



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 10:39 PM UTC

PDB ID : 1EVW / pdb_00001evw
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

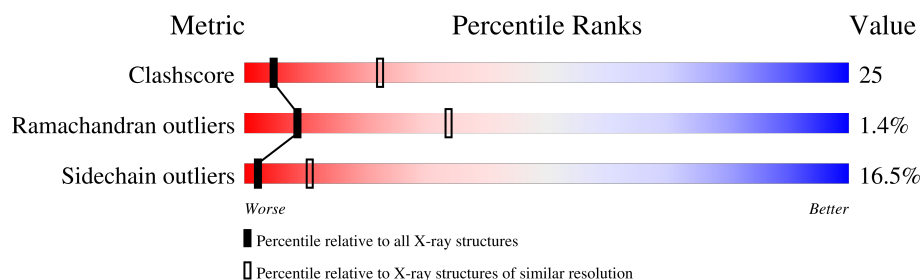
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (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 ≥ 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% 83% 8%
2	M	8	50% 38% 12%
2	N	8	12% 88%
3	F	12	42% 50% 8%
3	H	12	25% 58% 17%
4	O	8	25% 25% 50%
4	P	8	12% 38% 38% 12%

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Mol	Chain	Length	Quality of chain
5	A	163	56%36%7%
5	B	163	55%37%6%
5	C	163	52%40%7%
5	D	163	52%39%8%

2 Entry composition [i](#)

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
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
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
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
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
5	A	162	Total	C	N	O	S	0	0	0
			1242	783	232	219	8			
5	B	162	Total	C	N	O	S	0	0	0
			1242	783	232	219	8			
5	C	162	Total	C	N	O	S	0	0	0
			1242	783	232	219	8			
5	D	162	Total	C	N	O	S	0	0	0
			1242	783	232	219	8			

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 (CCD ID: MG) (formula: Mg).

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

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

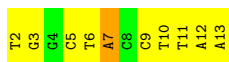
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

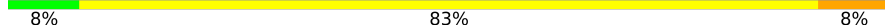
Note EDS was not executed.

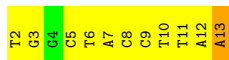
- Molecule 1: DNA (5'-D(*TP*GP*GP*CP*TP*AP*CP*CP*TP*TP*AP*A)-3')

Chain E: 



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

Chain G: 



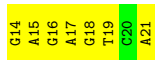
- Molecule 2: DNA (5'-D(P*GP*AP*GP*AP*GP*TP*CP*A)-3')

Chain M: 



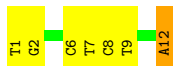
- Molecule 2: DNA (5'-D(P*GP*AP*GP*AP*GP*TP*CP*A)-3')

Chain N: 

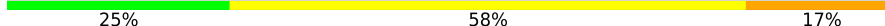


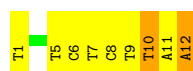
- Molecule 3: DNA (5'-D(*TP*GP*AP*CP*TP*CP*TP*CP*TP*TP*AP*A)-3')

Chain F: 

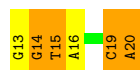
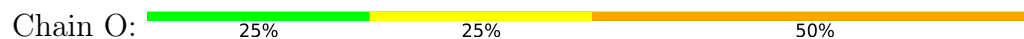


- Molecule 3: DNA (5'-D(*TP*GP*AP*CP*TP*CP*TP*CP*TP*TP*AP*A)-3')

Chain H: 



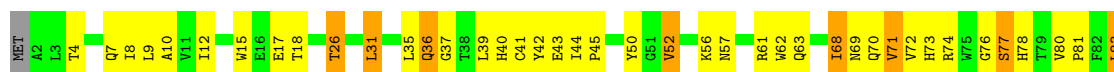
- Molecule 4: DNA (5'-D(P*GP*GP*TP*AP*GP*CP*CP*A)-3')



- 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



MET	A2	L3	T4	N5	A6	Q7	I8	L9	A10	V11	I12		W15	E16	E17	T18	V19	G20	Q21	F22	P23	V24	I25	T26		L31	G32		Q36	G37	T38	L39	H40	C41	Y42		Y50	G51	V52		A55	K56	R57	G58	P59	T60	R61	W62	Q63	Y64	K65	R66	T67	I68		V72	H73	R74	W75
	H78	T79	V80	P81	F82	L83	L84		N88	I89		K92		T95	A96	S97	H98	L99		T103		H106	N107	P108	L109	H110	L111	C112	W113	E114		K120	N123		P126		N129		V137	C138	L139	R140	Q141		L144		T150		P154	Q155	Q156	R157	G158	S159	H160	F161	V162	V163	

4 Data and refinement statistics

Xtriage (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, α , β , γ	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.	Xtriage
Total number of atoms	6612	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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	0.37	0/269	0.80	0/413
1	G	0.38	0/269	0.92	2/413 (0.5%)
2	M	0.47	0/190	0.65	0/290
2	N	0.50	0/190	0.78	1/290 (0.3%)
3	F	0.33	0/266	0.78	1/408 (0.2%)
3	H	0.36	0/266	0.76	1/408 (0.2%)
4	O	0.53	0/187	0.90	1/285 (0.4%)
4	P	0.49	0/187	0.98	1/285 (0.4%)
5	A	0.63	0/1283	1.00	4/1756 (0.2%)
5	B	0.75	2/1283 (0.2%)	1.07	7/1756 (0.4%)
5	C	0.65	0/1283	0.97	2/1756 (0.1%)
5	D	0.72	1/1283 (0.1%)	1.06	8/1756 (0.5%)
All	All	0.63	3/6956 (0.0%)	0.97	28/9816 (0.3%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	52	VAL	CA-CB	8.09	1.62	1.53
5	B	52	VAL	CA-C	5.24	1.58	1.53
5	D	157	ARG	CB-CG	-5.06	1.37	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	157	ARG	CG-CD-NE	-8.45	93.40	112.00
5	B	21	GLN	CA-CB-CG	-8.11	97.88	114.10
1	G	13	DA	C4'-C3'-O3'	8.04	122.06	110.00
4	O	20	DA	C2'-C3'-O3'	-7.64	100.04	111.50
4	P	20	DA	C2'-C3'-O3'	-7.25	100.62	111.50
5	D	157	ARG	CB-CA-C	-7.01	100.09	110.95
3	H	12	DA	C2'-C3'-O3'	6.68	121.52	111.50
5	B	21	GLN	N-CA-C	6.63	120.28	112.72
2	N	21	DA	C2'-C3'-O3'	6.49	121.23	111.50
5	A	97	SER	CB-CA-C	-6.33	98.76	109.72
5	B	139	LEU	N-CA-CB	6.15	119.59	110.49
5	A	74	ARG	NE-CZ-NH2	6.09	124.68	119.20
5	B	17	GLU	CB-CA-C	-6.09	101.52	110.95
5	A	161	PHE	N-CA-C	5.85	118.31	109.41
5	C	151	VAL	N-CA-C	5.82	116.03	110.74
3	F	12	DA	C2'-C3'-O3'	5.75	120.13	111.50
5	D	5	ASN	CB-CA-C	-5.75	101.30	110.84
5	D	157	ARG	CD-NE-CZ	-5.51	116.69	124.40
5	B	161	PHE	N-CA-C	5.46	117.99	109.52
5	D	52	VAL	CB-CA-C	-5.43	106.04	111.80
1	G	13	DA	C2'-C3'-O3'	5.42	119.62	111.50
5	D	57	ASN	N-CA-C	-5.27	106.62	113.16
5	A	43	GLU	N-CA-C	5.24	118.10	109.76
5	B	139	LEU	N-CA-C	-5.21	106.61	113.17
5	B	21	GLN	CA-C-O	5.16	125.92	119.78
5	D	55	ALA	CA-C-N	-5.16	115.83	123.05
5	D	55	ALA	C-N-CA	-5.16	115.83	123.05
5	C	52	VAL	CB-CA-C	-5.05	106.44	111.80

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

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Mol	Chain	Res	Type	Group
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

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	63	2
5	C	1242	0	1185	74	2
5	D	1242	0	1185	75	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	311	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 (311) 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
5:D:88:ASN:C	5:D:88:ASN:HD22	1.76	0.94
1:G:7:DA:C2	4:P:15:DT:H71	2.03	0.92
1:G:12:DA:H2''	1:G:13:DA:C8	2.05	0.91
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
5:C:163:VAL:C	5:D:40:HIS:HD1	2.05	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
5:A:31:LEU:HD11	5:A:36:GLN:C	2.33	0.53
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:D:31:LEU:HD11	5:D:36:GLN:C	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:42:TYR:CD1	5:B:107:ASN:HB2	2.47	0.49
5:C:31:LEU:HD11	5:C:36:GLN:C	2.37	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:88:ASN:C	5:D:88:ASN:ND2	2.51	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
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:D:107:ASN:OD1	5:D:107:ASN:C	2.57	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
5:C:11:VAL:O	5:C:12:ILE:C	2.57	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:B:25:ILE:HG13	5:B:43:GLU:CD	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:107:ASN:C	5:C:107:ASN:OD1	2.58	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
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: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:D:11:VAL:O	5:D:12:ILE:C	2.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:58:GLY:O	5:D:59:PRO:C	2.62	0.42
5:B:61:ARG:HA	5:B:61:ARG:HD2	1.61	0.42
5:C:38:THR:O	5:C:39:LEU:HD12	2.19	0.42
5:B:141:GLN:O	5:B:142:GLY:C	2.62	0.42
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
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:4:THR:O	5:D:5:ASN:C	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:83:LEU:HD12	5:C:83:LEU:HA	1.78	0.41
5:D:22:PHE:O	5:D:23:PRO:C	2.64	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
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: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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	9	35
5	B	160/163 (98%)	147 (92%)	10 (6%)	3 (2%)	6	27
5	C	160/163 (98%)	144 (90%)	14 (9%)	2 (1%)	9	35
5	D	160/163 (98%)	140 (88%)	18 (11%)	2 (1%)	9	35
All	All	640/652 (98%)	577 (90%)	54 (8%)	9 (1%)	9	34

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 ⓘ

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%)	111 (84%)	21 (16%)	2	12
5	B	132/133 (99%)	113 (86%)	19 (14%)	3	14
5	C	132/133 (99%)	111 (84%)	21 (16%)	2	12
5	D	132/133 (99%)	106 (80%)	26 (20%)	1	6
All	All	528/532 (99%)	441 (84%)	87 (16%)	2	11

All (87) 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	52	VAL
5	A	68	ILE
5	A	71	VAL
5	A	72	VAL
5	A	83	LEU
5	A	84	LEU
5	A	89	ILE
5	A	93	THR
5	A	99	LEU
5	A	103	THR
5	A	129	ASN
5	A	144	LEU
5	A	157	ARG
5	A	162	VAL
5	B	3	LEU
5	B	28	HIS
5	B	31	LEU
5	B	38	THR
5	B	39	LEU
5	B	52	VAL
5	B	61	ARG
5	B	67	THR
5	B	68	ILE
5	B	71	VAL
5	B	72	VAL
5	B	83	LEU
5	B	84	LEU
5	B	89	ILE
5	B	99	LEU
5	B	103	THR
5	B	129	ASN
5	B	139	LEU
5	B	144	LEU
5	C	3	LEU
5	C	17	GLU
5	C	21	GLN

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Mol	Chain	Res	Type
5	C	26	THR
5	C	31	LEU
5	C	35	LEU
5	C	39	LEU
5	C	61	ARG
5	C	65	LYS
5	C	67	THR
5	C	68	ILE
5	C	71	VAL
5	C	72	VAL
5	C	83	LEU
5	C	84	LEU
5	C	85	GLU
5	C	89	ILE
5	C	103	THR
5	C	129	ASN
5	C	144	LEU
5	C	157	ARG
5	D	3	LEU
5	D	5	ASN
5	D	17	GLU
5	D	21	GLN
5	D	26	THR
5	D	31	LEU
5	D	39	LEU
5	D	56	LYS
5	D	57	ASN
5	D	61	ARG
5	D	67	THR
5	D	68	ILE
5	D	72	VAL
5	D	83	LEU
5	D	84	LEU
5	D	88	ASN
5	D	89	ILE
5	D	99	LEU
5	D	103	THR
5	D	120	LYS
5	D	129	ASN
5	D	138	CYS
5	D	144	LEU
5	D	155	GLN

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Mol	Chain	Res	Type
5	D	159	SER
5	D	162	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
5	A	27	HIS
5	A	36	GLN
5	A	90	ASN
5	B	27	HIS
5	B	28	HIS
5	B	78	HIS
5	B	90	ASN
5	B	119	ASN
5	C	63	GLN
5	C	70	GLN
5	C	90	ASN
5	D	27	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [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.