



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:39 PM GMT

PDB ID : 1GNS  
Title : SUBTILISIN BPN'  
Authors : Almog, O.; Gallagher, D.T.; Ladner, J.E.; Strausberg, S.; Alexander, P.  
Deposited on : 2001-10-06  
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](mailto: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.

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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) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

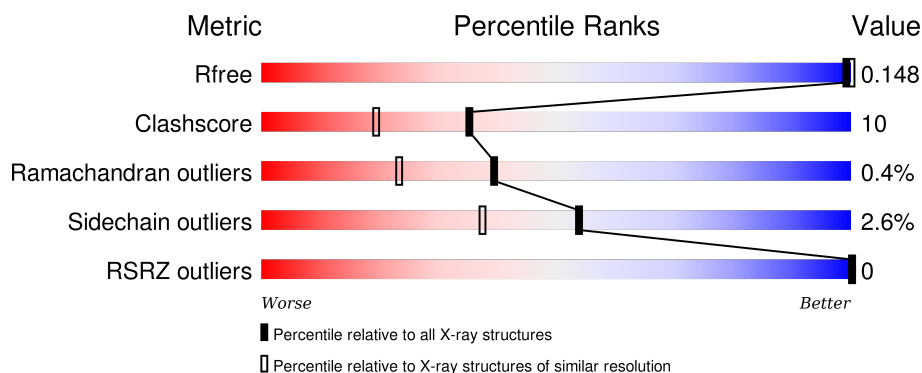
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


The reported resolution of this entry is 1.80 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))
$R_{free}$	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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.

Mol	Chain	Length	Quality of chain
1	A	263	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2017 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.

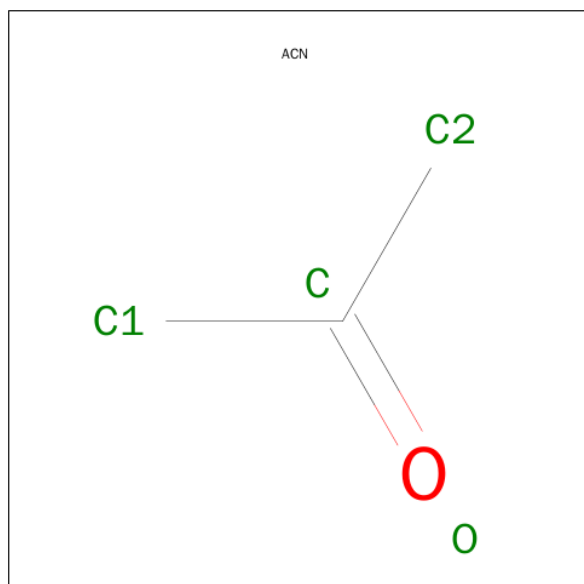
- Molecule 1 is a protein called SUBTILISIN BPN'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			1858	1160	319	374	5			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	GLY	VAL	CONFLICT	UNP P00782
A	41	ALA	ASP	ENGINEERED MUTATION	UNP P00782
A	50	PHE	MET	ENGINEERED MUTATION	UNP P00782
A	73	LEU	ALA	ENGINEERED MUTATION	UNP P00782
A	206	TRP	GLN	ENGINEERED MUTATION	UNP P00782
A	217	LYS	TYR	ENGINEERED MUTATION	UNP P00782
A	218	SER	ASN	ENGINEERED MUTATION	UNP P00782
A	221	CSO	SER	ENGINEERED MUTATION	UNP P00782
A	271	GLU	GLN	ENGINEERED MUTATION	UNP P00782

- Molecule 2 is ACETONE (three-letter code: ACN) (formula: C<sub>3</sub>H<sub>6</sub>O).



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

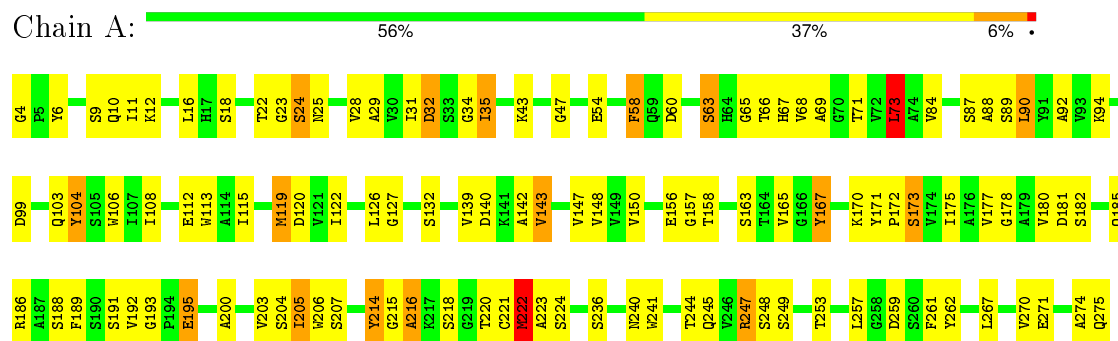
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	155	Total	O	0	0
			155	155		

### 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 ( $\text{RSRZ} > 2$ ). 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.

- Molecule 1: SUBTILISIN BPN'



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	41.17Å 78.06Å 36.70Å 90.00° 114.60° 90.00°	Depositor
Resolution (Å)	8.00 – 1.80 10.01 – 1.80	Depositor EDS
% Data completeness (in resolution range)	77.0 (8.00-1.80) 80.0 (10.01-1.80)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.66 (at 1.80Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.165 , (Not available) 0.148 , 0.148	Depositor DCC
$R_{free}$ test set	503 reflections (3.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	10.3	Xtriage
Anisotropy	0.516	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 51.4	EDS
Estimated twinning fraction	0.045 for -h-l,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 15589 reflections (0.006%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2017	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.73% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CSO, 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	1.84	19/1890 (1.0%)	2.36	98/2578 (3.8%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	222	MET	CG-SD	-11.86	1.50	1.81
1	A	248	SER	CA-CB	8.54	1.65	1.52
1	A	112	GLU	CD-OE1	-8.23	1.16	1.25
1	A	4	GLY	N-CA	7.29	1.56	1.46
1	A	54	GLU	CD-OE1	-6.98	1.18	1.25
1	A	214	TYR	CG-CD2	6.72	1.47	1.39
1	A	178	GLY	CA-C	6.48	1.62	1.51
1	A	71	THR	CB-OG1	6.34	1.55	1.43
1	A	89	SER	CB-OG	-6.20	1.34	1.42
1	A	68	VAL	CB-CG1	6.00	1.65	1.52
1	A	67	HIS	CE1-NE2	5.90	1.46	1.32
1	A	214	TYR	CE1-CZ	5.80	1.46	1.38
1	A	224	SER	CA-CB	5.70	1.61	1.52
1	A	214	TYR	CE2-CZ	-5.66	1.31	1.38
1	A	68	VAL	N-CA	5.35	1.57	1.46
1	A	220	THR	N-CA	5.24	1.56	1.46
1	A	271	GLU	CD-OE1	-5.16	1.20	1.25
1	A	9	SER	CA-CB	5.07	1.60	1.52
1	A	157	GLY	CA-C	5.04	1.59	1.51

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247	ARG	NE-CZ-NH1	21.05	130.83	120.30
1	A	222	MET	CG-SD-CE	13.81	122.30	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	ASP	CB-CG-OD1	12.97	129.97	118.30
1	A	247	ARG	NE-CZ-NH2	-10.56	115.02	120.30
1	A	60	ASP	CB-CG-OD2	-9.86	109.42	118.30
1	A	259	ASP	CB-CG-OD2	-9.84	109.45	118.30
1	A	29	ALA	N-CA-CB	8.88	122.53	110.10
1	A	214	TYR	CB-CG-CD1	8.61	126.17	121.00
1	A	156	GLU	OE1-CD-OE2	8.44	133.43	123.30
1	A	32	ASP	CB-CG-OD1	8.42	125.88	118.30
1	A	189	PHE	CB-CG-CD1	-8.30	114.99	120.80
1	A	150	VAL	CA-CB-CG2	8.30	123.34	110.90
1	A	60	ASP	CB-CG-OD1	8.00	125.50	118.30
1	A	259	ASP	OD1-CG-OD2	7.88	138.28	123.30
1	A	63	SER	N-CA-CB	7.31	121.47	110.50
1	A	259	ASP	CB-CG-OD1	-7.28	111.75	118.30
1	A	73	LEU	CB-CA-C	7.27	124.01	110.20
1	A	205	ILE	O-C-N	7.21	134.24	122.70
1	A	90	LEU	CA-CB-CG	7.02	131.46	115.30
1	A	271	GLU	CG-CD-OE1	7.00	132.30	118.30
1	A	112	GLU	CG-CD-OE2	-6.93	104.43	118.30
1	A	24	SER	N-CA-CB	-6.88	100.18	110.50
1	A	203	VAL	CG1-CB-CG2	-6.80	100.02	110.90
1	A	257	LEU	CB-CA-C	6.79	123.09	110.20
1	A	43	LYS	N-CA-CB	6.74	122.74	110.60
1	A	271	GLU	CG-CD-OE2	-6.71	104.89	118.30
1	A	143	VAL	CA-CB-CG1	6.55	120.72	110.90
1	A	99	ASP	CB-CA-C	6.55	123.49	110.40
1	A	223	ALA	N-CA-CB	-6.55	100.94	110.10
1	A	143	VAL	CG1-CB-CG2	-6.39	100.67	110.90
1	A	157	GLY	O-C-N	6.37	132.89	122.70
1	A	73	LEU	CB-CG-CD1	6.29	121.70	111.00
1	A	156	GLU	CG-CD-OE2	-6.28	105.73	118.30
1	A	132	SER	N-CA-CB	6.23	119.84	110.50
1	A	163	SER	N-CA-CB	-6.12	101.32	110.50
1	A	167	TYR	CB-CG-CD2	-6.12	117.33	121.00
1	A	66	THR	CA-CB-OG1	-6.07	96.26	109.00
1	A	148	VAL	CA-CB-CG2	6.04	119.96	110.90
1	A	112	GLU	OE1-CD-OE2	6.02	130.53	123.30
1	A	87	SER	O-C-N	-6.01	113.09	122.70
1	A	120	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	A	35	ILE	CA-C-N	-5.99	104.03	117.20
1	A	140	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	A	35	ILE	O-C-N	5.98	132.26	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	ALA	CA-C-O	5.96	132.62	120.10
1	A	218	SER	N-CA-CB	-5.95	101.58	110.50
1	A	186	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	A	244	THR	CA-CB-CG2	5.81	120.53	112.40
1	A	58	PHE	CB-CG-CD1	-5.79	116.74	120.80
1	A	99	ASP	CB-CG-OD1	5.79	123.52	118.30
1	A	193	GLY	CA-C-O	5.79	131.03	120.60
1	A	191	SER	CA-C-N	-5.79	104.47	117.20
1	A	16	LEU	CA-CB-CG	5.79	128.61	115.30
1	A	22	THR	O-C-N	-5.77	113.39	123.20
1	A	113	TRP	CD1-NE1-CE2	5.76	114.18	109.00
1	A	248	SER	CA-CB-OG	-5.71	95.79	111.20
1	A	104	TYR	CG-CD2-CE2	5.71	125.86	121.30
1	A	167	TYR	CB-CG-CD1	5.64	124.39	121.00
1	A	261	PHE	CG-CD2-CE2	-5.58	114.66	120.80
1	A	244	THR	CA-CB-OG1	-5.56	97.32	109.00
1	A	181	ASP	N-CA-CB	-5.55	100.60	110.60
1	A	16	LEU	CB-CA-C	5.55	120.74	110.20
1	A	99	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	A	214	TYR	CZ-CE2-CD2	5.52	124.77	119.80
1	A	25	ASN	N-CA-CB	5.37	120.27	110.60
1	A	241	TRP	CA-CB-CG	5.35	123.87	113.70
1	A	171	TYR	CA-CB-CG	5.35	123.57	113.40
1	A	165	VAL	CA-CB-CG2	5.35	118.92	110.90
1	A	12	LYS	O-C-N	-5.34	114.16	122.70
1	A	181	ASP	CA-C-O	5.30	131.24	120.10
1	A	4	GLY	N-CA-C	-5.28	99.89	113.10
1	A	103	GLN	CA-CB-CG	5.28	125.02	113.40
1	A	185	GLN	CB-CG-CD	5.28	125.32	111.60
1	A	177	VAL	CA-CB-CG2	5.27	118.81	110.90
1	A	205	ILE	CA-C-N	-5.24	105.66	117.20
1	A	188	SER	CA-C-O	5.24	131.10	120.10
1	A	68	VAL	CB-CA-C	5.24	121.36	111.40
1	A	215	GLY	O-C-N	5.24	131.08	122.70
1	A	94	LYS	CA-C-N	-5.23	105.69	117.20
1	A	253	THR	OG1-CB-CG2	5.22	122.01	110.00
1	A	163	SER	CB-CA-C	5.21	120.00	110.10
1	A	69	ALA	CB-CA-C	5.20	117.90	110.10
1	A	126	LEU	CB-CG-CD2	-5.18	102.19	111.00
1	A	274	ALA	CB-CA-C	5.18	117.87	110.10
1	A	119	MET	CA-CB-CG	5.16	122.07	113.30
1	A	18	SER	CB-CA-C	5.12	119.83	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	VAL	CG1-CB-CG2	-5.12	102.71	110.90
1	A	200	ALA	CB-CA-C	5.11	117.77	110.10
1	A	139	VAL	N-CA-CB	5.11	122.74	111.50
1	A	58	PHE	CG-CD2-CE2	-5.09	115.19	120.80
1	A	10	GLN	O-C-N	5.07	130.81	122.70
1	A	245	GLN	CG-CD-OE1	5.03	131.67	121.60
1	A	173	SER	O-C-N	5.03	130.75	122.70
1	A	106	TRP	CB-CG-CD1	5.02	133.52	127.00
1	A	192	VAL	CA-CB-CG2	5.01	118.42	110.90
1	A	28	VAL	CA-CB-CG2	5.01	118.42	110.90
1	A	84	VAL	CG1-CB-CG2	-5.01	102.88	110.90
1	A	195	GLU	OE1-CD-OE2	-5.00	117.30	123.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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	1858	0	1817	36	0
2	A	4	0	6	0	0
3	A	155	0	0	8	0
All	All	2017	0	1823	36	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 10.

All (36) 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:73:LEU:HD13	1:A:90:LEU:HD22	1.61	0.81
1:A:104:TYR:HD2	3:A:2068:HOH:O	1.71	0.72
1:A:206:TRP:CD1	1:A:216:ALA:HB2	2.29	0.67
1:A:73:LEU:HD22	3:A:2026:HOH:O	2.00	0.61
1:A:240:ASN:HB3	3:A:2132:HOH:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ILE:HD11	3:A:2068:HOH:O	2.03	0.58
1:A:23:GLY:HA2	1:A:236:SER:HB3	1.86	0.58
1:A:240:ASN:HA	3:A:2131:HOH:O	2.04	0.56
1:A:31:ILE:HD12	1:A:122:ILE:HG23	1.87	0.56
1:A:115:ILE:HG12	1:A:142:ALA:HA	1.90	0.52
1:A:31:ILE:HD12	1:A:122:ILE:CG2	2.41	0.50
1:A:205:ILE:O	1:A:216:ALA:HA	2.11	0.50
1:A:73:LEU:CD1	1:A:90:LEU:HD22	2.38	0.50
1:A:122:ILE:HD12	1:A:147:VAL:HG11	1.94	0.50
1:A:158:THR:HG22	1:A:262:TYR:HE1	1.77	0.49
1:A:34:GLY:O	1:A:65:GLY:HA3	2.13	0.48
1:A:221:CSO:SG	1:A:222:MET:HE2	2.53	0.48
1:A:11:ILE:O	1:A:270:VAL:HG12	2.14	0.48
1:A:175:ILE:HG12	1:A:247:ARG:HG3	1.95	0.47
1:A:221:CSO:SG	1:A:222:MET:CE	3.05	0.45
1:A:104:TYR:HB3	3:A:2068:HOH:O	2.16	0.45
1:A:207:SER:O	1:A:214:TYR:HA	2.17	0.45
1:A:170:LYS:HE3	1:A:195:GLU:OE1	2.18	0.44
1:A:170:LYS:HG2	1:A:195:GLU:HG2	2.00	0.44
1:A:73:LEU:HD11	1:A:88:ALA:O	2.18	0.43
1:A:6:TYR:CE1	1:A:182:SER:HB2	2.53	0.43
1:A:180:VAL:HG21	1:A:267:LEU:HD13	2.01	0.43
1:A:119:MET:O	1:A:147:VAL:HG22	2.18	0.43
1:A:195:GLU:HB3	3:A:2095:HOH:O	2.19	0.42
1:A:249:SER:OG	1:A:275:GLN:NE2	2.53	0.42
1:A:127:GLY:HA2	1:A:167:TYR:O	2.21	0.41
1:A:143:VAL:HG21	1:A:173:SER:HB2	2.02	0.41
1:A:73:LEU:HD21	3:A:2040:HOH:O	2.21	0.41
1:A:172:PRO:O	1:A:247:ARG:NH1	2.47	0.41
1:A:47:GLY:HA3	1:A:92:ALA:O	2.21	0.40
1:A:35:ILE:O	1:A:58:PHE:HA	2.21	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	260/263 (99%)	253 (97%)	6 (2%)	1 (0%)	39	23

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	SER

### 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	194/194 (100%)	189 (97%)	5 (3%)	54	37

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	SER
1	A	32	ASP
1	A	73	LEU
1	A	204	SER
1	A	222	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
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	CSO	A	221	1	3,6,7	0.87	0	1,6,8	0.41	0

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	CSO	A	221	1	-	0/1/5/7	0/0/0/0

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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	221	CSO	2	0

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

1 ligand 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	$\# Z  > 2$
2	ACN	A	298	-	3,3,3	0.76	0	3,3,3	1.18	0

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	ACN	A	298	-	-	0/0/0/0	0/0/0/0

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 [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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	262/263 (99%)	-0.47	0 100 100	4, 8, 17, 24	0

There are no RSRZ outliers to report.

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	CSO	A	221	7/8	0.93	0.09	-	4,5,11,13	1

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ACN	A	298	4/4	0.95	0.09	-0.01	16,17,17,17	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.