



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:09 PM GMT

PDB ID : 1SCN
Title : INACTIVATION OF SUBTILISIN CARLSBERG BY N-(TERT-BUTOXY CARBONYL-ALANYL-PROLYL-PHENYLALANYL)-O-BENZOL HYDROXYLAMINE: FORMATION OF COVALENT ENZYME-INHIBITOR LINKAGE IN THE FORM OF A CARBAMATE DERIVATIVE
Authors : Steinmetz, A.C.U.; Demuth, H.-U.; Ringe, D.
Deposited on : 1994-03-02
Resolution : 1.90 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

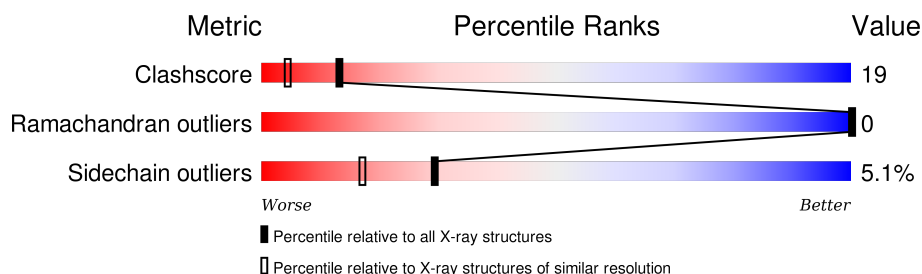
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)

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	E	276	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2094 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.

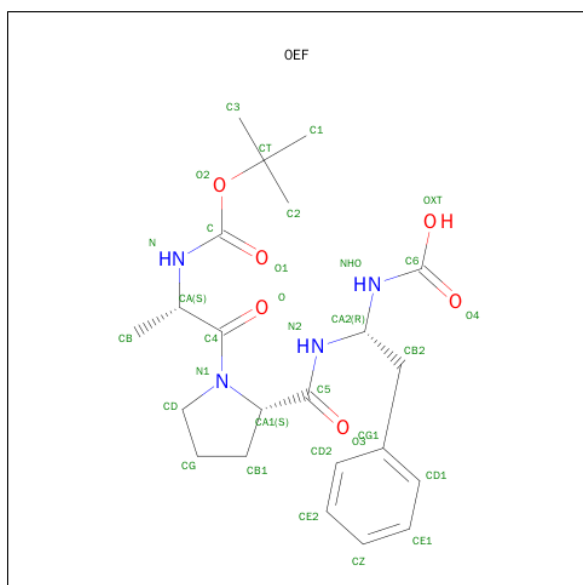
- Molecule 1 is a protein called SUBTILISIN CARLSBERG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	E	274	1919	1190	332	392	5	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	103	SER	THR	CONFLICT	UNP P00780
E	129	ALA	PRO	CONFLICT	UNP P00780
E	158	ASN	SER	CONFLICT	UNP P00780
E	161	SER	ASN	CONFLICT	UNP P00780
E	212	ASN	SER	CONFLICT	UNP P00780

- Molecule 2 is N-(TERT-BUTOXYCARBONYL)-L-ALANYL-N-[(1R)-1-(CARBOXYAMINO)-2-PHENYLETHYL]-L-PROLINAMIDE (three-letter code: 0EF) (formula: $C_{22}H_{32}N_4O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	E	1	Total	C	N	O	0	0
			31	22	4	5		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	2	Total	Ca	0	0
			2	2		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	1	Total	Na	0	0
			1	1		

- Molecule 5 is water.

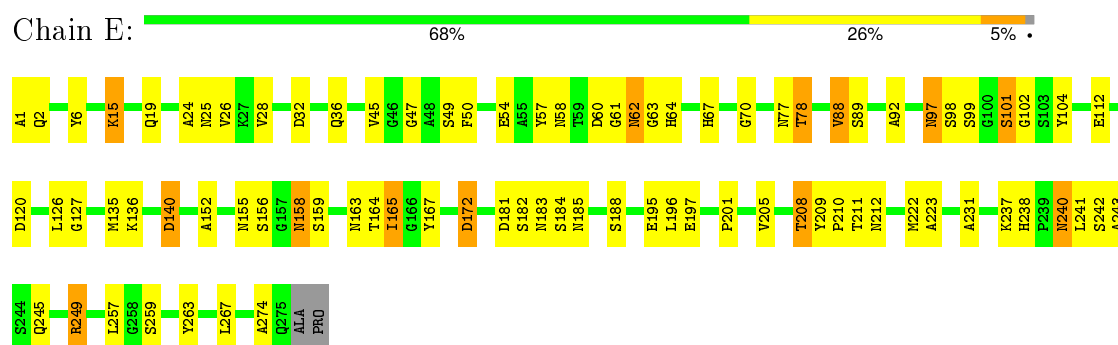
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	141	Total	O	0	0
			141	141		

3 Residue-property plots

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: SUBTILISIN CARLSBERG



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	76.50 Å 55.40 Å 53.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.191 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2094	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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: NA, CA, OEF

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	E	0.80	4/1951 (0.2%)	1.64	28/2662 (1.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	15	LYS	CE-NZ	8.77	1.71	1.49
1	E	54	GLU	CD-OE1	6.56	1.32	1.25
1	E	197	GLU	CD-OE1	6.48	1.32	1.25
1	E	112	GLU	CD-OE2	5.89	1.32	1.25

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	181	ASP	CB-CG-OD2	-12.98	106.62	118.30
1	E	181	ASP	CB-CG-OD1	12.12	129.21	118.30
1	E	167	TYR	CB-CG-CD1	-9.94	115.03	121.00
1	E	32	ASP	CB-CG-OD1	-9.39	109.85	118.30
1	E	140	ASP	CB-CG-OD2	-7.93	111.16	118.30
1	E	140	ASP	CB-CG-OD1	7.82	125.34	118.30
1	E	263	TYR	CB-CG-CD2	-7.63	116.42	121.00
1	E	172	ASP	CB-CG-OD2	-7.58	111.48	118.30
1	E	249	ARG	NE-CZ-NH2	-7.09	116.76	120.30
1	E	120	ASP	CB-CG-OD1	-6.90	112.09	118.30
1	E	50	PHE	CB-CG-CD1	6.71	125.50	120.80
1	E	159	SER	N-CA-CB	6.70	120.54	110.50
1	E	167	TYR	CB-CA-C	-6.62	97.15	110.40
1	E	60	ASP	CB-CG-OD1	-6.53	112.42	118.30
1	E	32	ASP	CB-CG-OD2	6.48	124.13	118.30
1	E	120	ASP	CB-CG-OD2	6.45	124.11	118.30
1	E	98	SER	CB-CA-C	-6.41	97.93	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	88	VAL	CG1-CB-CG2	-6.31	100.80	110.90
1	E	249	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	E	259	SER	N-CA-CB	-6.12	101.31	110.50
1	E	167	TYR	CA-CB-CG	-5.79	102.40	113.40
1	E	208	THR	CA-CB-CG2	-5.74	104.37	112.40
1	E	60	ASP	CB-CG-OD2	5.70	123.43	118.30
1	E	243	ALA	CB-CA-C	-5.64	101.64	110.10
1	E	49	SER	N-CA-CB	5.62	118.92	110.50
1	E	195	GLU	CG-CD-OE2	-5.62	107.07	118.30
1	E	165	ILE	CA-CB-CG1	-5.49	100.58	111.00
1	E	231	ALA	N-CA-CB	-5.08	102.99	110.10

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	E	1919	0	1879	64	5
2	E	31	0	31	12	8
3	E	2	0	0	0	0
4	E	1	0	0	0	0
5	E	141	0	0	8	4
All	All	2094	0	1910	73	9

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 19.

All (73) 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:E:15:LYS:NZ	1:E:15:LYS:CE	1.71	1.51
2:E:447:0EF:N2	2:E:447:0EF:CA2	1.84	1.36
1:E:158:ASN:N	1:E:158:ASN:HD22	1.53	1.03
1:E:242:SER:H	1:E:245:GLN:NE2	1.56	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:158:ASN:H	1:E:158:ASN:ND2	1.63	0.96
1:E:242:SER:H	1:E:245:GLN:HE21	1.03	0.95
1:E:2:GLN:HE22	1:E:77:ASN:H	0.94	0.93
2:E:447:0EF:CB2	2:E:447:0EF:N2	2.32	0.93
1:E:28:VAL:HG23	1:E:88:VAL:HG21	1.53	0.91
2:E:447:0EF:HB21	5:E:802:HOH:O	1.76	0.84
2:E:447:0EF:N2	2:E:447:0EF:HB22	1.95	0.82
1:E:242:SER:N	1:E:245:GLN:HE21	1.77	0.82
1:E:36:GLN:HE22	1:E:212:ASN:H	1.27	0.82
1:E:2:GLN:NE2	1:E:77:ASN:H	1.77	0.81
1:E:97:ASN:C	1:E:97:ASN:HD22	1.84	0.80
1:E:242:SER:N	1:E:245:GLN:NE2	2.31	0.76
1:E:26:VAL:O	1:E:88:VAL:HG23	1.87	0.73
1:E:28:VAL:CG2	1:E:88:VAL:HG21	2.19	0.72
1:E:2:GLN:HE22	1:E:77:ASN:N	1.79	0.70
1:E:62:ASN:HD22	1:E:64:HIS:H	1.40	0.69
1:E:97:ASN:ND2	1:E:99:SER:H	1.95	0.65
1:E:158:ASN:HD22	1:E:158:ASN:H	0.78	0.64
2:E:447:0EF:CA2	2:E:447:0EF:C5	2.73	0.64
1:E:126:LEU:C	1:E:126:LEU:HD12	2.19	0.62
1:E:158:ASN:N	1:E:158:ASN:ND2	2.28	0.60
1:E:183:ASN:O	1:E:184:SER:HB2	2.00	0.60
1:E:240:ASN:HD22	1:E:240:ASN:H	1.50	0.60
1:E:104:TYR:HD1	1:E:135:MET:CE	2.15	0.59
1:E:165:ILE:HD11	1:E:196:LEU:HB2	1.85	0.59
1:E:63:GLY:HA2	1:E:210:PRO:CG	2.34	0.57
2:E:447:0EF:HB31	5:E:861:HOH:O	2.04	0.57
1:E:209:TYR:CG	1:E:210:PRO:HD2	2.40	0.57
1:E:15:LYS:NZ	1:E:15:LYS:CD	2.63	0.56
1:E:97:ASN:C	1:E:97:ASN:ND2	2.58	0.55
1:E:61:GLY:N	5:E:595:HOH:O	2.34	0.55
1:E:19:GLN:HE22	1:E:237:LYS:NZ	2.04	0.55
1:E:205:VAL:HG22	5:E:501:HOH:O	2.07	0.54
1:E:238:HIS:O	1:E:241:LEU:HG	2.08	0.54
1:E:185:ASN:ND2	5:E:774:HOH:O	2.40	0.54
1:E:63:GLY:HA2	1:E:210:PRO:HG3	1.90	0.53
1:E:257:LEU:HD11	1:E:267:LEU:HB2	1.90	0.53
1:E:240:ASN:HB3	5:E:525:HOH:O	2.09	0.52
1:E:237:LYS:HD3	1:E:274:ALA:O	2.11	0.51
1:E:6:TYR:CD1	1:E:6:TYR:C	2.84	0.51
1:E:28:VAL:HG23	1:E:88:VAL:CG2	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:88:VAL:HG22	1:E:89:SER:N	2.27	0.50
1:E:240:ASN:ND2	1:E:240:ASN:H	2.08	0.50
2:E:447:0EF:H1	2:E:447:0EF:HB22	1.74	0.49
1:E:152:ALA:HB3	2:E:447:0EF:HE1	1.94	0.48
1:E:104:TYR:HD1	1:E:135:MET:HE3	1.78	0.48
1:E:70:GLY:HA3	1:E:208:THR:OG1	2.13	0.48
1:E:127:GLY:HA3	2:E:447:0EF:CZ	2.45	0.47
1:E:136:LYS:NZ	1:E:140:ASP:OD2	2.48	0.47
2:E:447:0EF:N2	2:E:447:0EF:NHO	2.59	0.46
1:E:19:GLN:HE22	1:E:237:LYS:HZ2	1.62	0.46
1:E:211:THR:O	1:E:212:ASN:HB2	2.15	0.46
1:E:6:TYR:CE1	1:E:182:SER:HA	2.51	0.45
1:E:249:ARG:NH2	5:E:756:HOH:O	2.30	0.45
1:E:57:TYR:C	1:E:57:TYR:CD2	2.89	0.45
1:E:155:ASN:ND2	2:E:447:0EF:HA2	2.34	0.43
1:E:1:ALA:HB3	1:E:78:THR:O	2.18	0.43
1:E:102:GLY:HA2	5:E:856:HOH:O	2.17	0.43
1:E:97:ASN:ND2	1:E:101:SER:H	2.16	0.43
1:E:58:ASN:N	1:E:58:ASN:OD1	2.41	0.43
2:E:447:0EF:NHO	2:E:447:0EF:HD1	2.33	0.43
1:E:97:ASN:ND2	1:E:99:SER:N	2.66	0.42
1:E:45:VAL:O	1:E:45:VAL:HG12	2.19	0.42
1:E:36:GLN:NE2	1:E:210:PRO:HA	2.35	0.41
1:E:201:PRO:O	1:E:223:ALA:HA	2.20	0.41
1:E:47:GLY:HA3	1:E:92:ALA:O	2.20	0.41
1:E:67:HIS:HA	1:E:208:THR:O	2.21	0.41
1:E:24:ALA:O	1:E:25:ASN:CB	2.69	0.41
1:E:156:SER:HB2	1:E:164:THR:HB	2.02	0.40

All (9) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:447:0EF:C3	5:E:852:HOH:O[4_477]	0.79	1.41
2:E:447:0EF:C1	5:E:650:HOH:O[4_477]	1.07	1.13
1:E:249:ARG:CG	2:E:447:0EF:C2[4_577]	1.38	0.82
1:E:249:ARG:CD	2:E:447:0EF:C2[4_577]	1.44	0.76
2:E:447:0EF:CT	5:E:852:HOH:O[4_477]	1.62	0.58
1:E:249:ARG:NE	2:E:447:0EF:C2[4_577]	1.68	0.52
1:E:249:ARG:NE	2:E:447:0EF:C3[4_577]	1.72	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:249:ARG:NE	2:E:447:0EF:CT[4_577]	1.91	0.29
5:E:859:HOH:O	5:E:879:HOH:O[3_757]	2.08	0.12

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	E	272/276 (99%)	263 (97%)	9 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	E	198/199 (100%)	188 (95%)	10 (5%)	29	17

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	62	ASN
1	E	78	THR
1	E	97	ASN
1	E	101	SER
1	E	158	ASN
1	E	163	ASN

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Mol	Chain	Res	Type
1	E	172	ASP
1	E	188	SER
1	E	222	MET
1	E	240	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	19	GLN
1	E	36	GLN
1	E	62	ASN
1	E	97	ASN
1	E	141	ASN
1	E	158	ASN
1	E	185	ASN
1	E	212	ASN
1	E	238	HIS
1	E	240	ASN
1	E	245	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are 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
2	0EF	E	447	1	31,32,33	6.01	4 (12%)	40,44,46	2.47	14 (35%)

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	0EF	E	447	1	-	0/30/42/43	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	447	0EF	CB2-CG1	-2.89	1.44	1.51
2	E	447	0EF	C-N	2.71	1.42	1.34
2	E	447	0EF	CD-N1	4.18	1.55	1.47
2	E	447	0EF	CA2-N2	32.60	1.84	1.45

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	447	0EF	CT-O2-C	-7.61	108.76	121.05
2	E	447	0EF	CA1-C5-N2	-4.93	105.56	116.64
2	E	447	0EF	CD-N1-CA1	-4.65	105.12	112.00
2	E	447	0EF	O2-C-O1	-4.24	116.98	125.55
2	E	447	0EF	O2-C-N	-3.35	103.78	110.07
2	E	447	0EF	CA2-N2-C5	-3.21	119.93	123.30
2	E	447	0EF	C2-CT-C1	-2.72	103.44	111.16
2	E	447	0EF	C3-CT-C2	-2.69	103.54	111.16
2	E	447	0EF	CD-N1-C4	-2.15	117.86	125.58
2	E	447	0EF	CA-N-C	2.16	124.89	120.64
2	E	447	0EF	O2-CT-C1	2.25	116.19	107.21
2	E	447	0EF	C4-CA-N	2.50	114.95	108.83
2	E	447	0EF	CB1-CA1-N1	3.15	107.49	102.99
2	E	447	0EF	O3-C5-CA1	4.75	131.43	120.51

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	447	0EF	12	8

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.