



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:53 AM UTC

PDB ID : 1SUC / pdb_00001suc
Title : CALCIUM-INDEPENDENT SUBTILISIN BY DESIGN
Authors : Gallagher, T.; Bryan, P.; Gilliland, G.L.
Deposited on : 1992-06-10
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

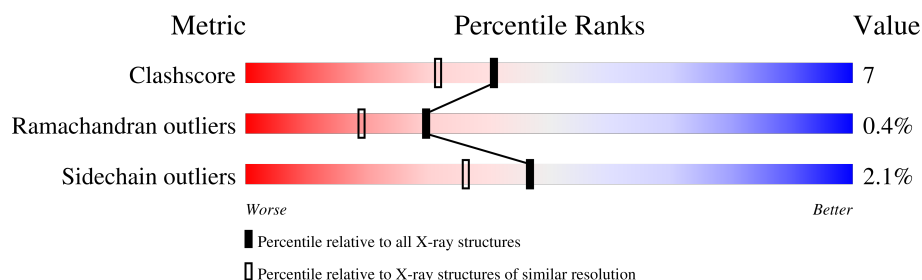
1 Overall quality at a glance

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	275	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2019 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 SUBTILISIN BPN' CRB-S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			1854	1152	320	377	5			

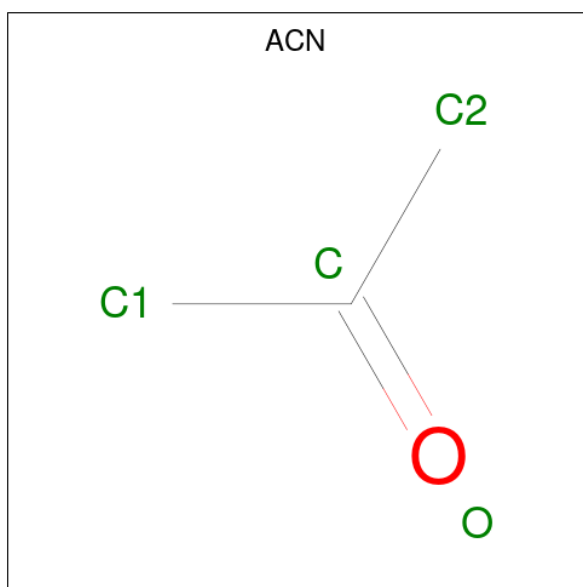
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	50	PHE	MET	engineered mutation	UNP P00782
A	217	LYS	TYR	engineered mutation	UNP P00782
A	218	SER	ASN	engineered mutation	UNP P00782
A	221	CSD	SER	engineered mutation	UNP P00782

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 3 is ACETONE (CCD ID: ACN) (formula: C₃H₆O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	3	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	160	Total	O	0	0
			160	160		

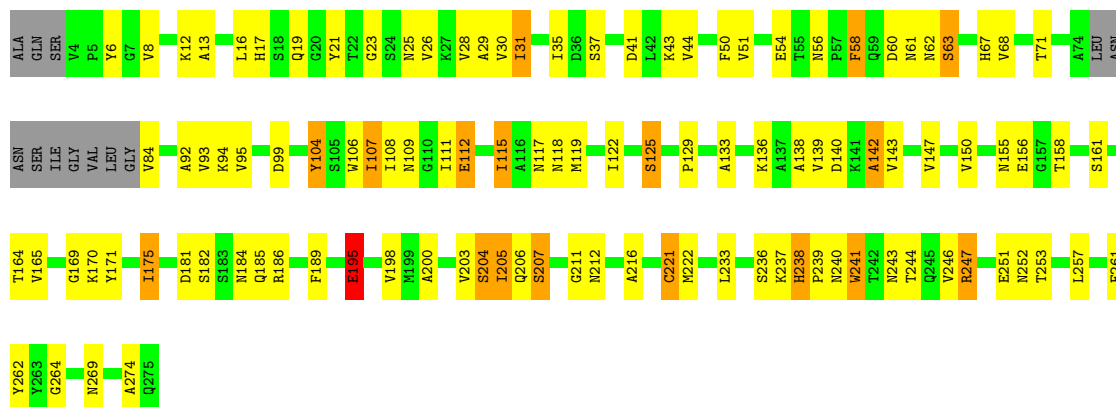
3 Residue-property plots

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: SUBTILISIN BPN' CRB-S3

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 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	41.37Å 78.67Å 36.78Å 90.00° 114.73° 90.00°	Depositor
Resolution (Å)	8.00 – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROFFT	Depositor
R, R_{free}	0.177 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2019	wwPDB-VP
Average B, all atoms (Å ²)	9.0	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: CSD, K, ACN

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	1.36	8/1884 (0.4%)	2.40	116/2570 (4.5%)

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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	30	VAL	N-CA	5.76	1.53	1.46
1	A	200	ALA	N-CA	5.55	1.50	1.45
1	A	165	VAL	CA-C	5.50	1.58	1.52
1	A	181	ASP	N-CA	5.40	1.52	1.45
1	A	68	VAL	N-CA	5.38	1.52	1.46
1	A	164	THR	N-CA	5.16	1.52	1.46
1	A	125	SER	N-CA	5.02	1.52	1.46
1	A	175	ILE	N-CA	5.01	1.52	1.46

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	99	ASP	CA-CB-CG	10.33	122.93	112.60
1	A	118	ASN	CA-CB-CG	9.74	122.34	112.60
1	A	243	ASN	CA-CB-CG	9.40	122.00	112.60
1	A	41	ASP	CA-CB-CG	9.30	121.91	112.60
1	A	212	ASN	CA-CB-CG	9.28	121.88	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	ASN	CA-CB-CG	9.10	121.70	112.60
1	A	181	ASP	CA-CB-CG	8.94	121.53	112.60
1	A	184	ASN	CA-CB-CG	8.69	121.29	112.60
1	A	257	LEU	CB-CA-C	8.11	126.56	110.42
1	A	58	PHE	CA-CB-CG	7.94	121.74	113.80
1	A	63	SER	N-CA-CB	7.81	123.68	110.49
1	A	239	PRO	CA-C-N	7.77	133.88	120.68
1	A	239	PRO	C-N-CA	7.77	133.88	120.68
1	A	12	LYS	CA-C-N	7.73	130.79	120.58
1	A	12	LYS	C-N-CA	7.73	130.79	120.58
1	A	238	HIS	CA-CB-CG	7.65	121.45	113.80
1	A	109	ASN	CA-CB-CG	7.45	120.05	112.60
1	A	207	SER	CA-C-N	7.42	131.25	120.71
1	A	207	SER	C-N-CA	7.42	131.25	120.71
1	A	56	ASN	CB-CA-C	7.29	118.16	109.85
1	A	25	ASN	CA-CB-CG	7.17	119.77	112.60
1	A	142	ALA	CA-C-N	7.16	129.58	120.56
1	A	142	ALA	C-N-CA	7.16	129.58	120.56
1	A	251	GLU	CB-CG-CD	6.83	124.21	112.60
1	A	150	VAL	CA-C-O	6.80	128.63	120.67
1	A	206	GLN	CB-CG-CD	6.77	124.10	112.60
1	A	43	LYS	CA-CB-CG	6.74	127.58	114.10
1	A	51	VAL	N-CA-C	-6.72	100.90	107.55
1	A	56	ASN	CA-CB-CG	6.71	119.31	112.60
1	A	150	VAL	CA-CB-CG2	6.71	121.81	110.40
1	A	93	VAL	CB-CA-C	6.69	120.22	111.53
1	A	50	PHE	CA-C-N	6.67	130.45	122.85
1	A	50	PHE	C-N-CA	6.67	130.45	122.85
1	A	51	VAL	O-C-N	6.56	125.50	121.37
1	A	244	THR	CA-CB-CG2	6.54	121.63	110.50
1	A	106	TRP	CA-CB-CG	6.38	125.71	113.60
1	A	28	VAL	CA-CB-CG2	6.24	121.01	110.40
1	A	17	HIS	CA-CB-CG	6.17	119.97	113.80
1	A	44	VAL	CB-CA-C	6.15	119.21	110.84
1	A	125	SER	CA-C-O	6.13	131.52	122.38
1	A	186	ARG	CD-NE-CZ	6.11	132.95	124.40
1	A	169	GLY	CA-C-N	6.08	129.03	120.28
1	A	169	GLY	C-N-CA	6.08	129.03	120.28
1	A	189	PHE	CA-CB-CG	6.08	119.88	113.80
1	A	117	ASN	CA-C-O	6.05	126.64	119.56
1	A	68	VAL	CA-C-N	6.03	128.36	120.28
1	A	68	VAL	C-N-CA	6.03	128.36	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	VAL	CB-CA-C	5.92	119.55	111.97
1	A	60	ASP	CA-CB-CG	5.90	118.50	112.60
1	A	117	ASN	O-C-N	-5.89	115.27	122.34
1	A	8	VAL	CB-CA-C	5.88	119.72	112.02
1	A	247	ARG	NE-CZ-NH1	5.86	127.36	121.50
1	A	211	GLY	CA-C-N	5.83	130.63	122.36
1	A	211	GLY	C-N-CA	5.83	130.63	122.36
1	A	95	VAL	CB-CA-C	5.78	116.07	110.63
1	A	43	LYS	CB-CA-C	5.77	120.19	110.79
1	A	175	ILE	N-CA-C	-5.75	99.43	108.23
1	A	155	ASN	CA-CB-CG	5.75	118.35	112.60
1	A	115	ILE	CA-C-N	5.73	127.96	120.28
1	A	115	ILE	C-N-CA	5.73	127.96	120.28
1	A	156	GLU	CB-CG-CD	5.73	122.34	112.60
1	A	51	VAL	CB-CA-C	5.70	117.76	111.04
1	A	252	ASN	CA-CB-CG	5.69	118.29	112.60
1	A	112	GLU	CB-CG-CD	5.67	122.24	112.60
1	A	205	ILE	CB-CA-C	5.62	117.65	111.08
1	A	269	ASN	CA-CB-CG	5.60	118.20	112.60
1	A	240	ASN	CA-CB-CG	5.58	118.18	112.60
1	A	243	ASN	CA-C-N	5.57	127.68	120.44
1	A	243	ASN	C-N-CA	5.57	127.68	120.44
1	A	244	THR	CA-C-N	5.56	128.18	120.29
1	A	244	THR	C-N-CA	5.56	128.18	120.29
1	A	94	LYS	CA-C-O	5.56	126.53	120.58
1	A	204	SER	CA-C-O	5.54	128.27	121.84
1	A	207	SER	CA-C-O	5.53	127.36	121.45
1	A	19	GLN	OE1-CD-NE2	-5.52	117.08	122.60
1	A	26	VAL	N-CA-CB	5.51	117.60	110.99
1	A	195	GLU	CB-CG-CD	5.51	121.97	112.60
1	A	62	ASN	CA-C-N	5.50	132.04	121.54
1	A	62	ASN	C-N-CA	5.50	132.04	121.54
1	A	68	VAL	CB-CA-C	5.47	118.98	111.97
1	A	253	THR	CA-C-N	5.47	129.01	120.75
1	A	253	THR	C-N-CA	5.47	129.01	120.75
1	A	111	ILE	N-CA-CB	5.37	117.44	110.57
1	A	139	VAL	CA-CB-CG2	5.36	119.51	110.40
1	A	140	ASP	CA-CB-CG	5.35	117.95	112.60
1	A	156	GLU	N-CA-C	5.33	119.78	113.28
1	A	207	SER	O-C-N	-5.32	116.99	123.10
1	A	246	VAL	CA-CB-CG1	5.30	119.42	110.40
1	A	30	VAL	CB-CA-C	5.30	119.07	111.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	ASP	CB-CA-C	5.29	120.20	111.31
1	A	117	ASN	CA-C-N	5.26	129.65	122.34
1	A	117	ASN	C-N-CA	5.26	129.65	122.34
1	A	60	ASP	N-CA-CB	5.25	119.05	110.39
1	A	203	VAL	CA-C-N	5.24	129.79	122.36
1	A	203	VAL	C-N-CA	5.24	129.79	122.36
1	A	161	SER	CA-C-O	5.21	124.92	119.03
1	A	54	GLU	CA-C-O	5.20	129.18	120.81
1	A	54	GLU	CA-CB-CG	5.14	124.38	114.10
1	A	241	TRP	CA-CB-CG	5.14	123.36	113.60
1	A	71	THR	CA-C-N	5.13	127.22	120.60
1	A	71	THR	C-N-CA	5.13	127.22	120.60
1	A	185	GLN	CA-CB-CG	5.10	124.30	114.10
1	A	261	PHE	CA-CB-CG	5.09	118.89	113.80
1	A	233	LEU	CA-C-N	5.08	126.96	120.56
1	A	233	LEU	C-N-CA	5.08	126.96	120.56
1	A	118	ASN	CA-C-O	5.04	127.55	121.65
1	A	13	ALA	CA-C-N	5.04	125.32	119.47
1	A	13	ALA	C-N-CA	5.04	125.32	119.47
1	A	31	ILE	CB-CG1-CD1	5.04	124.38	113.80
1	A	106	TRP	CA-C-N	5.03	126.90	120.56
1	A	106	TRP	C-N-CA	5.03	126.90	120.56
1	A	212	ASN	CB-CA-C	5.02	119.02	111.89
1	A	37	SER	CA-C-N	5.01	129.10	120.72
1	A	37	SER	C-N-CA	5.01	129.10	120.72
1	A	161	SER	CA-C-N	5.00	130.63	122.07
1	A	161	SER	C-N-CA	5.00	130.63	122.07

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	TYR	Mainchain
1	A	112	GLU	Mainchain
1	A	133	ALA	Mainchain
1	A	198	VAL	Mainchain
1	A	264	GLY	Mainchain
1	A	84	VAL	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	1854	0	1808	24	0
2	A	1	0	0	0	0
3	A	4	0	6	0	0
4	A	160	0	0	2	0
All	All	2019	0	1814	24	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 7.

All (24) 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:31:ILE:HD12	1:A:122:ILE:HG23	1.63	0.79
1:A:6:TYR:HB3	4:A:447:HOH:O	1.96	0.66
1:A:31:ILE:HD12	1:A:122:ILE:CG2	2.27	0.64
1:A:104:TYR:HA	1:A:107:ILE:HD12	1.80	0.63
1:A:115:ILE:HG12	1:A:142:ALA:HA	1.87	0.57
1:A:21:TYR:CZ	1:A:237:LYS:HG3	2.42	0.54
1:A:125:SER:HB3	1:A:221:CSD:HB2	1.89	0.54
1:A:205:ILE:O	1:A:216:ALA:HA	2.08	0.52
1:A:35:ILE:HD12	1:A:92:ALA:HB2	1.91	0.52
1:A:158:THR:HG22	1:A:262:TYR:HE1	1.74	0.51
1:A:170:LYS:HG2	1:A:195:GLU:HG2	1.91	0.51
1:A:129:PRO:HB3	4:A:438:HOH:O	2.10	0.50
1:A:175:ILE:HG12	1:A:247:ARG:HG3	1.95	0.47
1:A:23:GLY:HA2	1:A:236:SER:HB3	1.96	0.46
1:A:67:HIS:CD2	1:A:207:SER:HB3	2.52	0.44
1:A:122:ILE:HD12	1:A:147:VAL:HG11	2.00	0.43
1:A:16:LEU:HD21	1:A:274:ALA:HB3	2.00	0.43
1:A:108:ILE:HG23	1:A:138:ALA:HB2	2.00	0.42
1:A:29:ALA:HB2	1:A:119:MET:HG3	2.02	0.42
1:A:238:HIS:HB3	1:A:241:TRP:CD1	2.56	0.41
1:A:35:ILE:O	1:A:58:PHE:HA	2.20	0.41
1:A:119:MET:O	1:A:147:VAL:HG22	2.21	0.41
1:A:6:TYR:CE1	1:A:182:SER:HB2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:LYS:HG3	1:A:171:TYR:CD1	2.56	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	260/275 (94%)	251 (96%)	8 (3%)	1 (0%)	30 19

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	SER

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	194/204 (95%)	190 (98%)	4 (2%)	47 36

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	ILE
1	A	195	GLU

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Mol	Chain	Res	Type
1	A	204	SER
1	A	222	MET

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	271	GLN
1	A	275	GLN

5.3.3 RNA ⓘ

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	CSD	A	221	1	4,7,8	14.70	1 (25%)	1,8,10	6.77	1 (100%)

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	CSD	A	221	1	-	0/2/6/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	221	CSD	OD1-SG	29.36	1.74	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	CSD	OD1-SG-CB	-6.77	93.13	105.60

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	221	CSD	1	0

5.5 Carbohydrates

There are no oligosaccharides 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	ACN	A	298	-	3,3,3	0.58	0	3,3,3	0.74	0

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

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.