



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2017 – 05:28 AM EST

PDB ID : 2SNS  
Title : STAPHYLOCOCCAL NUCLEASE. PROPOSED MECHANISM OF ACTION BASED ON STRUCTURE OF ENZYME-THYMIDINE 3(PRIME),5(PRIME)-BIPHOSPHATE-CALCIUM ION COMPLEX AT 1.5-ANGSTROMS RESOLUTION  
Authors : Legg, M.J.; Cotton, F.A.; Hazen Jr., E.E.  
Deposited on : unknown  
Resolution : 1.50 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

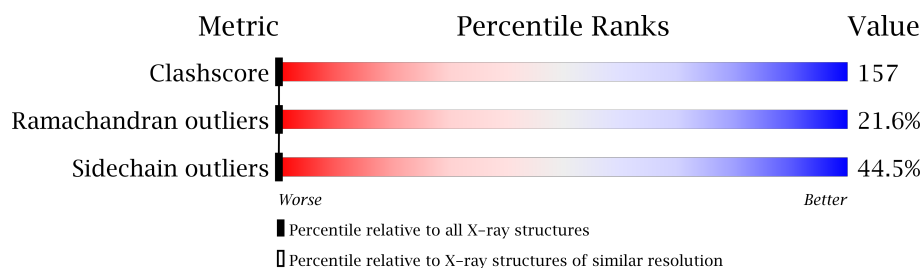
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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	112137	2503 (1.50-1.50)
Ramachandran outliers	110173	2445 (1.50-1.50)
Sidechain outliers	110143	2443 (1.50-1.50)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	149	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1151 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 THERMONUCLEASE PRECURSOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	0	0
			1125	717	199	205	4			

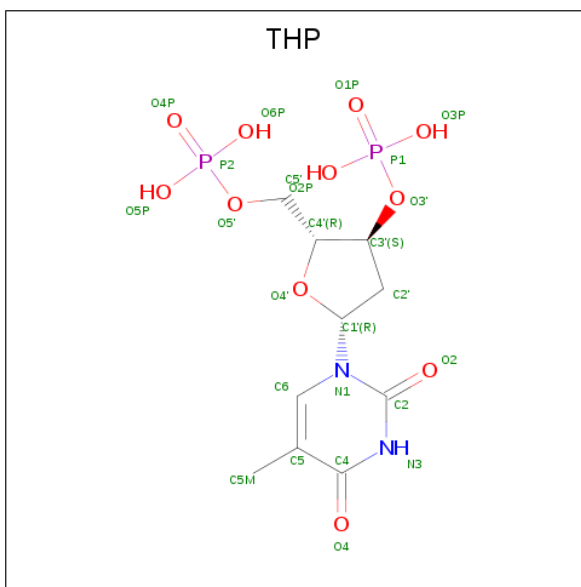
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	ASN	ASP	CONFLICT	UNP P00644
A	143	ASN	ASP	CONFLICT	UNP P00644
A	144	ASP	ASN	CONFLICT	UNP P00644

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is THYMIDINE-3',5'-DIPHOSPHATE (three-letter code: THP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>2</sub>O<sub>11</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			25	10	2	11	2		

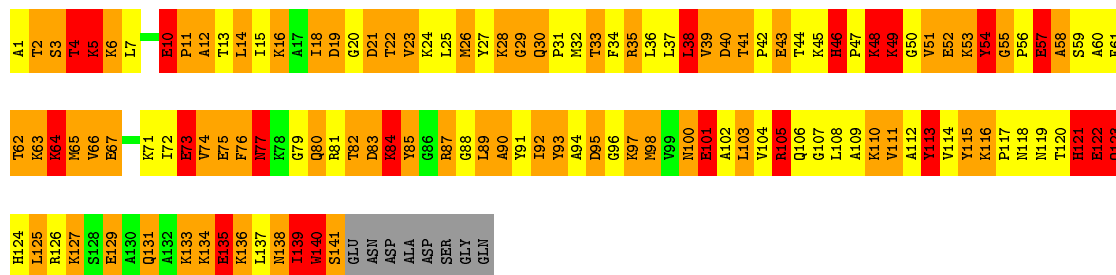
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: THERMONUCLEASE PRECURSOR

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 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.19 Å 48.19 Å 63.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	unknown	Depositor
R, $R_{free}$	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1151	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	0.0	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, THP

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	1.35	17/1146 (1.5%)	2.17	41/1536 (2.7%)

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	3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	76	PHE	CA-CB	-10.12	1.31	1.53
1	A	140	TRP	NE1-CE2	-7.54	1.27	1.37
1	A	123	GLN	CA-CB	6.93	1.69	1.53
1	A	52	GLU	CD-OE1	-6.33	1.18	1.25
1	A	55	GLY	CA-C	-6.05	1.42	1.51
1	A	75	GLU	CD-OE1	-6.02	1.19	1.25
1	A	122	GLU	CD-OE1	-5.82	1.19	1.25
1	A	57	GLU	CD-OE1	-5.78	1.19	1.25
1	A	73	GLU	CD-OE1	-5.76	1.19	1.25
1	A	101	GLU	CD-OE1	-5.72	1.19	1.25
1	A	131	GLN	CD-NE2	-5.42	1.19	1.32
1	A	46	HIS	CA-C	-5.15	1.39	1.52
1	A	138	ASN	CG-ND2	-5.10	1.20	1.32
1	A	27	TYR	CD1-CE1	5.10	1.47	1.39
1	A	129	GLU	CD-OE1	-5.07	1.20	1.25
1	A	67	GLU	CD-OE1	-5.03	1.20	1.25
1	A	135	GLU	CD-OE1	-5.01	1.20	1.25

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	76	PHE	CB-CG-CD2	-58.87	79.59	120.80
1	A	109	ALA	N-CA-CB	-15.82	87.95	110.10
1	A	46	HIS	N-CA-CB	-9.99	92.62	110.60
1	A	22	THR	N-CA-CB	-8.39	94.36	110.30
1	A	23	VAL	N-CA-CB	-8.07	93.75	111.50
1	A	38	LEU	N-CA-CB	7.76	125.92	110.40
1	A	21	ASP	CB-CG-OD1	7.46	125.02	118.30
1	A	34	PHE	N-CA-CB	-7.34	97.39	110.60
1	A	90	ALA	N-CA-CB	7.29	120.31	110.10
1	A	19	ASP	CB-CG-OD1	7.24	124.81	118.30
1	A	93	TYR	CB-CG-CD1	-7.06	116.77	121.00
1	A	95	ASP	CB-CG-OD1	6.93	124.54	118.30
1	A	131	GLN	CG-CD-OE1	-6.91	107.79	121.60
1	A	40	ASP	CB-CG-OD1	6.70	124.33	118.30
1	A	123	GLN	N-CA-C	6.69	129.07	111.00
1	A	129	GLU	OE1-CD-OE2	6.46	131.06	123.30
1	A	21	ASP	N-CA-C	6.28	127.96	111.00
1	A	67	GLU	OE1-CD-OE2	6.08	130.60	123.30
1	A	10	GLU	OE1-CD-OE2	6.04	130.54	123.30
1	A	21	ASP	N-CA-CB	-6.03	99.74	110.60
1	A	135	GLU	OE1-CD-OE2	5.96	130.45	123.30
1	A	57	GLU	OE1-CD-OE2	5.93	130.42	123.30
1	A	101	GLU	OE1-CD-OE2	5.84	130.31	123.30
1	A	122	GLU	OE1-CD-OE2	5.81	130.27	123.30
1	A	83	ASP	CB-CG-OD1	5.79	123.51	118.30
1	A	75	GLU	OE1-CD-OE2	5.66	130.10	123.30
1	A	54	TYR	CB-CG-CD1	-5.59	117.64	121.00
1	A	73	GLU	OE1-CD-OE2	5.58	130.00	123.30
1	A	52	GLU	OE1-CD-OE2	5.50	129.90	123.30
1	A	22	THR	N-CA-C	5.50	125.84	111.00
1	A	52	GLU	CG-CD-OE2	-5.45	107.41	118.30
1	A	113	TYR	CB-CG-CD1	-5.41	117.76	121.00
1	A	75	GLU	CG-CD-OE2	-5.37	107.56	118.30
1	A	57	GLU	CG-CD-OE2	-5.36	107.58	118.30
1	A	122	GLU	CG-CD-OE2	-5.30	107.69	118.30
1	A	135	GLU	CG-CD-OE2	-5.25	107.79	118.30
1	A	67	GLU	CG-CD-OE2	-5.23	107.83	118.30
1	A	73	GLU	CG-CD-OE2	-5.20	107.89	118.30
1	A	101	GLU	CG-CD-OE2	-5.20	107.89	118.30
1	A	129	GLU	CG-CD-OE2	-5.13	108.03	118.30
1	A	123	GLN	CA-C-N	-5.12	105.92	117.20



There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	ARG	Sidechain
1	A	76	PHE	Sidechain
1	A	87	ARG	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	1125	0	1172	366	0
2	A	1	0	0	0	0
3	A	25	0	12	1	0
All	All	1151	0	1184	366	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 157.

All (366) 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:48:LYS:CD	1:A:48:LYS:O	1.75	1.32
1:A:38:LEU:O	1:A:39:VAL:HG23	1.15	1.29
1:A:20:GLY:HA2	1:A:62:THR:CG2	1.62	1.29
1:A:138:ASN:O	1:A:141:SER:HB2	1.18	1.29
1:A:134:LYS:CB	1:A:134:LYS:NZ	1.94	1.28
1:A:91:TYR:HA	1:A:100:ASN:ND2	1.48	1.27
1:A:63:LYS:O	1:A:66:VAL:HG23	1.25	1.24
1:A:122:GLU:CD	1:A:126:ARG:HH21	1.39	1.24
1:A:72:ILE:HG23	1:A:93:TYR:O	1.10	1.22
1:A:112:ALA:CB	1:A:113:TYR:CE1	2.22	1.21
1:A:100:ASN:O	1:A:104:VAL:HG23	1.39	1.21
1:A:20:GLY:CA	1:A:62:THR:HG21	1.70	1.20
1:A:48:LYS:HD3	1:A:48:LYS:O	1.31	1.20
1:A:80:GLN:OE1	1:A:80:GLN:N	1.73	1.19
1:A:114:VAL:O	1:A:119:ASN:HB3	1.42	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:LYS:NZ	1:A:110:LYS:HB2	1.36	1.17
1:A:64:LYS:HG2	1:A:65:MET:N	1.53	1.16
1:A:134:LYS:HB3	1:A:134:LYS:NZ	1.23	1.15
1:A:134:LYS:CB	1:A:134:LYS:HZ2	1.55	1.13
1:A:122:GLU:OE2	1:A:126:ARG:NH2	1.81	1.13
1:A:62:THR:O	1:A:66:VAL:CG2	1.96	1.13
1:A:112:ALA:HB1	1:A:113:TYR:CE1	1.83	1.12
1:A:110:LYS:NZ	1:A:110:LYS:CB	2.12	1.11
1:A:113:TYR:HB3	1:A:115:TYR:HE2	0.98	1.10
1:A:62:THR:O	1:A:66:VAL:HG22	1.48	1.10
1:A:91:TYR:CA	1:A:100:ASN:HD21	1.64	1.10
1:A:47:PRO:O	1:A:49:LYS:N	1.83	1.10
1:A:84:LYS:O	1:A:84:LYS:HG2	1.53	1.08
1:A:113:TYR:HB3	1:A:115:TYR:CE2	1.86	1.08
1:A:46:HIS:CD2	1:A:48:LYS:HB3	1.88	1.08
1:A:101:GLU:HB2	1:A:125:LEU:HD12	1.23	1.08
1:A:43:GLU:HB3	1:A:49:LYS:HZ3	1.10	1.07
1:A:112:ALA:C	1:A:113:TYR:CD1	2.27	1.07
1:A:115:TYR:O	1:A:119:ASN:ND2	1.86	1.06
1:A:112:ALA:HB3	1:A:113:TYR:CE1	1.85	1.05
1:A:72:ILE:CG2	1:A:93:TYR:O	2.04	1.04
1:A:101:GLU:CB	1:A:125:LEU:HD12	1.86	1.04
1:A:38:LEU:O	1:A:39:VAL:CG2	2.05	1.03
1:A:138:ASN:O	1:A:141:SER:CB	2.06	1.03
1:A:14:LEU:HD22	1:A:15:ILE:N	1.74	1.01
1:A:64:LYS:O	1:A:67:GLU:N	1.95	1.00
1:A:112:ALA:C	1:A:113:TYR:HD1	1.64	1.00
1:A:28:LYS:O	1:A:29:GLY:O	1.80	1.00
1:A:122:GLU:OE2	1:A:126:ARG:NE	1.95	1.00
1:A:114:VAL:O	1:A:119:ASN:CB	2.09	0.99
1:A:112:ALA:CB	1:A:113:TYR:CD1	2.45	0.98
1:A:139:ILE:O	1:A:141:SER:N	1.96	0.98
1:A:110:LYS:HZ3	1:A:110:LYS:HB2	1.15	0.97
1:A:54:TYR:O	1:A:58:ALA:HB2	1.63	0.97
1:A:64:LYS:HG2	1:A:65:MET:H	1.11	0.96
1:A:43:GLU:CB	1:A:49:LYS:HZ3	1.77	0.96
1:A:101:GLU:HB2	1:A:125:LEU:CD1	1.95	0.96
1:A:46:HIS:HD2	1:A:48:LYS:HB3	1.27	0.95
1:A:26:MET:CE	1:A:31:PRO:N	2.29	0.95
1:A:134:LYS:HB2	1:A:134:LYS:HZ2	1.31	0.94
1:A:37:LEU:HD21	1:A:89:LEU:HB2	1.46	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:LYS:O	1:A:49:LYS:HB2	1.65	0.94
1:A:114:VAL:O	1:A:119:ASN:ND2	2.00	0.94
1:A:122:GLU:OE2	1:A:126:ARG:CZ	2.16	0.93
1:A:4:THR:HG22	1:A:5:LYS:H	1.30	0.93
1:A:36:LEU:CD2	1:A:92:ILE:HD13	1.99	0.93
1:A:131:GLN:HA	1:A:134:LYS:HD2	1.49	0.92
1:A:122:GLU:CD	1:A:126:ARG:NH2	2.21	0.92
1:A:43:GLU:HG3	1:A:49:LYS:NZ	1.85	0.92
1:A:61:PHE:CD2	1:A:103:LEU:CD1	2.53	0.91
1:A:63:LYS:HG2	1:A:64:LYS:N	1.85	0.91
1:A:97:LYS:HZ3	1:A:97:LYS:N	1.70	0.90
1:A:135:GLU:HG3	1:A:137:LEU:CD2	2.02	0.89
1:A:48:LYS:O	1:A:48:LYS:CG	2.18	0.89
1:A:42:PRO:HG3	1:A:54:TYR:O	1.72	0.89
1:A:110:LYS:HZ2	1:A:110:LYS:HB2	1.12	0.89
1:A:110:LYS:HZ3	1:A:110:LYS:CB	1.77	0.88
1:A:91:TYR:O	1:A:92:ILE:O	1.91	0.88
1:A:84:LYS:O	1:A:84:LYS:CG	2.20	0.88
1:A:37:LEU:CD2	1:A:89:LEU:HB2	2.03	0.87
1:A:101:GLU:CB	1:A:125:LEU:CD1	2.50	0.86
1:A:35:ARG:HB3	1:A:89:LEU:HD23	1.57	0.86
1:A:105:ARG:NH2	1:A:131:GLN:HG2	1.89	0.86
1:A:42:PRO:HG2	1:A:55:GLY:HA2	1.57	0.86
1:A:63:LYS:O	1:A:66:VAL:CG2	2.20	0.85
1:A:64:LYS:O	1:A:66:VAL:N	2.10	0.85
1:A:57:GLU:O	1:A:60:ALA:N	2.09	0.85
1:A:112:ALA:O	1:A:113:TYR:HD1	1.57	0.85
1:A:4:THR:CG2	1:A:5:LYS:N	2.39	0.84
1:A:20:GLY:HA2	1:A:62:THR:HG21	0.86	0.84
1:A:43:GLU:HG3	1:A:49:LYS:HZ1	1.40	0.84
1:A:134:LYS:HB3	1:A:134:LYS:HZ3	0.87	0.84
1:A:120:THR:O	1:A:120:THR:HG22	1.76	0.84
1:A:64:LYS:CG	1:A:65:MET:N	2.36	0.83
1:A:26:MET:HE3	1:A:30:GLN:C	1.99	0.83
1:A:112:ALA:HB3	1:A:113:TYR:HE1	1.36	0.83
1:A:55:GLY:H	1:A:56:PRO:HD2	1.42	0.83
1:A:139:ILE:C	1:A:141:SER:H	1.79	0.82
1:A:26:MET:CE	1:A:30:GLN:C	2.47	0.82
1:A:4:THR:HG22	1:A:5:LYS:N	1.93	0.82
1:A:49:LYS:HB3	1:A:49:LYS:NZ	1.94	0.82
1:A:43:GLU:CG	1:A:49:LYS:NZ	2.43	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:GLU:HG3	1:A:137:LEU:HD23	1.62	0.81
1:A:131:GLN:NE2	1:A:134:LYS:CD	2.43	0.81
1:A:21:ASP:HB3	1:A:41:THR:OG1	1.80	0.81
1:A:55:GLY:N	1:A:56:PRO:HD2	1.94	0.81
1:A:80:GLN:H	1:A:80:GLN:CD	1.83	0.81
1:A:111:VAL:CG1	1:A:129:GLU:OE2	2.29	0.80
1:A:131:GLN:NE2	1:A:134:LYS:HD2	1.97	0.80
1:A:6:LYS:HG3	1:A:7:LEU:H	1.46	0.80
1:A:91:TYR:HA	1:A:100:ASN:HD21	0.71	0.79
1:A:112:ALA:HB3	1:A:113:TYR:CD1	2.13	0.79
1:A:35:ARG:O	1:A:89:LEU:HA	1.83	0.78
1:A:43:GLU:CG	1:A:49:LYS:CE	2.61	0.78
1:A:77:ASN:OD1	1:A:118:ASN:C	2.21	0.78
1:A:97:LYS:N	1:A:97:LYS:NZ	2.31	0.78
1:A:83:ASP:OD1	1:A:85:TYR:HB2	1.84	0.77
1:A:75:GLU:O	1:A:90:ALA:HB1	1.84	0.77
1:A:54:TYR:CD1	1:A:138:ASN:HB3	2.19	0.77
1:A:114:VAL:HG21	1:A:122:GLU:OE1	1.85	0.77
1:A:29:GLY:O	1:A:30:GLN:HB2	1.85	0.77
1:A:97:LYS:CA	1:A:97:LYS:NZ	2.47	0.77
1:A:61:PHE:HD2	1:A:103:LEU:CD1	1.98	0.76
1:A:63:LYS:NZ	1:A:67:GLU:OE2	2.17	0.76
1:A:14:LEU:C	1:A:14:LEU:HD22	2.05	0.76
1:A:97:LYS:HZ3	1:A:97:LYS:CA	1.98	0.76
1:A:123:GLN:HA	1:A:126:ARG:HG3	1.67	0.76
1:A:43:GLU:CB	1:A:49:LYS:NZ	2.49	0.76
1:A:111:VAL:CG1	1:A:129:GLU:CD	2.54	0.75
1:A:49:LYS:HB3	1:A:49:LYS:HZ2	1.53	0.74
1:A:38:LEU:HA	1:A:113:TYR:O	1.87	0.74
1:A:62:THR:O	1:A:66:VAL:HG23	1.88	0.73
1:A:4:THR:O	1:A:5:LYS:CB	2.37	0.73
1:A:36:LEU:HD23	1:A:92:ILE:HD13	1.70	0.73
1:A:91:TYR:O	1:A:92:ILE:C	2.27	0.73
1:A:112:ALA:HB1	1:A:113:TYR:CD1	2.17	0.73
1:A:63:LYS:HG2	1:A:64:LYS:H	1.53	0.72
1:A:131:GLN:O	1:A:135:GLU:HG2	1.88	0.72
1:A:133:LYS:HG3	1:A:140:TRP:CD2	2.24	0.72
1:A:111:VAL:HG12	1:A:129:GLU:CD	2.10	0.72
1:A:4:THR:O	1:A:5:LYS:HB2	1.90	0.72
1:A:29:GLY:O	1:A:30:GLN:CB	2.38	0.72
1:A:3:SER:O	1:A:5:LYS:N	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:VAL:CG2	1:A:122:GLU:OE1	2.37	0.71
1:A:114:VAL:O	1:A:119:ASN:CG	2.29	0.71
1:A:100:ASN:N	1:A:100:ASN:OD1	2.23	0.71
1:A:134:LYS:CB	1:A:134:LYS:HZ3	1.78	0.71
1:A:3:SER:O	1:A:4:THR:C	2.28	0.71
1:A:62:THR:HG22	1:A:103:LEU:HD21	1.71	0.71
1:A:42:PRO:CG	1:A:54:TYR:O	2.39	0.71
1:A:43:GLU:HB3	1:A:49:LYS:NZ	1.97	0.70
1:A:53:LYS:O	1:A:54:TYR:HB2	1.91	0.70
1:A:111:VAL:O	1:A:111:VAL:HG22	1.92	0.70
1:A:20:GLY:HA3	1:A:41:THR:HG21	1.73	0.70
1:A:48:LYS:HD2	1:A:48:LYS:O	1.86	0.70
1:A:80:GLN:N	1:A:118:ASN:HD21	1.89	0.69
1:A:66:VAL:HG12	1:A:72:ILE:HD13	1.74	0.69
1:A:61:PHE:CD2	1:A:103:LEU:HD11	2.27	0.69
1:A:72:ILE:HG22	1:A:73:GLU:N	2.07	0.69
1:A:122:GLU:OE1	1:A:126:ARG:NH2	2.23	0.69
1:A:113:TYR:CD1	1:A:113:TYR:N	2.61	0.69
1:A:105:ARG:NH2	1:A:131:GLN:CG	2.54	0.69
1:A:131:GLN:NE2	1:A:134:LYS:HD3	2.06	0.69
1:A:37:LEU:CD2	1:A:89:LEU:CB	2.71	0.69
1:A:45:LYS:O	1:A:46:HIS:O	2.11	0.68
1:A:5:LYS:O	1:A:6:LYS:HB3	1.91	0.68
1:A:133:LYS:HE2	1:A:140:TRP:CZ3	2.28	0.68
1:A:135:GLU:HG3	1:A:137:LEU:HD21	1.74	0.68
1:A:139:ILE:C	1:A:141:SER:N	2.41	0.68
1:A:6:LYS:HG3	1:A:7:LEU:N	2.08	0.68
1:A:98:MET:O	1:A:102:ALA:N	2.16	0.68
1:A:131:GLN:HA	1:A:134:LYS:CD	2.24	0.68
1:A:100:ASN:O	1:A:104:VAL:CG2	2.31	0.67
1:A:36:LEU:HD21	1:A:92:ILE:HD13	1.75	0.67
1:A:5:LYS:O	1:A:6:LYS:CB	2.42	0.67
1:A:57:GLU:O	1:A:59:SER:N	2.28	0.67
1:A:96:GLY:C	1:A:97:LYS:NZ	2.48	0.67
1:A:14:LEU:CD2	1:A:15:ILE:N	2.56	0.67
1:A:46:HIS:HD2	1:A:48:LYS:CB	2.05	0.66
1:A:120:THR:CG2	1:A:120:THR:O	2.44	0.66
1:A:51:VAL:CG1	1:A:51:VAL:O	2.43	0.66
1:A:64:LYS:O	1:A:65:MET:C	2.34	0.66
1:A:54:TYR:CE2	1:A:139:ILE:HA	2.31	0.65
1:A:123:GLN:N	1:A:123:GLN:OE1	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:GLN:O	1:A:138:ASN:ND2	2.31	0.64
1:A:19:ASP:HA	1:A:59:SER:HB3	1.79	0.64
1:A:61:PHE:CD2	1:A:103:LEU:HD13	2.32	0.64
1:A:77:ASN:HD21	1:A:120:THR:HB	1.63	0.64
1:A:131:GLN:HE21	1:A:134:LYS:HD2	1.62	0.63
1:A:21:ASP:OD2	1:A:22:THR:OG1	2.07	0.63
1:A:97:LYS:HZ3	1:A:97:LYS:CB	2.10	0.63
1:A:80:GLN:N	1:A:118:ASN:ND2	2.46	0.63
1:A:53:LYS:O	1:A:54:TYR:CB	2.47	0.62
1:A:38:LEU:HA	1:A:112:ALA:O	2.00	0.62
1:A:49:LYS:NZ	1:A:49:LYS:CB	2.62	0.62
1:A:101:GLU:HB3	1:A:125:LEU:CD1	2.29	0.62
1:A:123:GLN:HA	1:A:126:ARG:CG	2.30	0.62
1:A:97:LYS:HZ2	1:A:97:LYS:HA	1.64	0.62
1:A:101:GLU:HG3	1:A:102:ALA:N	2.15	0.62
1:A:51:VAL:HG13	1:A:51:VAL:O	1.99	0.62
1:A:131:GLN:O	1:A:134:LYS:HG2	2.00	0.62
1:A:77:ASN:OD1	1:A:119:ASN:N	2.32	0.61
1:A:43:GLU:HG2	1:A:48:LYS:NZ	2.14	0.61
1:A:77:ASN:HD21	1:A:120:THR:H	1.48	0.61
1:A:133:LYS:HG3	1:A:140:TRP:CG	2.35	0.61
1:A:28:LYS:O	1:A:29:GLY:C	2.38	0.61
1:A:101:GLU:HB3	1:A:125:LEU:HD11	1.83	0.60
1:A:91:TYR:CA	1:A:100:ASN:ND2	2.40	0.60
1:A:48:LYS:C	1:A:48:LYS:CD	2.67	0.60
1:A:43:GLU:CG	1:A:49:LYS:HE2	2.31	0.59
1:A:26:MET:HE3	1:A:31:PRO:N	2.12	0.59
1:A:134:LYS:HB3	1:A:134:LYS:HZ2	1.18	0.59
1:A:15:ILE:HG22	1:A:16:LYS:N	2.17	0.59
1:A:84:LYS:O	1:A:85:TYR:CG	2.56	0.59
1:A:43:GLU:HG2	1:A:49:LYS:CE	2.32	0.58
1:A:36:LEU:CD2	1:A:92:ILE:CD1	2.77	0.58
1:A:36:LEU:HD23	1:A:92:ILE:CD1	2.34	0.58
1:A:127:LYS:HB2	1:A:127:LYS:NZ	2.19	0.58
1:A:57:GLU:C	1:A:59:SER:N	2.56	0.58
1:A:54:TYR:O	1:A:58:ALA:CB	2.45	0.58
1:A:72:ILE:CG2	1:A:73:GLU:N	2.67	0.58
1:A:26:MET:HE2	1:A:30:GLN:C	2.25	0.57
1:A:26:MET:CE	1:A:31:PRO:CA	2.82	0.57
1:A:55:GLY:N	1:A:56:PRO:CD	2.67	0.57
1:A:125:LEU:HD22	1:A:125:LEU:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ALA:O	1:A:113:TYR:CD1	2.45	0.57
1:A:6:LYS:HG3	1:A:7:LEU:HG	1.86	0.57
1:A:114:VAL:O	1:A:115:TYR:O	2.23	0.56
1:A:133:LYS:HE2	1:A:140:TRP:CE3	2.40	0.56
1:A:107:GLY:O	1:A:139:ILE:HG13	2.06	0.56
1:A:77:ASN:ND2	1:A:120:THR:HB	2.20	0.56
1:A:26:MET:CE	1:A:31:PRO:CD	2.84	0.56
1:A:97:LYS:CB	1:A:97:LYS:NZ	2.69	0.56
1:A:112:ALA:CB	1:A:113:TYR:HE1	1.92	0.56
1:A:1:ALA:O	1:A:2:THR:C	2.43	0.56
1:A:122:GLU:HB3	1:A:123:GLN:OE1	2.06	0.56
1:A:114:VAL:HB	1:A:122:GLU:OE1	2.06	0.56
1:A:43:GLU:HG2	1:A:49:LYS:HE2	1.87	0.56
1:A:22:THR:C	1:A:23:VAL:HG12	2.26	0.56
1:A:26:MET:HE1	1:A:31:PRO:N	2.19	0.56
1:A:111:VAL:CG2	1:A:111:VAL:O	2.54	0.55
1:A:114:VAL:CB	1:A:122:GLU:OE1	2.54	0.55
1:A:71:LYS:O	1:A:72:ILE:HG13	2.07	0.55
1:A:82:THR:HA	1:A:88:GLY:HA2	1.89	0.55
1:A:14:LEU:CD2	1:A:14:LEU:C	2.75	0.55
1:A:63:LYS:CG	1:A:64:LYS:N	2.57	0.55
1:A:61:PHE:HD2	1:A:103:LEU:HD11	1.66	0.55
1:A:64:LYS:C	1:A:66:VAL:N	2.61	0.54
1:A:64:LYS:HA	1:A:67:GLU:HB2	1.89	0.54
1:A:22:THR:C	1:A:23:VAL:CG1	2.71	0.54
1:A:43:GLU:H	1:A:52:GLU:CD	2.09	0.54
1:A:63:LYS:C	1:A:66:VAL:HG23	2.20	0.54
1:A:64:LYS:CG	1:A:65:MET:H	2.00	0.54
1:A:57:GLU:C	1:A:59:SER:H	2.10	0.54
1:A:61:PHE:HD2	1:A:103:LEU:HD13	1.71	0.53
1:A:129:GLU:O	1:A:133:LYS:HB2	2.08	0.53
1:A:26:MET:HE1	1:A:31:PRO:CA	2.38	0.53
1:A:66:VAL:HG12	1:A:72:ILE:CD1	2.38	0.53
1:A:111:VAL:HG13	1:A:129:GLU:CD	2.29	0.53
1:A:43:GLU:CB	1:A:49:LYS:HE2	2.38	0.53
1:A:47:PRO:C	1:A:49:LYS:N	2.60	0.53
1:A:51:VAL:HG22	1:A:56:PRO:HD3	1.91	0.53
1:A:111:VAL:HG13	1:A:129:GLU:OE2	2.07	0.53
1:A:83:ASP:O	1:A:85:TYR:N	2.42	0.53
1:A:133:LYS:HG2	1:A:140:TRP:HB3	1.91	0.52
1:A:121:HIS:O	1:A:125:LEU:HD22	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:GLU:CB	1:A:49:LYS:CE	2.87	0.52
1:A:42:PRO:CG	1:A:55:GLY:HA2	2.34	0.52
1:A:131:GLN:HA	1:A:134:LYS:HG2	1.92	0.52
1:A:26:MET:HE2	1:A:31:PRO:N	2.20	0.51
1:A:93:TYR:CE1	1:A:98:MET:HG2	2.45	0.51
1:A:35:ARG:HD2	1:A:36:LEU:H	1.75	0.51
1:A:79:GLY:C	1:A:118:ASN:HD21	2.14	0.51
1:A:19:ASP:OD2	1:A:19:ASP:N	2.42	0.51
1:A:46:HIS:CD2	1:A:48:LYS:CB	2.78	0.51
1:A:43:GLU:HG2	1:A:48:LYS:HZ2	1.76	0.51
1:A:48:LYS:O	1:A:48:LYS:HG2	2.09	0.50
1:A:53:LYS:O	1:A:54:TYR:CD2	2.64	0.50
1:A:35:ARG:HH21	3:A:151:THP:P2	2.33	0.50
1:A:21:ASP:C	1:A:22:THR:OG1	2.49	0.50
1:A:43:GLU:HB2	1:A:49:LYS:HE2	1.92	0.50
1:A:101:GLU:CA	1:A:125:LEU:HD12	2.41	0.50
1:A:43:GLU:HG3	1:A:49:LYS:CE	2.34	0.50
1:A:38:LEU:HD13	1:A:125:LEU:HD23	1.93	0.49
1:A:112:ALA:CA	1:A:113:TYR:CD1	2.95	0.49
1:A:20:GLY:C	1:A:62:THR:HG21	2.30	0.49
1:A:84:LYS:O	1:A:85:TYR:CD1	2.66	0.49
1:A:75:GLU:O	1:A:90:ALA:CB	2.55	0.49
1:A:138:ASN:O	1:A:141:SER:N	2.40	0.49
1:A:24:LYS:HG2	1:A:33:THR:HG22	1.93	0.48
1:A:110:LYS:HZ3	1:A:110:LYS:HB3	1.72	0.48
1:A:75:GLU:HB2	1:A:93:TYR:CE2	2.48	0.48
1:A:37:LEU:HG	1:A:89:LEU:C	2.34	0.48
1:A:94:ALA:O	1:A:97:LYS:HB2	2.13	0.48
1:A:121:HIS:O	1:A:122:GLU:O	2.32	0.48
1:A:37:LEU:CG	1:A:89:LEU:HB2	2.44	0.48
1:A:26:MET:HE2	1:A:30:GLN:CA	2.43	0.48
1:A:43:GLU:OE2	1:A:45:LYS:O	2.31	0.47
1:A:43:GLU:N	1:A:52:GLU:CD	2.67	0.47
1:A:137:LEU:O	1:A:138:ASN:C	2.51	0.47
1:A:42:PRO:CG	1:A:58:ALA:CB	2.92	0.47
1:A:91:TYR:CE1	1:A:121:HIS:HB2	2.49	0.47
1:A:4:THR:HG23	1:A:5:LYS:N	2.27	0.47
1:A:75:GLU:HB2	1:A:93:TYR:HE2	1.79	0.47
1:A:26:MET:HE2	1:A:31:PRO:CD	2.45	0.47
1:A:15:ILE:HG22	1:A:16:LYS:HB2	1.97	0.47
1:A:94:ALA:O	1:A:95:ASP:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:PRO:CG	1:A:58:ALA:HB2	2.45	0.46
1:A:26:MET:HE2	1:A:31:PRO:HD3	1.97	0.46
1:A:10:GLU:O	1:A:74:VAL:N	2.46	0.46
1:A:65:MET:CE	1:A:97:LYS:HB3	2.45	0.46
1:A:38:LEU:HD23	1:A:119:ASN:HB2	1.97	0.46
1:A:63:LYS:O	1:A:64:LYS:C	2.54	0.46
1:A:131:GLN:HE22	1:A:134:LYS:HD3	1.79	0.46
1:A:98:MET:HB2	1:A:101:GLU:HG2	1.97	0.46
1:A:49:LYS:HB3	1:A:50:GLY:H	1.49	0.46
1:A:80:GLN:CD	1:A:80:GLN:N	2.54	0.45
1:A:5:LYS:HA	1:A:5:LYS:HD2	1.48	0.45
1:A:131:GLN:HA	1:A:134:LYS:CG	2.46	0.45
1:A:42:PRO:O	1:A:43:GLU:C	2.54	0.45
1:A:37:LEU:HG	1:A:89:LEU:CB	2.46	0.45
1:A:29:GLY:O	1:A:30:GLN:CG	2.65	0.45
1:A:138:ASN:O	1:A:139:ILE:C	2.54	0.45
1:A:38:LEU:O	1:A:39:VAL:CB	2.62	0.45
1:A:122:GLU:O	1:A:124:HIS:N	2.50	0.44
1:A:45:LYS:O	1:A:46:HIS:HB3	2.17	0.44
1:A:116:LYS:HA	1:A:117:PRO:HA	1.56	0.44
1:A:131:GLN:O	1:A:135:GLU:CG	2.63	0.44
1:A:54:TYR:CE1	1:A:138:ASN:HB3	2.53	0.44
1:A:52:GLU:O	1:A:53:LYS:C	2.56	0.44
1:A:83:ASP:C	1:A:83:ASP:OD1	2.56	0.44
1:A:10:GLU:O	1:A:73:GLU:HA	2.18	0.44
1:A:14:LEU:HA	1:A:25:LEU:HD23	1.99	0.44
1:A:46:HIS:HA	1:A:47:PRO:HD2	1.65	0.43
1:A:11:PRO:O	1:A:12:ALA:HB2	2.18	0.43
1:A:18:ILE:HG13	1:A:22:THR:HG22	2.00	0.43
1:A:103:LEU:HA	1:A:103:LEU:HD12	1.77	0.43
1:A:21:ASP:OD2	1:A:21:ASP:C	2.56	0.43
1:A:37:LEU:O	1:A:38:LEU:C	2.56	0.43
1:A:114:VAL:O	1:A:114:VAL:HG23	2.19	0.43
1:A:79:GLY:CA	1:A:118:ASN:ND2	2.80	0.43
1:A:26:MET:HE3	1:A:30:GLN:O	2.17	0.43
1:A:26:MET:CE	1:A:31:PRO:HD3	2.48	0.43
1:A:43:GLU:CG	1:A:48:LYS:HZ2	2.31	0.43
1:A:57:GLU:O	1:A:58:ALA:C	2.58	0.43
1:A:71:LYS:C	1:A:72:ILE:HG13	2.39	0.43
1:A:98:MET:HB3	1:A:101:GLU:CG	2.49	0.42
1:A:15:ILE:HB	1:A:24:LYS:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ARG:HD2	1:A:36:LEU:N	2.34	0.42
1:A:46:HIS:HD2	1:A:48:LYS:HD2	1.84	0.42
1:A:105:ARG:HH21	1:A:131:GLN:HG2	1.79	0.42
1:A:107:GLY:O	1:A:138:ASN:HB2	2.20	0.42
1:A:79:GLY:C	1:A:118:ASN:ND2	2.73	0.42
1:A:139:ILE:O	1:A:140:TRP:C	2.56	0.42
1:A:37:LEU:HD21	1:A:89:LEU:CD1	2.50	0.42
1:A:37:LEU:O	1:A:38:LEU:O	2.38	0.42
1:A:6:LYS:CG	1:A:7:LEU:H	2.12	0.41
1:A:108:LEU:HD23	1:A:138:ASN:ND2	2.36	0.41
1:A:98:MET:CB	1:A:101:GLU:HG2	2.49	0.41
1:A:18:ILE:CG1	1:A:22:THR:O	2.69	0.41
1:A:91:TYR:HB3	1:A:98:MET:SD	2.61	0.41
1:A:42:PRO:HG2	1:A:58:ALA:CB	2.50	0.41
1:A:26:MET:HE3	1:A:31:PRO:CA	2.50	0.41
1:A:105:ARG:CZ	1:A:131:GLN:HG2	2.46	0.41
1:A:40:ASP:HB2	1:A:113:TYR:HE1	1.86	0.41
1:A:18:ILE:HG13	1:A:22:THR:O	2.20	0.41
1:A:48:LYS:HD3	1:A:49:LYS:HB2	2.02	0.41
1:A:81:ARG:C	1:A:82:THR:CG2	2.89	0.40
1:A:125:LEU:HD13	1:A:125:LEU:N	2.36	0.40
1:A:62:THR:O	1:A:63:LYS:O	2.39	0.40
1:A:42:PRO:HD2	1:A:58:ALA:HB1	2.03	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	139/149 (93%)	89 (64%)	20 (14%)	30 (22%)	<b>0</b> <b>0</b>

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	5	LYS
1	A	6	LYS
1	A	29	GLY
1	A	30	GLN
1	A	39	VAL
1	A	46	HIS
1	A	48	LYS
1	A	49	LYS
1	A	63	LYS
1	A	65	MET
1	A	92	ILE
1	A	115	TYR
1	A	122	GLU
1	A	123	GLN
1	A	136	LYS
1	A	139	ILE
1	A	140	TRP
1	A	2	THR
1	A	58	ALA
1	A	77	ASN
1	A	85	TYR
1	A	113	TYR
1	A	11	PRO
1	A	38	LEU
1	A	84	LYS
1	A	121	HIS
1	A	12	ALA
1	A	54	TYR
1	A	64	LYS

### 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	119/125 (95%)	66 (56%)	53 (44%)	<b>0</b> <b>0</b>

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	4	THR
1	A	5	LYS
1	A	10	GLU
1	A	13	THR
1	A	14	LEU
1	A	16	LYS
1	A	18	ILE
1	A	26	MET
1	A	28	LYS
1	A	32	MET
1	A	33	THR
1	A	35	ARG
1	A	38	LEU
1	A	41	THR
1	A	43	GLU
1	A	44	THR
1	A	48	LYS
1	A	49	LYS
1	A	51	VAL
1	A	53	LYS
1	A	57	GLU
1	A	62	THR
1	A	64	LYS
1	A	66	VAL
1	A	73	GLU
1	A	74	VAL
1	A	77	ASN
1	A	80	GLN
1	A	82	THR
1	A	84	LYS
1	A	87	ARG
1	A	89	LEU
1	A	97	LYS
1	A	98	MET
1	A	100	ASN
1	A	101	GLU
1	A	103	LEU
1	A	105	ARG
1	A	110	LYS
1	A	111	VAL
1	A	113	TYR

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Mol	Chain	Res	Type
1	A	116	LYS
1	A	121	HIS
1	A	123	GLN
1	A	125	LEU
1	A	127	LYS
1	A	133	LYS
1	A	134	LYS
1	A	135	GLU
1	A	136	LYS
1	A	139	ILE
1	A	141	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	HIS
1	A	124	HIS
1	A	131	GLN
1	A	138	ASN

### 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 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	THP	A	151	1,2	21,26,26	5.21	13 (61%)	30,40,40	2.46	10 (33%)

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	THP	A	151	1,2	-	0/11/27/27	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	151	THP	O4'-C1'	-5.45	1.30	1.42
3	A	151	THP	P1-O3'	-5.02	1.50	1.59
3	A	151	THP	C5M-C5	-4.61	1.42	1.51
3	A	151	THP	C2-N3	-2.34	1.33	1.38
3	A	151	THP	C2'-C1'	2.83	1.60	1.52
3	A	151	THP	P1-O2P	2.87	1.66	1.54
3	A	151	THP	O4'-C4'	4.66	1.55	1.45
3	A	151	THP	C2'-C3'	4.69	1.63	1.52
3	A	151	THP	P1-O1P	5.35	1.68	1.50
3	A	151	THP	P2-O6P	5.44	1.77	1.54
3	A	151	THP	O4-C4	6.02	1.39	1.24
3	A	151	THP	P2-O5'	9.75	1.91	1.60
3	A	151	THP	C4-N3	15.14	1.60	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	151	THP	C4-N3-C2	-9.02	107.27	115.16
3	A	151	THP	C5-C6-N1	-4.42	117.36	122.15
3	A	151	THP	C2'-C1'-N1	-3.46	106.06	114.23
3	A	151	THP	O2P-P1-O1P	-2.66	100.08	110.50
3	A	151	THP	C5'-C4'-C3'	-2.24	109.42	114.57
3	A	151	THP	O5P-P2-O5'	-2.19	100.91	106.73
3	A	151	THP	C2'-C3'-C4'	2.07	107.09	102.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	151	THP	O6P-P2-O5P	2.21	116.52	107.61
3	A	151	THP	O4'-C1'-C2'	2.47	110.98	106.25
3	A	151	THP	O3P-P1-O3'	2.66	118.10	106.00

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
3	A	151	THP	1	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 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.