG-CD2	6.72	111.68	106.30
1	A	257	TRP	CG-CD2-CE3	6.64	139.87	133.90
1	A	294	TRP	CD1-CG-CD2	6.62	111.59	106.30
1	A	276	ARG	NE-CZ-NH2	6.59	123.59	120.30
1	A	206	TYR	CB-CG-CD2	-6.46	117.13	121.00
1	A	147	TRP	CE2-CD2-CG	-6.21	102.33	107.30
1	A	257	TRP	CB-CG-CD1	-6.11	119.05	127.00
1	A	147	TRP	CG-CD2-CE3	6.05	139.35	133.90
1	A	257	TRP	CG-CD1-NE1	-6.01	104.08	110.10
1	A	73	TRP	CE2-CD2-CG	-5.96	102.53	107.30
1	A	164	THR	N-CA-CB	-5.77	99.34	110.30
1	A	72	GLU	OE1-CD-OE2	-5.76	116.38	123.30
1	A	71	ARG	NE-CZ-NH2	5.74	123.17	120.30
1	A	294	TRP	CE2-CD2-CG	-5.74	102.71	107.30
1	A	147	TRP	CG-CD1-NE1	-5.68	104.42	110.10
1	A	205	PRO	CA-C-N	5.66	129.65	117.20
1	A	203	LEU	CA-CB-CG	5.55	128.07	115.30
1	A	63	TRP	CG-CD1-NE1	-5.46	104.64	110.10
1	A	90	TYR	CB-CG-CD2	-5.24	117.86	121.00
1	A	126	TRP	CG-CD2-CE3	5.05	138.45	133.90
1	A	12	TYR	CB-CG-CD1	-5.00	118.00	121.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	124	ARG	Sidechain
1	A	133	THR	Peptide
1	A	169	TYR	Sidechain
1	A	198	TYR	Sidechain
1	A	90	TYR	Sidechain

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	2437	0	2352	78	0
2	A	1	0	0	0	0
3	A	33	0	25	3	0
4	A	148	0	0	21	0
All	All	2619	0	2377	78	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 16.

All (78) 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:255:ILE:HG21	4:A:665:HOH:O	1.20	1.37
1:A:293:THR:HB	4:A:653:HOH:O	1.19	1.30
1:A:131:SER:CB	4:A:463:HOH:O	1.86	1.22
1:A:247:ILE:HG21	4:A:391:HOH:O	1.42	1.19
1:A:134:SER:HA	4:A:651:HOH:O	1.49	1.11
1:A:131:SER:HB2	4:A:463:HOH:O	1.47	1.05
1:A:103:MET:SD	4:A:570:HOH:O	2.26	0.92
1:A:185:ASN:HB2	4:A:541:HOH:O	1.75	0.86
1:A:186:HIS:HD2	1:A:188:ASN:H	1.24	0.86
1:A:198:TYR:CD1	4:A:663:HOH:O	2.35	0.80
1:A:247:ILE:CG2	4:A:391:HOH:O	2.14	0.77
1:A:45:ARG:HH21	1:A:114:ASN:HD22	1.33	0.77
1:A:255:ILE:CG2	4:A:665:HOH:O	1.96	0.75
1:A:304:THR:HB	4:A:412:HOH:O	1.86	0.74
1:A:103:MET:HE2	1:A:305:VAL:HG13	1.70	0.74
1:A:276:ARG:HG3	1:A:276:ARG:HH21	1.54	0.72
1:A:81:TRP:CH2	1:A:85:LYS:HD2	2.23	0.72
1:A:45:ARG:HH21	1:A:114:ASN:ND2	1.88	0.71
1:A:145:ARG:NH2	4:A:636:HOH:O	2.18	0.69
1:A:127:ARG:HD3	1:A:163:GLU:HG2	1.76	0.68
1:A:153:LYS:HB3	1:A:153:LYS:NZ	2.08	0.68
1:A:164:THR:HG21	4:A:311:HOH:O	1.95	0.67
1:A:239:LYS:HE3	1:A:239:LYS:N	2.09	0.66
1:A:133:THR:HB	1:A:134:SER:OG	1.99	0.63
1:A:233:LEU:HD13	1:A:234:TYR:CE1	2.33	0.63
1:A:54:THR:HG21	1:A:101:ASP:HA	1.81	0.63
1:A:242:SER:OG	1:A:245:THR:HB	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:LYS:H	1:A:239:LYS:HE3	1.64	0.62
1:A:247:ILE:HD12	1:A:248:TYR:H	1.63	0.62
1:A:81:TRP:CZ3	1:A:85:LYS:HD2	2.37	0.59
1:A:270:GLU:OE2	3:A:309:ZAF:O3B	2.21	0.58
1:A:243:ILE:HG23	1:A:247:ILE:HD11	1.85	0.58
1:A:71:ARG:O	1:A:124:ARG:NH1	2.36	0.57
1:A:186:HIS:CD2	1:A:188:ASN:H	2.13	0.57
1:A:119:THR:HA	1:A:123:ASN:O	2.07	0.55
1:A:145:ARG:HH12	3:A:309:ZAF:C1	2.19	0.55
1:A:301:MET:O	1:A:305:VAL:HG23	2.06	0.54
1:A:99:ILE:HG12	1:A:305:VAL:HG21	1.90	0.54
1:A:127:ARG:CD	1:A:163:GLU:HG2	2.38	0.53
1:A:145:ARG:NH1	3:A:309:ZAF:O1A	2.41	0.53
1:A:281:LEU:HD22	1:A:282:PRO:HD2	1.91	0.53
1:A:54:THR:HG22	1:A:59:ARG:HH22	1.74	0.52
1:A:205:PRO:HB2	1:A:213:ILE:HG21	1.93	0.51
1:A:145:ARG:HG2	1:A:156:ALA:CB	2.40	0.51
1:A:103:MET:CE	1:A:305:VAL:HG22	2.41	0.51
1:A:255:ILE:HG13	1:A:266:SER:HB3	1.92	0.50
1:A:86:PHE:HE1	1:A:294:TRP:CZ3	2.28	0.50
1:A:157:SER:HB3	1:A:164:THR:HG22	1.93	0.50
1:A:164:THR:CG2	4:A:311:HOH:O	2.55	0.50
1:A:198:TYR:HA	1:A:271:LEU:O	2.11	0.50
1:A:186:HIS:HD2	1:A:188:ASN:N	2.03	0.50
1:A:276:ARG:CG	1:A:276:ARG:HH21	2.22	0.49
1:A:293:THR:CG2	4:A:653:HOH:O	2.51	0.49
1:A:60:PRO:HB3	1:A:190:LYS:HE2	1.95	0.48
1:A:54:THR:HB	1:A:100:LEU:O	2.14	0.47
1:A:186:HIS:HE1	4:A:321:HOH:O	1.98	0.47
1:A:204:TYR:HB2	1:A:205:PRO:CD	2.45	0.46
1:A:103:MET:HE2	1:A:305:VAL:HG22	1.97	0.46
1:A:99:ILE:HG12	1:A:305:VAL:CG2	2.45	0.46
1:A:59:ARG:NH2	4:A:523:HOH:O	2.49	0.45
1:A:194:SER:O	1:A:268:THR:HG23	2.15	0.45
1:A:198:TYR:O	1:A:199:SER:CB	2.65	0.45
1:A:145:ARG:HG3	1:A:251:SER:O	2.18	0.44
1:A:145:ARG:HG2	1:A:156:ALA:HB2	1.98	0.44
1:A:203:LEU:HG	1:A:243:ILE:HA	1.98	0.44
1:A:45:ARG:HD2	1:A:114:ASN:HD22	1.82	0.44
1:A:247:ILE:CB	4:A:391:HOH:O	2.53	0.44
1:A:199:SER:HB3	1:A:201:LEU:HG	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:VAL:O	1:A:133:THR:OG1	2.35	0.43
1:A:9:TYR:OH	1:A:84:LYS:HD3	2.19	0.43
1:A:159:SER:HA	1:A:160:PRO:HD3	1.69	0.43
1:A:272:ARG:HD2	1:A:292:GLU:OE1	2.20	0.42
1:A:134:SER:HB2	1:A:135:SER:OG	2.19	0.41
1:A:201:LEU:HD11	1:A:247:ILE:HG23	2.01	0.41
1:A:255:ILE:HG12	4:A:665:HOH:O	2.20	0.41
1:A:289:THR:O	1:A:293:THR:HG22	2.20	0.41
1:A:103:MET:HE1	4:A:412:HOH:O	2.21	0.41
1:A:200:GLN:HA	1:A:270:GLU:O	2.20	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	305/307 (99%)	288 (94%)	14 (5%)	3 (1%)	19 11

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	199	SER
1	A	3	SER
1	A	2	ARG

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	263/263 (100%)	238 (90%)	25 (10%)	11 6

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	54	THR
1	A	59	ARG
1	A	85	LYS
1	A	112	ASN
1	A	130	ARG
1	A	131	SER
1	A	135	SER
1	A	145	ARG
1	A	164	THR
1	A	199	SER
1	A	202	LEU
1	A	203	LEU
1	A	227	VAL
1	A	233	LEU
1	A	239	LYS
1	A	245	THR
1	A	247	ILE
1	A	248	TYR
1	A	255	ILE
1	A	261	GLN
1	A	271	LEU
1	A	281	LEU
1	A	298	LEU
1	A	305	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	ASN
1	A	114	ASN
1	A	185	ASN
1	A	186	HIS
1	A	220	ASN
1	A	285	GLN

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Mol	Chain	Res	Type
1	A	291	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 ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\# Z > 2$
3	ZAF	A	309	2	27,34,34	3.47	6 (22%)	36,46,46	1.99	8 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ZAF	A	309	2	-	0/31/36/36	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	309	ZAF	P3-C4	-11.44	1.73	1.84
3	A	309	ZAF	C7-C6	-3.38	1.43	1.52
3	A	309	ZAF	C2A-CP1	-3.10	1.43	1.51
3	A	309	ZAF	C11-C1X	-2.81	1.44	1.50
3	A	309	ZAF	O10-C11	-2.16	1.41	1.45
3	A	309	ZAF	P3-O3	11.09	1.70	1.57

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	309	ZAF	C4A-C4-N5	-4.94	104.72	110.69
3	A	309	ZAF	O9-C9-N8	-4.50	116.99	124.86
3	A	309	ZAF	O3A-P3-C4	-3.64	108.90	114.70
3	A	309	ZAF	O3-P3-O3A	-2.84	109.75	114.91
3	A	309	ZAF	C7-N8-C9	3.56	127.63	120.64
3	A	309	ZAF	O10-C11-C1X	3.67	118.61	109.36
3	A	309	ZAF	O10-C9-N8	3.93	119.25	110.54
3	A	309	ZAF	CP1-C2A-C2	4.30	120.66	113.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	309	ZAF	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.