



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:48 AM UTC

PDB ID : 1N29 / pdb_00001n29
Title : Crystal structure of the N1A mutant of human group IIA phospholipase A2
Authors : Edwards, S.H.; Thompson, D.; Baker, S.F.; Wood, S.P.; Wilton, D.C.
Deposited on : 2002-10-22
Resolution : 2.60 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
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

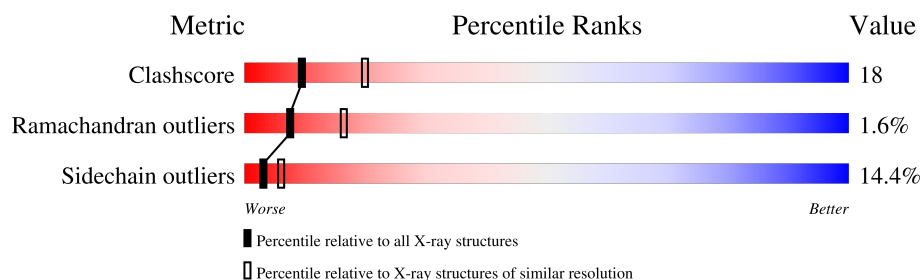
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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	124	42% 35% 15% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 990 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 Phospholipase A2, membrane associated.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	124	Total	C	N	O	S	71	0	0
			963	588	183	177	15			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	ASN	engineered mutation	UNP P14555

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

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

- Molecule 3 is water.

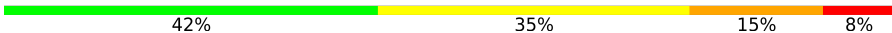
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	25	Total	O	0	0
			25	25		

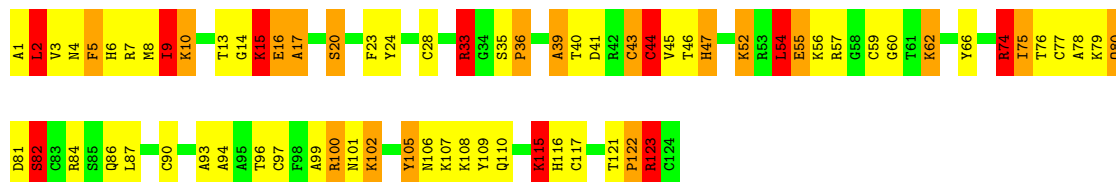
3 Residue-property plots [i](#)

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: Phospholipase A2, membrane associated

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 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	74.79Å 74.79Å 88.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.242 , 0.320	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	990	wwPDB-VP
Average B, all atoms (Å ²)	37.0	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: CA

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	2.64	50/981 (5.1%)	3.13	99/1308 (7.6%)

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	6

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	59	CYS	CA-C	-28.74	1.13	1.53
1	A	16	GLU	C-N	25.81	1.70	1.33
1	A	79	LYS	CB-CG	22.93	2.21	1.52
1	A	43	CYS	C-N	18.90	1.60	1.33
1	A	17	ALA	CA-C	-17.06	1.30	1.53
1	A	17	ALA	C-N	15.70	1.55	1.33
1	A	10	LYS	CB-CG	-15.49	1.05	1.52
1	A	55	GLU	N-CA	-13.82	1.29	1.46
1	A	2	LEU	C-O	-13.43	1.07	1.24
1	A	55	GLU	CA-C	-11.81	1.37	1.52
1	A	59	CYS	N-CA	11.54	1.60	1.45
1	A	107	LYS	CB-CG	-11.48	1.18	1.52
1	A	16	GLU	CA-C	-11.18	1.38	1.53
1	A	121	THR	CA-C	-11.00	1.39	1.52
1	A	9	ILE	CA-CB	-10.96	1.40	1.54
1	A	33	ARG	CB-CG	-10.41	1.21	1.52
1	A	16	GLU	N-CA	-10.39	1.32	1.46
1	A	56	LYS	CB-CG	-9.70	1.23	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	82	SER	N-CA	-8.30	1.36	1.46
1	A	60	GLY	CA-C	-7.78	1.42	1.52
1	A	57	ARG	NE-CZ	-7.77	1.24	1.33
1	A	123	ARG	CA-CB	7.70	1.66	1.53
1	A	54	LEU	C-N	7.60	1.44	1.33
1	A	75	ILE	C-N	7.31	1.43	1.33
1	A	55	GLU	C-O	-7.22	1.15	1.24
1	A	117	CYS	N-CA	-7.22	1.37	1.46
1	A	3	VAL	CA-CB	7.06	1.62	1.54
1	A	60	GLY	N-CA	-6.90	1.35	1.45
1	A	117	CYS	CA-C	-6.88	1.44	1.52
1	A	15	LYS	N-CA	-6.67	1.37	1.45
1	A	82	SER	CA-C	-6.56	1.44	1.52
1	A	17	ALA	N-CA	-6.52	1.38	1.46
1	A	15	LYS	CA-C	-6.34	1.44	1.52
1	A	110	GLN	CD-OE1	6.15	1.35	1.23
1	A	121	THR	CA-CB	-6.03	1.44	1.53
1	A	101	ASN	CG-OD1	5.93	1.34	1.23
1	A	57	ARG	CA-CB	-5.74	1.43	1.53
1	A	17	ALA	CA-CB	-5.71	1.44	1.53
1	A	14	GLY	C-N	-5.53	1.25	1.33
1	A	47	HIS	CG-CD2	5.42	1.41	1.35
1	A	77	CYS	CA-C	-5.37	1.45	1.52
1	A	23	PHE	N-CA	-5.35	1.38	1.45
1	A	44	CYS	CA-CB	-5.33	1.44	1.53
1	A	80	GLN	CD-OE1	5.33	1.33	1.23
1	A	57	ARG	N-CA	-5.21	1.39	1.46
1	A	110	GLN	CD-NE2	-5.16	1.22	1.33
1	A	39	ALA	N-CA	-5.11	1.40	1.46
1	A	52	LYS	CB-CG	5.09	1.67	1.52
1	A	77	CYS	CA-CB	-5.08	1.45	1.53
1	A	76	THR	N-CA	-5.02	1.40	1.46

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	SER	O-C-N	-23.85	97.29	122.09
1	A	55	GLU	O-C-N	-19.88	99.49	122.15
1	A	10	LYS	CA-CB-CG	19.83	153.76	114.10
1	A	33	ARG	CA-CB-CG	19.34	152.78	114.10
1	A	107	LYS	CA-CB-CG	18.69	151.48	114.10
1	A	79	LYS	N-CA-CB	-18.08	82.91	109.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	ARG	NE-CZ-NH2	-17.82	103.16	119.20
1	A	33	ARG	NE-CZ-NH2	-17.33	103.60	119.20
1	A	33	ARG	CB-CA-C	-17.24	82.23	109.99
1	A	59	CYS	CA-C-N	16.54	139.22	120.53
1	A	59	CYS	C-N-CA	16.54	139.22	120.53
1	A	23	PHE	O-C-N	16.26	138.93	122.19
1	A	55	GLU	CA-C-N	15.59	141.17	120.28
1	A	55	GLU	C-N-CA	15.59	141.17	120.28
1	A	82	SER	CA-C-N	15.25	141.13	120.54
1	A	82	SER	C-N-CA	15.25	141.13	120.54
1	A	10	LYS	N-CA-CB	14.63	135.19	110.32
1	A	33	ARG	NE-CZ-NH1	14.49	135.99	121.50
1	A	59	CYS	N-CA-C	14.09	129.56	110.55
1	A	33	ARG	CB-CG-CD	13.85	143.15	111.30
1	A	59	CYS	O-C-N	-13.62	107.32	122.85
1	A	10	LYS	CB-CG-CD	13.46	142.26	111.30
1	A	110	GLN	CG-CD-NE2	13.20	136.19	116.40
1	A	74	ARG	NE-CZ-NH1	13.06	134.56	121.50
1	A	17	ALA	O-C-N	-12.86	104.89	121.74
1	A	79	LYS	CA-CB-CG	-11.86	90.38	114.10
1	A	107	LYS	CB-CG-CD	11.68	138.16	111.30
1	A	33	ARG	N-CA-CB	11.61	129.70	111.24
1	A	56	LYS	N-CA-CB	10.72	125.89	110.12
1	A	100	ARG	CD-NE-CZ	-10.40	109.83	124.40
1	A	110	GLN	CG-CD-OE1	-10.15	100.51	120.80
1	A	13	THR	O-C-N	10.00	133.34	122.34
1	A	10	LYS	CB-CA-C	-9.50	90.28	110.32
1	A	107	LYS	N-CA-CB	9.33	126.17	110.32
1	A	33	ARG	CD-NE-CZ	-9.30	111.38	124.40
1	A	23	PHE	CA-C-O	-9.08	108.25	118.69
1	A	74	ARG	CG-CD-NE	-8.70	92.86	112.00
1	A	107	LYS	CB-CA-C	-8.50	92.39	110.32
1	A	121	THR	CA-C-N	8.48	130.44	119.84
1	A	121	THR	C-N-CA	8.48	130.44	119.84
1	A	54	LEU	CA-C-N	8.42	132.25	120.29
1	A	54	LEU	C-N-CA	8.42	132.25	120.29
1	A	116	HIS	O-C-N	-8.29	111.70	122.39
1	A	106	ASN	O-C-N	8.19	132.65	123.48
1	A	14	GLY	CA-C-N	8.12	135.96	122.07
1	A	14	GLY	C-N-CA	8.12	135.96	122.07
1	A	14	GLY	O-C-N	-7.93	112.79	122.23
1	A	56	LYS	CG-CD-CE	7.64	128.88	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	55	GLU	N-CA-C	-7.51	103.18	111.36
1	A	102	LYS	CG-CD-CE	7.40	128.31	111.30
1	A	52	LYS	CB-CG-CD	-7.23	94.67	111.30
1	A	100	ARG	CG-CD-NE	7.14	127.72	112.00
1	A	110	GLN	CA-CB-CG	7.12	128.35	114.10
1	A	52	LYS	CG-CD-CE	7.11	127.64	111.30
1	A	110	GLN	CB-CG-CD	7.08	124.63	112.60
1	A	115	LYS	CG-CD-CE	-7.01	95.17	111.30
1	A	57	ARG	CD-NE-CZ	-7.01	114.59	124.40
1	A	100	ARG	CA-CB-CG	6.92	127.95	114.10
1	A	39	ALA	N-CA-C	6.81	119.33	111.02
1	A	75	ILE	O-C-N	-6.78	115.86	123.18
1	A	115	LYS	CA-CB-CG	6.73	127.56	114.10
1	A	107	LYS	CG-CD-CE	6.64	126.56	111.30
1	A	74	ARG	CA-CB-CG	6.57	127.24	114.10
1	A	17	ALA	CA-C-N	6.56	134.06	121.54
1	A	17	ALA	C-N-CA	6.56	134.06	121.54
1	A	81	ASP	CA-C-N	6.55	129.38	120.54
1	A	81	ASP	C-N-CA	6.55	129.38	120.54
1	A	13	THR	CA-C-O	-6.54	111.51	118.77
1	A	115	LYS	CA-C-N	6.52	133.77	122.56
1	A	115	LYS	C-N-CA	6.52	133.77	122.56
1	A	79	LYS	CG-CD-CE	6.50	126.25	111.30
1	A	100	ARG	CB-CG-CD	-6.43	96.50	111.30
1	A	122	PRO	O-C-N	-6.34	114.08	122.64
1	A	62	LYS	CA-CB-CG	6.22	126.53	114.10
1	A	102	LYS	CB-CG-CD	-6.19	97.07	111.30
1	A	116	HIS	CA-C-N	6.13	131.81	122.93
1	A	116	HIS	C-N-CA	6.13	131.81	122.93
1	A	79	LYS	CB-CG-CD	6.01	125.13	111.30
1	A	36	PRO	CA-C-N	-5.89	111.72	122.38
1	A	36	PRO	C-N-CA	-5.89	111.72	122.38
1	A	56	LYS	CD-CE-NZ	-5.76	93.47	111.90
1	A	5	PHE	O-C-N	5.74	130.23	122.59
1	A	60	GLY	N-CA-C	-5.73	105.21	112.54
1	A	79	LYS	CD-CE-NZ	-5.71	93.63	111.90
1	A	106	ASN	N-CA-C	5.69	117.75	108.76
1	A	100	ARG	NE-CZ-NH1	-5.69	115.81	121.50
1	A	115	LYS	CD-CE-NZ	-5.64	93.86	111.90
1	A	102	LYS	CD-CE-NZ	-5.60	93.98	111.90
1	A	14	GLY	N-CA-C	-5.58	108.23	115.59
1	A	116	HIS	CA-CB-CG	-5.32	108.48	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	ALA	O-C-N	5.30	127.75	122.08
1	A	105	TYR	CA-C-N	-5.29	111.48	121.63
1	A	105	TYR	C-N-CA	-5.29	111.48	121.63
1	A	79	LYS	N-CA-C	-5.26	102.06	109.96
1	A	109	TYR	O-C-N	5.25	128.84	122.48
1	A	9	ILE	O-C-N	-5.19	116.48	121.83
1	A	84	ARG	CD-NE-CZ	-5.14	117.21	124.40
1	A	45	VAL	N-CA-C	-5.13	105.60	110.42
1	A	10	LYS	CD-CE-NZ	-5.10	95.59	111.90

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	ARG	Sidechain
1	A	105	TYR	Mainchain
1	A	33	ARG	Sidechain
1	A	55	GLU	Mainchain
1	A	74	ARG	Sidechain
1	A	82	SER	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	963	0	925	31	0
2	A	2	0	0	0	0
3	A	25	0	0	2	0
All	All	990	0	925	31	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 18.

All (31) 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:16:GLU:C	1:A:17:ALA:N	1.70	1.47
1:A:16:GLU:O	1:A:20:SER:HB2	1.87	0.74
1:A:15:LYS:HD3	1:A:20:SER:OG	1.88	0.73
1:A:16:GLU:C	1:A:17:ALA:CA	2.65	0.67
1:A:40:THR:O	1:A:43:CYS:HB2	1.99	0.62
1:A:94:ALA:O	1:A:97:CYS:HB3	2.05	0.55
1:A:44:CYS:HA	1:A:47:HIS:CB	2.38	0.53
1:A:54:LEU:HD11	1:A:86:GLN:HB2	1.90	0.53
1:A:16:GLU:CA	1:A:17:ALA:N	2.61	0.53
1:A:36:PRO:HA	1:A:41:ASP:OD2	2.10	0.52
1:A:35:SER:HB2	3:A:148:HOH:O	2.11	0.50
1:A:87:LEU:O	1:A:90:CYS:HB2	2.11	0.50
1:A:1:ALA:O	1:A:4:ASN:HB2	2.12	0.49
1:A:82:SER:O	1:A:86:GLN:HG3	2.12	0.49
1:A:24:TYR:O	1:A:28:CYS:HB2	2.13	0.47
1:A:5:PHE:O	1:A:9:ILE:HG12	2.13	0.47
1:A:44:CYS:HA	1:A:47:HIS:HB3	1.97	0.46
1:A:2:LEU:O	1:A:5:PHE:HB3	2.15	0.45
1:A:44:CYS:HA	1:A:47:HIS:HB2	1.98	0.45
1:A:2:LEU:CD2	1:A:62:LYS:HG2	2.47	0.44
1:A:54:LEU:HD13	1:A:54:LEU:HA	1.73	0.43
1:A:93:ALA:O	1:A:97:CYS:HB2	2.19	0.42
1:A:4:ASN:O	1:A:7:ARG:HB2	2.19	0.42
1:A:78:ALA:O	1:A:80:GLN:HG2	2.20	0.42
1:A:6:HIS:HA	1:A:9:ILE:HG13	2.02	0.42
1:A:24:TYR:CE2	1:A:40:THR:HB	2.55	0.41
1:A:39:ALA:HB3	3:A:141:HOH:O	2.21	0.41
1:A:96:THR:O	1:A:99:ALA:HB3	2.20	0.41
1:A:66:TYR:CD1	1:A:66:TYR:C	2.98	0.41
1:A:115:LYS:HZ3	1:A:115:LYS:HG3	1.04	0.41
1:A:8:MET:HG2	1:A:75:ILE:HD13	2.02	0.40

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	122/124 (98%)	113 (93%)	7 (6%)	2 (2%)	7	16

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	ARG
1	A	122	PRO

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	104/104 (100%)	89 (86%)	15 (14%)	3	6

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	9	ILE
1	A	10	LYS
1	A	15	LYS
1	A	20	SER
1	A	33	ARG
1	A	44	CYS
1	A	46	THR
1	A	52	LYS
1	A	54	LEU
1	A	74	ARG
1	A	102	LYS
1	A	108	LYS
1	A	115	LYS
1	A	123	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	27	HIS

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 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	16:GLU	C	17:ALA	N	1.70
1	A	43:CYS	C	44:CYS	N	1.60

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.