



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2021 – 03:48 PM EDT

PDB ID : 1EVW  
Title : L116A MUTANT OF THE HOMING ENDONUCLEASE I-PPOI COM-  
PLEXED TO HOMING SITE DNA.  
Authors : Galburt, E.A.; Jurica, M.S.; Chevalier, B.S.; Erho, D.; Stoddard, B.L.  
Deposited on : 2000-04-20  
Resolution : 3.10 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

<https://www.wwpdb.org/validation/2017/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  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

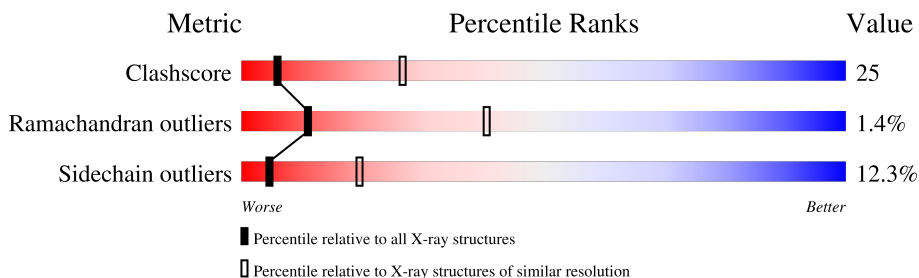
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)





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  $\geq 3$ , 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	E	12	17% 75% 8%
1	G	12	8% 92%
2	M	8	50% 25% 25%
2	N	8	25% 62% 12%
3	F	12	42% 58%
3	H	12	25% 67% 8%
4	O	8	25% 25% 50%
4	P	8	12% 25% 62%

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Mol	Chain	Length	Quality of chain
5	A	163	 58% 36% 6% .
5	B	163	 58% 37% . . .
5	C	163	 55% 39% 6% .
5	D	163	 57% 36% 7% .

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6612 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 DNA chain called DNA (5'-D(\*TP\*GP\*GP\*CP\*TP\*AP\*CP\*CP\*TP\*TP\*AP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	E	12	Total	C	N	O	P	0	0	0
			241	117	42	71	11			
1	G	12	Total	C	N	O	P	0	0	0
			241	117	42	71	11			

- Molecule 2 is a DNA chain called DNA (5'-D(P\*GP\*AP\*GP\*AP\*GP\*TP\*CP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	M	8	Total	C	N	O	P	0	0	0
			169	79	35	47	8			
2	N	8	Total	C	N	O	P	0	0	0
			169	79	35	47	8			

- Molecule 3 is a DNA chain called DNA (5'-D(\*TP\*GP\*AP\*CP\*TP\*CP\*TP\*CP\*TP\*TP\*AP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	F	12	Total	C	N	O	P	0	0	0
			239	117	39	72	11			
3	H	12	Total	C	N	O	P	0	0	0
			239	117	39	72	11			

- Molecule 4 is a DNA chain called DNA (5'-D(P\*GP\*GP\*TP\*AP\*GP\*CP\*CP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	O	8	Total	C	N	O	P	0	0	0
			167	78	33	48	8			
4	P	8	Total	C	N	O	P	0	0	0
			167	78	33	48	8			

- Molecule 5 is a protein called I-PPOI HOMING ENDONUCLEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	A	162	1242	783	232	219	8	0	0	0
5	B	162	1242	783	232	219	8	0	0	0
5	C	162	1242	783	232	219	8	0	0	0
5	D	162	1242	783	232	219	8	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	116	ALA	LEU	engineered mutation	UNP Q94702
B	116	ALA	LEU	engineered mutation	UNP Q94702
C	116	ALA	LEU	engineered mutation	UNP Q94702
D	116	ALA	LEU	engineered mutation	UNP Q94702

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	N	1	1	1	0	0
6	P	1	1	1	0	0
6	A	1	1	1	0	0
6	B	1	1	1	0	0

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
7	A	2	2	2	0	0
7	B	2	2	2	0	0
7	C	2	2	2	0	0
7	D	2	2	2	0	0

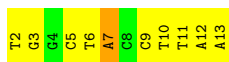
### 3 Residue-property plots [i](#)

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.

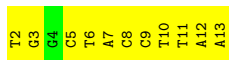
- Molecule 1: DNA (5'-D(\*TP\*GP\*GP\*CP\*TP\*AP\*CP\*CP\*TP\*TP\*AP\*A)-3')

Chain E: 



- Molecule 1: DNA (5'-D(\*TP\*GP\*GP\*CP\*TP\*AP\*CP\*CP\*TP\*TP\*AP\*A)-3')

Chain G: 



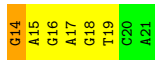
- Molecule 2: DNA (5'-D(P\*GP\*AP\*GP\*AP\*GP\*TP\*CP\*A)-3')

Chain M: 



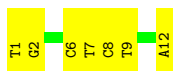
- Molecule 2: DNA (5'-D(P\*GP\*AP\*GP\*AP\*GP\*TP\*CP\*A)-3')

Chain N: 

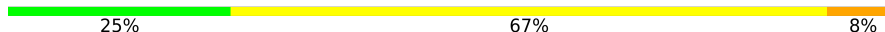


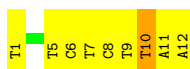
- Molecule 3: DNA (5'-D(\*TP\*GP\*AP\*CP\*TP\*CP\*TP\*CP\*TP\*TP\*AP\*A)-3')

Chain F: 

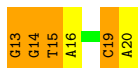
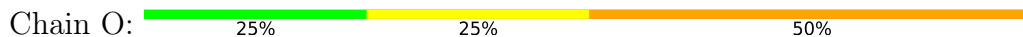


- Molecule 3: DNA (5'-D(\*TP\*GP\*AP\*CP\*TP\*CP\*TP\*CP\*TP\*TP\*AP\*A)-3')

Chain H: 



- Molecule 4: DNA (5'-D(P\*GP\*GP\*TP\*AP\*GP\*CP\*CP\*A)-3')



- Molecule 4: DNA (5'-D(P\*GP\*GP\*TP\*AP\*GP\*CP\*CP\*A)-3')



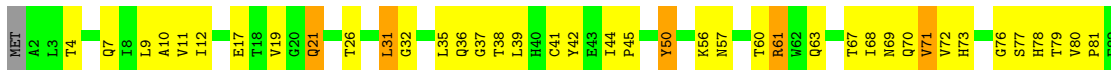
- Molecule 5: I-PPOI HOMING ENDONUCLEASE



- Molecule 5: I-PPOI HOMING ENDONUCLEASE

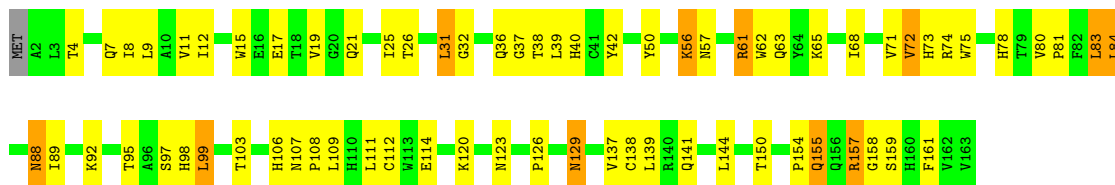


- Molecule 5: I-PPOI HOMING ENDONUCLEASE



- Molecule 5: I-PPOI HOMING ENDONUCLEASE







## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	182.00Å 73.10Å 92.70Å 90.00° 95.40° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-3.10)	Depositor
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.273 , 0.320	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	6612	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	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: MG, ZN

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	0.48	0/269	0.74	0/413
1	G	0.61	0/269	0.95	0/413
2	M	0.81	1/190 (0.5%)	0.74	0/290
2	N	0.98	1/190 (0.5%)	0.91	0/290
3	F	0.50	0/266	0.78	0/408
3	H	0.56	0/266	0.79	0/408
4	O	0.97	1/187 (0.5%)	0.99	0/285
4	P	0.95	2/187 (1.1%)	1.10	1/285 (0.4%)
5	A	0.56	0/1283	0.75	2/1756 (0.1%)
5	B	0.63	2/1283 (0.2%)	0.78	2/1756 (0.1%)
5	C	0.55	0/1283	0.68	0/1756
5	D	0.64	3/1283 (0.2%)	0.79	3/1756 (0.2%)
All	All	0.63	10/6956 (0.1%)	0.79	8/9816 (0.1%)

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	E	0	1
2	M	0	1
3	H	0	1
4	O	0	3
4	P	0	4
5	C	0	1
All	All	0	11

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	14	DG	OP3-P	-7.69	1.51	1.61
4	O	13	DG	OP3-P	-7.42	1.52	1.61
2	M	14	DG	OP3-P	-7.30	1.52	1.61
4	P	13	DG	OP3-P	-7.26	1.52	1.61
5	D	71	VAL	CB-CG2	-6.26	1.39	1.52
5	B	71	VAL	CB-CG2	-5.85	1.40	1.52
5	D	157	ARG	CB-CG	-5.66	1.37	1.52
5	D	71	VAL	CB-CG1	-5.38	1.41	1.52
5	B	52	VAL	CB-CG2	-5.10	1.42	1.52
4	P	13	DG	P-O5'	5.05	1.64	1.59

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	74	ARG	NE-CZ-NH2	8.77	124.68	120.30
5	D	157	ARG	CG-CD-NE	-8.76	93.40	111.80
5	B	139	LEU	CA-CB-CG	7.25	131.98	115.30
5	B	21	GLN	CA-CB-CG	-7.05	97.88	113.40
4	P	13	DG	OP1-P-OP2	-6.78	109.42	119.60
5	D	157	ARG	NE-CZ-NH2	-6.60	117.00	120.30
5	A	97	SER	CB-CA-C	-5.97	98.76	110.10
5	D	157	ARG	CB-CA-C	-5.15	100.09	110.40

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	C	50	TYR	Sidechain
1	E	7	DA	Sidechain
3	H	10	DT	Sidechain
2	M	17	DA	Sidechain
4	O	14	DG	Sidechain
4	O	15	DT	Sidechain
4	O	19	DC	Sidechain
4	P	14	DG	Sidechain
4	P	15	DT	Sidechain
4	P	19	DC	Sidechain
4	P	20	DA	Sidechain

## 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	E	241	0	138	20	0
1	G	241	0	138	25	0
2	M	169	0	90	19	0
2	N	169	0	90	14	0
3	F	239	0	139	6	0
3	H	239	0	139	11	0
4	O	167	0	90	17	0
4	P	167	0	90	21	0
5	A	1242	0	1185	57	0
5	B	1242	0	1186	62	2
5	C	1242	0	1185	74	2
5	D	1242	0	1185	71	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	N	1	0	0	0	0
6	P	1	0	0	0	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
7	C	2	0	0	0	0
7	D	2	0	0	0	0
All	All	6612	0	5655	306	2

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 25.

All (306) 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)
5:C:9:LEU:HD23	5:D:157:ARG:HH21	1.11	1.11
1:E:13:DA:H2'	2:M:14:DG:C8	1.87	1.10
2:M:14:DG:H5''	5:B:96:ALA:O	1.51	1.08
5:D:157:ARG:NH1	5:D:157:ARG:HG2	1.68	1.04
2:M:14:DG:H5'	5:B:119:ASN:ND2	1.78	0.98
5:B:99:LEU:HB3	5:B:139:LEU:HD21	1.50	0.94
1:G:7:DA:C2	4:P:15:DT:H71	2.03	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:12:DA:H2''	1:G:13:DA:C8	2.05	0.91
5:D:88:ASN:C	5:D:88:ASN:HD22	1.76	0.89
4:P:13:DG:H5''	5:C:96:ALA:O	1.73	0.89
5:C:9:LEU:CD2	5:D:157:ARG:HH21	1.86	0.88
1:G:7:DA:H2	4:P:15:DT:C7	1.85	0.88
5:D:157:ARG:HG2	5:D:157:ARG:HH11	1.39	0.87
5:B:99:LEU:HB3	5:B:139:LEU:CD2	2.04	0.86
5:C:9:LEU:HD23	5:D:157:ARG:NH2	1.92	0.85
5:C:9:LEU:HD22	5:D:157:ARG:HE	1.42	0.85
1:E:7:DA:H2	4:O:15:DT:H71	1.42	0.84
1:E:13:DA:H2'	2:M:14:DG:H8	1.36	0.83
2:N:17:DA:H62	5:D:63:GLN:HE22	1.25	0.83
1:G:7:DA:C2	4:P:15:DT:C7	2.63	0.82
5:C:50:TYR:CZ	5:C:56:LYS:HE3	2.16	0.81
5:D:88:ASN:O	5:D:88:ASN:ND2	2.13	0.81
2:M:16:DG:H2''	2:M:17:DA:H5'	1.62	0.80
1:G:2:DT:H2''	1:G:3:DG:OP2	1.79	0.80
1:G:7:DA:H2	4:P:15:DT:H71	1.45	0.79
1:E:7:DA:C2	4:O:15:DT:H71	2.17	0.79
1:G:6:DT:H2'	1:G:7:DA:C8	2.18	0.78
5:D:120:LYS:O	5:D:123:ASN:HB2	1.83	0.78
1:G:13:DA:H2''	2:N:14:DG:O5'	1.83	0.77
2:M:14:DG:H5'	5:B:119:ASN:HD21	1.49	0.77
5:C:80:VAL:HA	5:C:83:LEU:HD22	1.66	0.77
1:G:8:DC:H1'	1:G:9:DC:H5'	1.68	0.75
1:E:6:DT:H2'	1:E:7:DA:C8	2.21	0.75
5:C:50:TYR:OH	5:C:56:LYS:HE3	1.87	0.74
3:H:6:DC:H2''	3:H:7:DT:H5'	1.70	0.73
4:P:14:DG:H8	5:C:61:ARG:HH11	1.35	0.73
5:B:50:TYR:CZ	5:B:56:LYS:HE3	2.24	0.73
5:A:98:HIS:CE1	5:A:103:THR:HA	2.24	0.72
5:D:80:VAL:HA	5:D:83:LEU:HD22	1.72	0.72
5:D:50:TYR:OH	5:D:56:LYS:NZ	2.23	0.72
1:E:6:DT:O4	5:A:57:ASN:HA	1.90	0.71
5:B:120:LYS:O	5:B:123:ASN:HB2	1.89	0.71
1:E:12:DA:H2''	1:E:13:DA:C8	2.26	0.71
5:C:9:LEU:CD2	5:D:157:ARG:NH2	2.50	0.71
2:M:14:DG:OP3	5:B:97:SER:HA	1.92	0.70
5:D:42:TYR:HD1	5:D:107:ASN:HB2	1.57	0.70
1:E:7:DA:H2	4:O:15:DT:C7	2.06	0.69
4:P:13:DG:H5'	5:C:119:ASN:ND2	2.06	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:120:LYS:O	5:A:123:ASN:HB2	1.91	0.69
5:D:42:TYR:CD1	5:D:107:ASN:HB2	2.26	0.69
5:C:98:HIS:CE1	5:C:103:THR:HA	2.27	0.69
5:C:120:LYS:O	5:C:123:ASN:HB2	1.92	0.69
5:A:42:TYR:CZ	5:B:161:PHE:HD2	2.11	0.69
5:C:157:ARG:NH2	5:D:9:LEU:HD22	2.08	0.68
4:O:14:DG:H2''	4:O:15:DT:OP2	1.94	0.68
2:M:14:DG:H5'	5:B:119:ASN:HD22	1.59	0.68
5:A:98:HIS:CD2	5:A:111:LEU:HD21	2.29	0.67
5:C:9:LEU:CD2	5:D:157:ARG:HE	2.07	0.67
5:A:50:TYR:OH	5:A:56:LYS:NZ	2.27	0.66
4:P:19:DC:H2''	4:P:20:DA:OP2	1.96	0.66
5:A:4:THR:OG1	5:A:7:GLN:HG3	1.95	0.66
5:D:4:THR:HG23	5:D:7:GLN:OE1	1.97	0.65
5:A:98:HIS:HD2	5:A:111:LEU:CD2	2.09	0.65
5:D:80:VAL:HB	5:D:81:PRO:HD3	1.78	0.65
5:B:80:VAL:HA	5:B:83:LEU:HD22	1.79	0.65
4:O:19:DC:H2''	4:O:20:DA:OP2	1.95	0.64
2:N:17:DA:H62	5:D:63:GLN:NE2	1.96	0.64
5:D:157:ARG:HH11	5:D:157:ARG:CG	2.06	0.64
5:B:4:THR:HG23	5:B:7:GLN:OE1	1.97	0.64
1:E:13:DA:O3'	2:M:14:DG:OP2	2.15	0.64
5:C:80:VAL:HB	5:C:81:PRO:HD3	1.81	0.63
5:B:4:THR:OG1	5:B:7:GLN:HG3	1.98	0.63
1:E:5:DC:H2''	1:E:6:DT:H5'	1.79	0.63
5:B:99:LEU:CB	5:B:139:LEU:HD21	2.24	0.63
2:M:15:DA:H8	5:B:61:ARG:HH11	1.44	0.62
1:G:13:DA:H2'	2:N:14:DG:C8	2.34	0.62
5:D:4:THR:OG1	5:D:7:GLN:HG3	2.00	0.62
5:A:80:VAL:HB	5:A:81:PRO:HD3	1.82	0.62
5:B:99:LEU:HD23	5:B:139:LEU:HD21	1.82	0.61
1:G:6:DT:O4	5:C:57:ASN:HA	2.00	0.61
5:C:108:PRO:HA	5:C:111:LEU:HD12	1.81	0.61
5:C:114:GLU:HB3	5:D:150:THR:HG23	1.82	0.61
5:D:50:TYR:OH	5:D:56:LYS:CE	2.49	0.60
2:M:16:DG:C2'	2:M:17:DA:H5'	2.31	0.60
5:C:161:PHE:HA	5:D:42:TYR:OH	2.01	0.60
5:C:163:VAL:C	5:D:40:HIS:HD1	2.05	0.60
5:C:9:LEU:HD22	5:D:157:ARG:NE	2.15	0.60
4:P:13:DG:H5'	5:C:119:ASN:HD21	1.67	0.59
5:A:42:TYR:CD1	5:A:107:ASN:HB2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:150:THR:HG23	5:B:114:GLU:HB3	1.84	0.59
1:G:6:DT:H73	5:C:56:LYS:O	2.02	0.59
5:B:97:SER:HB3	5:B:112:CYS:SG	2.41	0.59
1:G:13:DA:H2'	2:N:14:DG:H8	1.69	0.58
5:A:50:TYR:CZ	5:A:56:LYS:HE3	2.39	0.58
1:G:12:DA:C2	3:H:10:DT:O2	2.57	0.57
5:A:80:VAL:HA	5:A:83:LEU:HD22	1.86	0.57
4:P:16:DA:H62	5:C:63:GLN:HE22	1.52	0.57
2:N:17:DA:N6	5:D:63:GLN:HE22	1.99	0.56
5:A:157:ARG:NH2	5:B:9:LEU:HD22	2.21	0.56
5:B:50:TYR:OH	5:B:56:LYS:NZ	2.36	0.56
5:C:42:TYR:CD1	5:C:107:ASN:HB2	2.40	0.56
5:B:12:ILE:O	5:B:15:TRP:HB3	2.06	0.55
4:P:13:DG:O3'	5:C:95:THR:HB	2.06	0.55
5:B:108:PRO:HA	5:B:111:LEU:HD12	1.89	0.55
5:C:80:VAL:HA	5:C:83:LEU:CD2	2.35	0.55
1:E:10:DT:H2''	1:E:11:DT:C5'	2.36	0.55
5:B:50:TYR:OH	5:B:56:LYS:HE3	2.05	0.55
4:O:13:DG:H2''	4:O:14:DG:H5'	1.89	0.55
5:A:26:THR:HG23	5:A:40:HIS:CD2	2.41	0.55
5:A:7:GLN:O	5:A:10:ALA:HB3	2.08	0.54
5:C:50:TYR:OH	5:C:56:LYS:CE	2.53	0.54
5:B:99:LEU:HB3	5:B:139:LEU:HD23	1.87	0.54
5:B:139:LEU:CD2	5:B:139:LEU:N	2.70	0.54
1:E:10:DT:H2''	1:E:11:DT:H5'	1.90	0.54
5:C:98:HIS:HE1	5:C:103:THR:HA	1.70	0.54
3:F:7:DT:H1'	3:F:8:DC:H5'	1.88	0.53
3:H:5:DT:H2'	3:H:6:DC:C6	2.44	0.53
5:C:69:ASN:O	5:C:70:GLN:HG2	2.08	0.53
5:A:98:HIS:HE1	5:A:103:THR:HA	1.69	0.53
5:A:109:LEU:HA	5:B:154:PRO:HB2	1.91	0.53
5:A:157:ARG:CZ	5:B:9:LEU:HD22	2.38	0.53
5:A:125:CYS:SG	5:A:126:PRO:HD2	2.49	0.53
5:C:9:LEU:CD2	5:D:157:ARG:NE	2.70	0.53
5:D:8:ILE:HG21	5:D:84:LEU:HD13	1.91	0.53
5:A:4:THR:HG23	5:A:7:GLN:OE1	2.08	0.53
1:G:7:DA:C2	4:P:15:DT:H72	2.43	0.53
5:B:80:VAL:HB	5:B:81:PRO:HD3	1.91	0.53
5:C:44:ILE:HG13	5:C:45:PRO:HD2	1.91	0.53
5:A:98:HIS:HD2	5:A:111:LEU:HD21	1.67	0.52
5:A:88:ASN:HA	5:A:92:LYS:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:157:ARG:CZ	5:D:9:LEU:HD22	2.40	0.52
5:D:108:PRO:HA	5:D:111:LEU:HD12	1.89	0.52
1:E:13:DA:HO3'	2:M:14:DG:P	2.32	0.52
1:G:12:DA:H2	3:H:10:DT:O2	1.92	0.52
5:A:42:TYR:HD1	5:A:107:ASN:HB2	1.75	0.52
5:A:44:ILE:HG13	5:A:45:PRO:HD2	1.92	0.52
4:O:14:DG:H8	5:A:61:ARG:HH11	1.56	0.52
2:N:14:DG:OP2	5:D:98:HIS:ND1	2.32	0.52
5:A:69:ASN:O	5:A:70:GLN:HB2	2.08	0.52
2:M:14:DG:O3'	5:B:95:THR:HB	2.10	0.52
4:P:14:DG:H2''	4:P:15:DT:OP2	2.09	0.52
5:C:4:THR:HG23	5:C:7:GLN:OE1	2.10	0.52
3:H:7:DT:H2''	3:H:8:DC:O5'	2.10	0.51
5:B:41:CYS:HB3	5:B:105:CYS:HB2	1.91	0.51
5:C:99:LEU:HD23	5:C:139:LEU:HG	1.92	0.51
5:C:42:TYR:HD1	5:C:107:ASN:HB2	1.76	0.51
5:A:148:GLY:HA3	5:B:118:ASP:OD1	2.11	0.51
1:G:11:DT:O2	3:H:11:DA:H2	1.94	0.50
5:A:18:THR:HG23	5:A:52:VAL:HG23	1.93	0.50
5:D:32:GLY:O	5:D:129:ASN:HB3	2.11	0.50
1:G:7:DA:N1	4:P:15:DT:H71	2.24	0.50
5:C:125:CYS:SG	5:C:126:PRO:HD2	2.52	0.50
5:A:41:CYS:HB3	5:A:105:CYS:HB2	1.92	0.50
5:C:71:VAL:HG22	5:C:73:HIS:CD2	2.46	0.50
5:D:50:TYR:CZ	5:D:56:LYS:HD2	2.47	0.50
5:D:88:ASN:HA	5:D:92:LYS:O	2.12	0.50
5:C:7:GLN:O	5:C:10:ALA:HB3	2.12	0.50
5:C:98:HIS:CD2	5:C:111:LEU:HD21	2.46	0.50
4:P:13:DG:H2''	4:P:14:DG:H5'	1.93	0.49
5:C:31:LEU:HD21	5:C:37:GLY:HA3	1.95	0.49
4:P:16:DA:H62	5:C:63:GLN:NE2	2.10	0.49
5:A:99:LEU:HD23	5:A:139:LEU:HG	1.95	0.49
1:E:2:DT:C2'	1:E:3:DG:O5'	2.61	0.49
5:A:31:LEU:HD11	5:A:36:GLN:C	2.33	0.49
5:B:42:TYR:CD1	5:B:107:ASN:HB2	2.47	0.49
5:C:80:VAL:CA	5:C:83:LEU:HD22	2.41	0.49
5:C:98:HIS:CD2	5:C:111:LEU:CD2	2.95	0.49
5:D:31:LEU:HD11	5:D:36:GLN:C	2.33	0.48
5:C:161:PHE:CE2	5:D:19:VAL:HG12	2.47	0.48
4:O:15:DT:H1'	4:O:16:DA:H5'	1.95	0.48
3:H:12:DA:H2'	4:P:13:DG:O4'	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:139:LEU:HD23	5:B:139:LEU:H	1.78	0.48
5:C:68:ILE:O	5:C:71:VAL:HG13	2.13	0.48
5:D:80:VAL:HA	5:D:83:LEU:CD2	2.43	0.48
2:M:14:DG:H2''	2:M:15:DA:O5'	2.14	0.48
4:O:13:DG:C5'	5:A:96:ALA:O	2.61	0.48
5:C:71:VAL:HG22	5:C:73:HIS:NE2	2.28	0.48
2:M:14:DG:OP3	5:B:98:HIS:N	2.42	0.48
5:B:32:GLY:O	5:B:129:ASN:HB3	2.14	0.48
5:A:98:HIS:HD2	5:A:111:LEU:HD23	1.78	0.47
5:C:41:CYS:HB3	5:C:105:CYS:HB2	1.96	0.47
5:B:50:TYR:OH	5:B:56:LYS:CE	2.61	0.47
5:D:57:ASN:OD1	5:D:57:ASN:N	2.37	0.47
2:N:15:DA:H8	5:D:61:ARG:HH11	1.62	0.47
2:N:18:DG:H2''	2:N:19:DT:H71	1.97	0.47
2:M:14:DG:C2'	2:M:15:DA:O5'	2.63	0.47
5:A:71:VAL:HG22	5:A:73:HIS:CD2	2.50	0.47
5:A:126:PRO:O	5:A:141:GLN:HB2	2.14	0.46
5:D:56:LYS:HB2	5:D:61:ARG:O	2.15	0.46
5:A:114:GLU:HB3	5:B:150:THR:HG23	1.97	0.46
1:E:13:DA:H2''	2:M:14:DG:O5'	2.15	0.46
1:E:7:DA:C2	4:O:15:DT:C7	2.88	0.46
5:C:161:PHE:HD2	5:D:42:TYR:CZ	2.33	0.46
5:D:38:THR:O	5:D:39:LEU:HD12	2.16	0.46
1:G:12:DA:H2''	1:G:13:DA:N7	2.31	0.46
3:H:6:DC:C2'	3:H:7:DT:H5'	2.44	0.46
4:P:14:DG:H8	5:C:61:ARG:NH1	2.10	0.46
5:B:3:LEU:HG	5:B:73:HIS:CE1	2.51	0.46
5:B:7:GLN:O	5:B:11:VAL:HG23	2.16	0.46
5:B:99:LEU:HD23	5:B:139:LEU:CD2	2.45	0.45
5:B:139:LEU:N	5:B:139:LEU:HD22	2.30	0.45
5:A:8:ILE:HG21	5:A:84:LEU:HD13	1.98	0.45
5:A:42:TYR:CE2	5:B:161:PHE:HD2	2.33	0.45
5:A:62:TRP:HB2	5:A:77:SER:OG	2.16	0.45
1:E:13:DA:H61	3:F:9:DT:H3	1.64	0.45
3:F:7:DT:H2''	3:F:8:DC:O5'	2.17	0.45
3:F:12:DA:O3'	4:O:13:DG:P	2.74	0.45
1:E:9:DC:H2'	1:E:10:DT:H72	1.99	0.45
5:A:98:HIS:CD2	5:A:111:LEU:CD2	2.90	0.45
5:B:69:ASN:O	5:B:70:GLN:HB2	2.16	0.45
5:C:163:VAL:OXT	5:D:40:HIS:N	2.45	0.45
2:N:14:DG:OP1	5:D:97:SER:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:5:DT:H2'	3:H:6:DC:H6	1.82	0.45
5:C:61:ARG:HA	5:C:61:ARG:HD2	1.56	0.45
5:D:61:ARG:HD2	5:D:61:ARG:HA	1.55	0.45
3:H:1:DT:C7	5:D:72:VAL:HG13	2.47	0.45
5:B:18:THR:OG1	5:B:52:VAL:HG13	2.17	0.45
5:D:31:LEU:HD21	5:D:37:GLY:HA3	1.99	0.45
5:A:157:ARG:CZ	5:A:157:ARG:HB3	2.46	0.44
5:D:78:HIS:CE1	5:D:106:HIS:CE1	3.05	0.44
2:M:15:DA:OP1	5:B:79:THR:HG22	2.16	0.44
5:C:88:ASN:HA	5:C:92:LYS:O	2.18	0.44
5:A:61:ARG:HD2	5:A:61:ARG:HA	1.60	0.44
5:D:88:ASN:C	5:D:88:ASN:ND2	2.51	0.44
5:A:12:ILE:O	5:A:15:TRP:HB3	2.17	0.44
5:C:9:LEU:CD2	5:D:157:ARG:CZ	2.96	0.44
5:C:97:SER:HB3	5:C:112:CYS:SG	2.57	0.44
5:B:88:ASN:HA	5:B:92:LYS:O	2.18	0.44
5:C:19:VAL:HG12	5:D:161:PHE:CE2	2.52	0.44
4:O:13:DG:H5'	5:A:96:ALA:O	2.18	0.44
5:C:80:VAL:O	5:C:83:LEU:HD22	2.18	0.43
5:C:31:LEU:HD11	5:C:36:GLN:C	2.37	0.43
5:D:97:SER:HB3	5:D:112:CYS:SG	2.58	0.43
4:O:13:DG:O3'	5:A:95:THR:HB	2.18	0.43
5:A:15:TRP:CZ3	5:A:81:PRO:HG3	2.53	0.43
5:A:76:GLY:O	5:A:78:HIS:N	2.51	0.43
5:C:124:TRP:CZ2	5:C:144:LEU:HD23	2.53	0.43
5:D:154:PRO:O	5:D:155:GLN:CB	2.67	0.43
5:C:32:GLY:O	5:C:129:ASN:HB3	2.18	0.43
5:C:76:GLY:O	5:C:78:HIS:N	2.51	0.43
5:D:65:LYS:HB2	5:D:74:ARG:HG3	2.01	0.43
5:A:68:ILE:O	5:A:71:VAL:HG13	2.19	0.43
5:B:83:LEU:HD12	5:B:83:LEU:HA	1.79	0.43
5:D:107:ASN:OD1	5:D:107:ASN:C	2.57	0.43
5:B:42:TYR:HD1	5:B:107:ASN:HB2	1.84	0.43
5:C:102:ASN:O	5:C:105:CYS:HB3	2.18	0.43
5:C:150:THR:HG23	5:D:114:GLU:HB3	2.01	0.43
1:G:5:DC:H2''	1:G:6:DT:H5'	2.00	0.43
5:B:102:ASN:O	5:B:105:CYS:HB3	2.19	0.42
2:N:15:DA:H2'	2:N:16:DG:C8	2.54	0.42
5:B:61:ARG:HA	5:B:61:ARG:HD2	1.61	0.42
5:C:11:VAL:O	5:C:12:ILE:C	2.57	0.42
5:C:38:THR:O	5:C:39:LEU:HD12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:25:ILE:O	5:D:40:HIS:HA	2.19	0.42
5:A:157:ARG:CZ	5:B:9:LEU:CD2	2.98	0.42
5:B:25:ILE:HG13	5:B:43:GLU:CD	2.40	0.42
1:G:5:DC:H2'	1:G:6:DT:O4'	2.19	0.42
5:A:57:ASN:OD1	5:A:57:ASN:N	2.50	0.42
1:G:10:DT:H2''	1:G:11:DT:C5'	2.50	0.42
5:D:7:GLN:O	5:D:11:VAL:HG23	2.20	0.42
5:D:109:LEU:HD23	5:D:109:LEU:HA	1.87	0.42
1:G:9:DC:H2'	1:G:10:DT:H72	2.02	0.41
4:P:18:DC:C2	4:P:19:DC:C5	3.08	0.41
2:M:14:DG:H2'	5:B:61:ARG:NH1	2.35	0.41
4:O:13:DG:H5''	5:A:96:ALA:O	2.20	0.41
5:C:98:HIS:HD2	5:C:111:LEU:CD2	2.32	0.41
5:A:57:ASN:HB3	5:A:63:GLN:OE1	2.20	0.41
5:D:126:PRO:O	5:D:141:GLN:HB2	2.20	0.41
4:O:14:DG:C2'	4:O:15:DT:OP2	2.63	0.41
1:G:7:DA:H2	4:P:15:DT:H72	1.71	0.41
5:C:98:HIS:HD2	5:C:111:LEU:HD23	1.85	0.41
5:D:97:SER:CB	5:D:114:GLU:OE2	2.68	0.41
3:F:6:DC:H2''	3:F:7:DT:H5'	2.02	0.41
5:A:36:GLN:HE21	5:A:36:GLN:HB3	1.15	0.41
5:D:12:ILE:O	5:D:15:TRP:HB3	2.21	0.41
5:D:56:LYS:HA	5:D:62:TRP:HA	2.02	0.41
3:F:1:DT:H2''	3:F:2:DG:O5'	2.20	0.41
5:A:31:LEU:HD11	5:A:37:GLY:N	2.36	0.41
5:B:99:LEU:CD2	5:B:139:LEU:HD21	2.50	0.41
2:N:16:DG:H2''	2:N:17:DA:H5'	2.02	0.41
5:C:19:VAL:HG12	5:D:161:PHE:HE2	1.86	0.41
5:C:83:LEU:HD12	5:C:83:LEU:HA	1.78	0.41
1:E:12:DA:H2''	1:E:13:DA:H8	1.77	0.41
4:O:14:DG:H8	5:A:61:ARG:NH1	2.18	0.41
1:G:5:DC:C2'	1:G:6:DT:H5'	2.51	0.41
2:N:18:DG:C2'	2:N:19:DT:H71	2.51	0.41
3:H:9:DT:H2''	3:H:10:DT:H71	2.01	0.41
4:P:14:DG:OP1	5:C:79:THR:HG22	2.21	0.41
5:B:109:LEU:HD23	5:B:109:LEU:HA	1.87	0.41
5:B:126:PRO:O	5:B:141:GLN:HB2	2.21	0.41
5:D:99:LEU:HD23	5:D:139:LEU:HG	2.03	0.41
4:O:19:DC:C2'	4:O:20:DA:OP2	2.67	0.41
1:E:5:DC:H2'	1:E:6:DT:C6	2.56	0.40
2:N:14:DG:O3'	5:D:95:THR:HB	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:38:THR:O	5:B:39:LEU:HD12	2.21	0.40
5:D:107:ASN:OD1	5:D:109:LEU:HB2	2.21	0.40
5:C:107:ASN:C	5:C:107:ASN:OD1	2.58	0.40
5:D:73:HIS:HB3	5:D:75:TRP:CZ2	2.56	0.40
5:B:57:ASN:HB3	5:B:63:GLN:OE1	2.21	0.40
5:B:78:HIS:HE1	5:B:105:CYS:O	2.03	0.40
5:C:50:TYR:OH	5:C:56:LYS:NZ	2.52	0.40
5:B:3:LEU:HG	5:B:73:HIS:HE1	1.86	0.40
5:C:60:THR:O	5:C:61:ARG:HD2	2.21	0.40
5:A:42:TYR:CE1	5:B:161:PHE:HD2	2.38	0.40
5:B:73:HIS:HB3	5:B:75:TRP:CZ2	2.56	0.40
5:D:78:HIS:NE2	5:D:106:HIS:ND1	2.70	0.40

All (2) 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)
5:B:28:HIS:ND1	5:C:21:GLN:NE2[1_545]	1.94	0.26
5:B:28:HIS:ND1	5:C:21:GLN:CD[1_545]	2.17	0.03

## 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	
5	A	160/163 (98%)	146 (91%)	12 (8%)	2 (1%)	12	42
5	B	160/163 (98%)	147 (92%)	10 (6%)	3 (2%)	8	33
5	C	160/163 (98%)	144 (90%)	14 (9%)	2 (1%)	12	42
5	D	160/163 (98%)	140 (88%)	18 (11%)	2 (1%)	12	42
All	All	640/652 (98%)	577 (90%)	54 (8%)	9 (1%)	11	40

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	A	77	SER
5	C	77	SER
5	C	159	SER
5	A	137	VAL
5	B	77	SER
5	B	137	VAL
5	B	159	SER
5	D	137	VAL
5	D	158	GLY

### 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	
5	A	132/133 (99%)	114 (86%)	18 (14%)	3	16
5	B	132/133 (99%)	119 (90%)	13 (10%)	8	29
5	C	132/133 (99%)	117 (89%)	15 (11%)	5	23
5	D	132/133 (99%)	113 (86%)	19 (14%)	3	14
All	All	528/532 (99%)	463 (88%)	65 (12%)	4	19

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	A	9	LEU
5	A	17	GLU
5	A	26	THR
5	A	31	LEU
5	A	35	LEU
5	A	36	GLN
5	A	39	LEU
5	A	61	ARG
5	A	71	VAL
5	A	72	VAL
5	A	83	LEU
5	A	84	LEU
5	A	93	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	A	103	THR
5	A	129	ASN
5	A	144	LEU
5	A	157	ARG
5	A	162	VAL
5	B	31	LEU
5	B	52	VAL
5	B	61	ARG
5	B	72	VAL
5	B	83	LEU
5	B	84	LEU
5	B	99	LEU
5	B	103	THR
5	B	118	ASP
5	B	129	ASN
5	B	139	LEU
5	B	144	LEU
5	B	155	GLN
5	C	17	GLU
5	C	21	GLN
5	C	26	THR
5	C	31	LEU
5	C	35	LEU
5	C	61	ARG
5	C	67	THR
5	C	71	VAL
5	C	72	VAL
5	C	83	LEU
5	C	84	LEU
5	C	85	GLU
5	C	103	THR
5	C	129	ASN
5	C	144	LEU
5	D	17	GLU
5	D	21	GLN
5	D	26	THR
5	D	31	LEU
5	D	56	LYS
5	D	61	ARG
5	D	68	ILE
5	D	72	VAL
5	D	83	LEU

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Mol	Chain	Res	Type
5	D	84	LEU
5	D	88	ASN
5	D	89	ILE
5	D	99	LEU
5	D	103	THR
5	D	129	ASN
5	D	138	CYS
5	D	144	LEU
5	D	155	GLN
5	D	159	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
5	A	36	GLN
5	A	90	ASN
5	B	28	HIS
5	B	78	HIS
5	B	119	ASN
5	C	63	GLN
5	C	70	GLN
5	C	90	ASN
5	C	101	HIS
5	D	63	GLN
5	D	88	ASN
5	D	90	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 monosaccharides in this entry.

## 5.6 Ligand geometry

Of 12 ligands modelled in this entry, 12 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

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

### 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.