Full wwPDB X-ray Structure Validation Report (i)

Jul 25, 2023 – 12:49 AM EDT

PDB ID	:	1BP7
Title	:	GROUP I MOBILE INTRON ENDONUCLEASE I-CREI COMPLEXED WITH HOMING SITE DNA
Authors	:	Jurica, M.S.; Monnat Junior, R.J.; Stoddard, B.L.
Deposited on	:	1998-08-13
Resolution	:	3.00 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 (i) 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 (i)) were used in the production of this report:

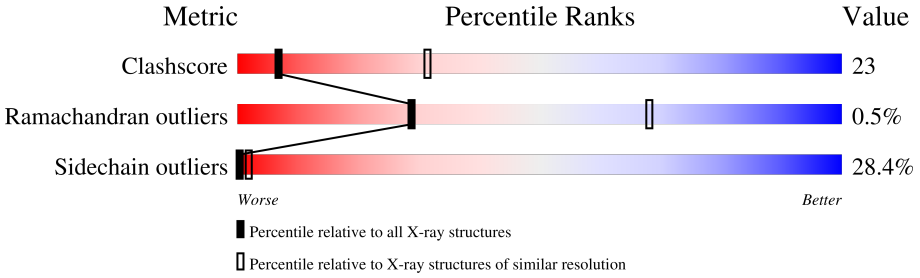
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 3.00 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	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1	24	38% 50% 12%
1	3	24	38% 54% 8%
2	2	24	25% 58% 17%
2	4	24	29% 58% 12%
3	A	152	51% 36% 13%
3	B	152	42% 47% 10% •
3	C	152	43% 46% 10% •
3	D	152	49% 37% 14%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6915 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(*GP*CP*AP*AP*AP*AP*CP*GP*TP*CP* GP*TP*GP*AP*GP*AP*CP*AP*GP*TP*TP*TP* CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	1	24	493	235	95	140	23	0	0	0
1	3	24	493	235	95	140	23	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	2	24	485	233	85	144	23	0	0	0
2	4	24	485	233	85	144	23	0	0	0

- Molecule 3 is a protein called PROTEIN (I-CREI).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	152	1237	796	210	230	1	0	0	0
3	B	152	1237	796	210	230	1	0	0	0
3	C	152	1237	796	210	230	1	0	0	0
3	D	152	1237	796	210	230	1	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	THR	ALA	SEE REMARK 999	UNP P05725
A	110	GLU	TRP	SEE REMARK 999	UNP P05725

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Chain	Residue	Modelled	Actual	Comment	Reference
A	111	GLN	ARG	SEE REMARK 999	UNP P05725
B	42	THR	ALA	SEE REMARK 999	UNP P05725
B	110	GLU	TRP	SEE REMARK 999	UNP P05725
B	111	GLN	ARG	SEE REMARK 999	UNP P05725
C	42	THR	ALA	SEE REMARK 999	UNP P05725
C	110	GLU	TRP	SEE REMARK 999	UNP P05725
C	111	GLN	ARG	SEE REMARK 999	UNP P05725
D	42	THR	ALA	SEE REMARK 999	UNP P05725
D	110	GLU	TRP	SEE REMARK 999	UNP P05725
D	111	GLN	ARG	SEE REMARK 999	UNP P05725

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	1	1	Total O 1 1	0	0
5	A	1	Total O 1 1	0	0
5	B	2	Total O 2 2	0	0
5	C	2	Total O 2 2	0	0
5	D	1	Total O 1 1	0	0

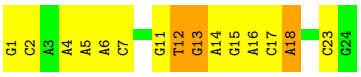
3 Residue-property plots (i)

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(*GP*CP*AP*AP*AP*AP*CP*GP*TP*CP*GP*TP*GP*AP*GP*AP *CP*AP*GP*TP*TP*TP* CP*G)-3')

Chain 1:



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

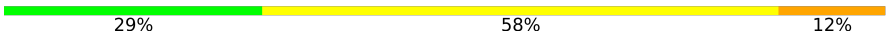
Chain 3:

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

Chain 2:

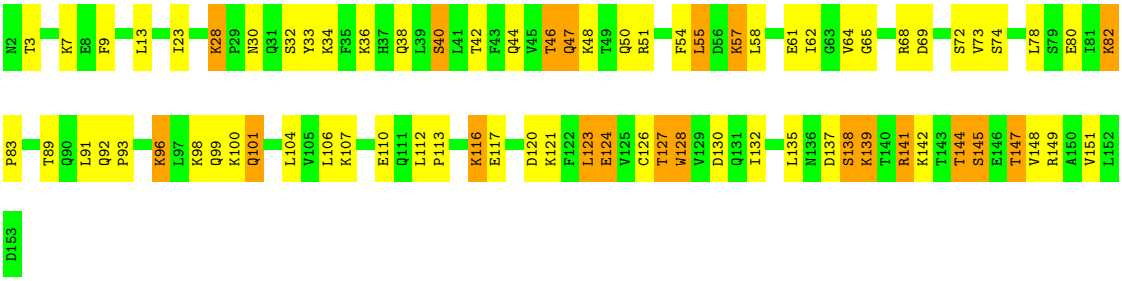
• Molecule 2: DNA (5'-D(*CP*GP*AP*AP*AP*CP*TP*GP*TP*CP*TP*CP*AP*CP*GP*AP *CP*GP*TP*TP*TP*TP* GP*C)-3')

Chain 4:



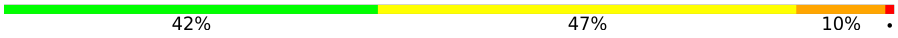
• Molecule 3: PROTEIN (I-CREI)

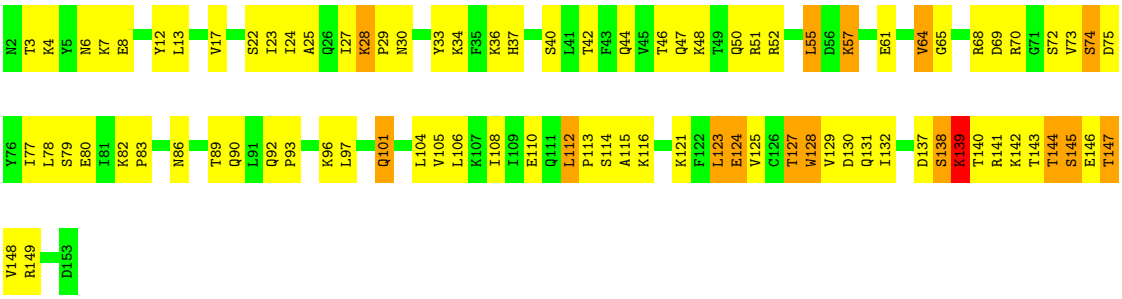
Chain A:



- Molecule 3: PROTEIN (I-CREI)

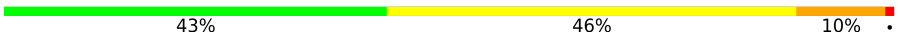
Chain B:

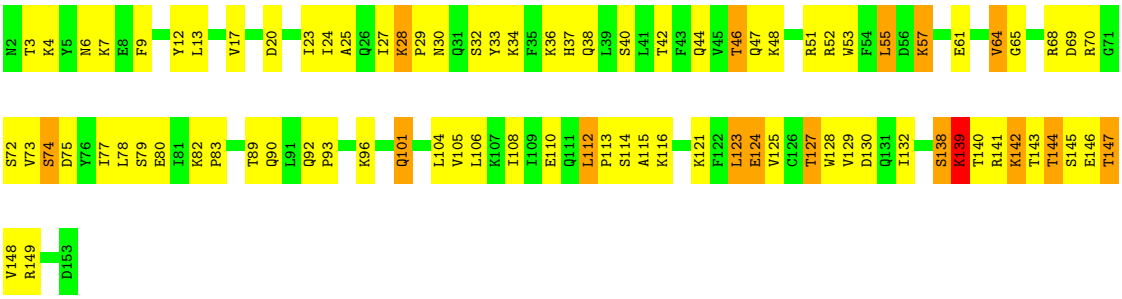




- Molecule 3: PROTEIN (I-CREI)

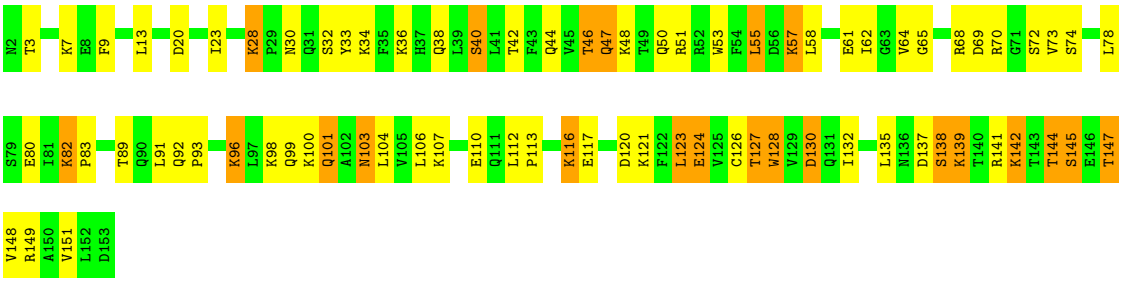
Chain C:





- Molecule 3: PROTEIN (I-CREI)

Chain D:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	67.56Å 89.26Å 177.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 3.00	Depositor
% Data completeness (in resolution range)	92.9 (100.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.234 , 0.281	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6915	wwPDB-VP
Average B, all atoms (Å^2)	16.0	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: CA

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	1	0.54	0/554	0.84	1/854 (0.1%)
1	3	0.67	0/554	0.82	0/854
2	2	0.88	1/542 (0.2%)	1.07	4/834 (0.5%)
2	4	0.74	1/542 (0.2%)	0.91	0/834
3	A	0.38	0/1260	0.59	0/1700
3	B	0.37	0/1260	0.59	0/1700
3	C	0.38	0/1260	0.58	0/1700
3	D	0.38	0/1260	0.59	0/1700
All	All	0.50	2/7232 (0.0%)	0.71	5/10176 (0.0%)

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	1	0	3
1	3	0	2
2	2	1	3
2	4	1	2
All	All	2	10

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	23	DG	C5'-C4'	7.09	1.59	1.51
2	4	24	DC	N1-C2	5.32	1.45	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	23	DG	O4'-C4'-C3'	-11.53	99.08	106.00
2	2	23	DG	O4'-C1'-N9	7.93	113.55	108.00
2	2	23	DG	O5'-P-OP1	5.92	117.80	110.70
1	1	23	DC	C1'-O4'-C4'	-5.72	104.38	110.10
2	2	24	DC	C2'-C3'-O3'	-5.14	95.62	112.60

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	2	22	DT	C3'
2	4	22	DT	C3'

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	12	DT	Sidechain
1	1	13	DG	Sidechain
1	1	18	DA	Sidechain
2	2	12	DC	Sidechain
2	2	14	DC	Sidechain
2	2	18	DG	Sidechain
1	3	12	DT	Sidechain
1	3	13	DG	Sidechain
2	4	12	DC	Sidechain
2	4	18	DG	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	1	493	0	271	18	0
1	3	493	0	271	23	0
2	2	485	0	273	27	0
2	4	485	0	273	31	0
3	A	1237	0	1270	60	0
3	B	1237	0	1270	63	0
3	C	1237	0	1270	62	0
3	D	1237	0	1270	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	1	1	0	0	0	0
4	3	1	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	1	1	0	0	1	0
5	A	1	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	1	0
5	D	1	0	0	0	0
All	All	6915	0	6168	299	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 23.

All (299) 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)
2:2:15:DG:H2"	2:2:16:DA:H5'	1.28	1.08
1:3:15:DG:H2"	1:3:16:DA:H5'	1.41	1.03
3:D:47:GLN:HE22	3:D:51:ARG:HH11	1.03	0.94
3:A:47:GLN:HE22	3:A:51:ARG:HH11	0.98	0.91
1:1:15:DG:H2"	1:1:16:DA:H5'	1.55	0.89
2:2:24:DC:H2"	3:D:53:TRP:NE1	1.86	0.88
2:2:13:DA:H2"	2:2:14:DC:H5"	1.59	0.85
3:A:47:GLN:HE22	3:A:51:ARG:NH1	1.76	0.84
2:2:19:DT:H72	3:B:28:LYS:HD2	1.58	0.84
3:D:47:GLN:HE22	3:D:51:ARG:NH1	1.77	0.83
2:4:19:DT:H72	3:C:28:LYS:HD2	1.60	0.83
2:2:19:DT:C7	3:B:28:LYS:HD2	2.07	0.82
2:4:15:DG:H2"	2:4:16:DA:H5'	1.59	0.82
3:D:64:VAL:HG22	3:D:65:GLY:H	1.45	0.82
3:A:47:GLN:NE2	3:A:51:ARG:HH11	1.79	0.79
2:4:19:DT:C7	3:C:28:LYS:HD2	2.14	0.77
2:4:23:DG:H2"	2:4:24:DC:O5'	1.84	0.77
2:4:23:DG:H2'	2:4:24:DC:C6	2.20	0.77
3:D:30:ASN:HB3	3:D:33:TYR:CD1	2.21	0.76
3:B:124:GLU:O	3:B:127:THR:HB	1.86	0.76
3:C:124:GLU:O	3:C:127:THR:HB	1.86	0.76
2:2:23:DG:H2"	2:2:24:DC:O5'	1.85	0.74
2:4:13:DA:H1'	2:4:14:DC:O4'	1.86	0.74
1:3:13:DG:H2"	1:3:14:DA:H5"	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:30:ASN:HB3	3:A:33:TYR:CD1	2.23	0.74
3:D:47:GLN:NE2	3:D:51:ARG:HH11	1.85	0.74
3:A:144:THR:O	3:A:147:THR:HG23	1.87	0.74
2:2:15:DG:C2'	2:2:16:DA:H5'	2.13	0.73
3:A:64:VAL:HG22	3:A:65:GLY:H	1.52	0.73
2:2:24:DC:H2"	3:D:53:TRP:CD1	2.24	0.72
3:B:4:LYS:HA	3:B:90:GLN:HE22	1.55	0.72
2:2:2:DG:H5"	3:A:116:LYS:HD2	1.72	0.71
3:A:144:THR:H	3:A:147:THR:CG2	2.04	0.71
1:3:5:DA:H2"	1:3:6:DA:H5'	1.73	0.70
2:4:13:DA:H2"	2:4:14:DC:H5"	1.73	0.70
3:D:144:THR:H	3:D:147:THR:CG2	2.06	0.69
1:1:5:DA:H2"	1:1:6:DA:H5'	1.74	0.68
1:3:14:DA:H2"	1:3:15:DG:C8	2.29	0.68
3:D:30:ASN:HB3	3:D:33:TYR:HD1	1.60	0.67
3:D:144:THR:O	3:D:147:THR:HG23	1.94	0.67
3:C:4:LYS:HA	3:C:90:GLN:HE22	1.59	0.66
3:D:64:VAL:HG22	3:D:65:GLY:N	2.10	0.65
2:4:23:DG:H2'	2:4:24:DC:C5	2.32	0.65
2:4:17:DC:OP1	3:C:138:SER:HB3	1.97	0.64
3:A:80:GLU:O	3:A:83:PRO:HD2	1.98	0.64
3:D:80:GLU:O	3:D:83:PRO:HD2	1.97	0.63
1:1:14:DA:H2"	1:1:15:DG:C8	2.34	0.63
3:A:46:THR:O	3:A:47:GLN:HG2	1.99	0.63
3:A:30:ASN:HB3	3:A:33:TYR:HD1	1.63	0.62
2:2:13:DA:H1'	2:2:14:DC:O4'	2.00	0.62
2:4:1:DC:HO5'	2:4:1:DC:H6	1.48	0.61
3:A:51:ARG:NH2	3:B:137:ASP:OD2	2.28	0.61
2:2:19:DT:H73	3:B:28:LYS:HD2	1.83	0.61
3:D:130:ASP:OD1	3:D:141:ARG:NH2	2.34	0.60
3:A:130:ASP:OD1	3:A:141:ARG:NH2	2.34	0.60
3:C:30:ASN:HB3	3:C:33:TYR:CD1	2.36	0.60
3:D:138:SER:C	3:D:139:LYS:HG2	2.22	0.60
3:A:138:SER:C	3:A:139:LYS:HG2	2.19	0.60
3:B:13:LEU:O	3:B:17:VAL:HG23	2.00	0.60
3:A:137:ASP:OD2	3:B:51:ARG:NH2	2.35	0.60
3:B:144:THR:H	3:B:147:THR:CG2	2.14	0.60
1:3:12:DT:O3'	3:C:139:LYS:HE3	2.02	0.59
3:C:28:LYS:HE2	3:C:40:SER:CB	2.32	0.59
2:2:15:DG:H3'	3:B:22:SER:HB2	1.83	0.59
1:3:19:DG:OP1	3:D:142:LYS:HE3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:144:THR:H	3:C:147:THR:CG2	2.14	0.59
3:C:51:ARG:NH2	3:D:137:ASP:OD2	2.35	0.58
1:1:5:DA:H2"	1:1:6:DA:C5'	2.32	0.58
2:2:1:DC:H2'	3:A:32:SER:O	2.04	0.58
1:3:16:DA:H2"	1:3:17:DC:O5'	2.03	0.58
3:B:28:LYS:HE2	3:B:40:SER:CB	2.34	0.58
3:C:144:THR:HG23	3:C:147:THR:CG2	2.34	0.58
3:A:64:VAL:HG22	3:A:65:GLY:N	2.16	0.58
3:C:70:ARG:HG3	3:C:70:ARG:O	2.04	0.57
3:D:46:THR:O	3:D:47:GLN:HG2	2.04	0.57
3:B:30:ASN:HB3	3:B:33:TYR:CD1	2.40	0.57
3:B:123:LEU:HD11	3:B:149:ARG:HG2	1.86	0.57
3:D:47:GLN:HE21	3:D:48:LYS:H	1.53	0.57
3:C:123:LEU:HD11	3:C:149:ARG:HG2	1.86	0.56
2:2:17:DC:OP1	3:B:138:SER:HB3	2.04	0.56
3:A:144:THR:HG23	3:A:147:THR:HG22	1.87	0.56
2:4:9:DT:H2"	2:4:10:DC:C5	2.41	0.56
1:3:1:DG:H2'	3:C:32:SER:O	2.05	0.56
2:4:23:DG:H4'	2:4:24:DC:OP1	2.06	0.55
2:4:9:DT:H2"	2:4:10:DC:C6	2.42	0.55
3:B:24:ILE:HG22	3:B:25:ALA:N	2.22	0.55
3:C:129:VAL:HA	3:C:132:ILE:HG13	1.89	0.55
3:B:144:THR:O	3:B:147:THR:HG23	2.07	0.55
3:B:57:LYS:O	3:B:61:GLU:HG3	2.06	0.55
3:C:57:LYS:O	3:C:61:GLU:HG3	2.07	0.55
3:B:70:ARG:O	3:B:70:ARG:HG3	2.05	0.54
3:D:73:VAL:HG12	3:D:74:SER:N	2.22	0.54
2:2:16:DA:H2"	2:2:17:DC:O5'	2.07	0.54
2:2:17:DC:H2"	2:2:18:DG:H5'	1.90	0.54
1:3:17:DC:C2'	1:3:18:DA:H5'	2.37	0.54
3:C:24:ILE:HG22	3:C:25:ALA:N	2.23	0.54
3:D:144:THR:HG23	3:D:147:THR:HG22	1.90	0.54
3:C:144:THR:H	3:C:147:THR:HG23	1.72	0.54
3:C:144:THR:O	3:C:147:THR:HG23	2.08	0.54
3:B:73:VAL:HG12	3:B:74:SER:N	2.24	0.53
3:B:144:THR:HG23	3:B:147:THR:CG2	2.38	0.53
1:1:16:DA:H2"	1:1:17:DC:O5'	2.08	0.53
2:4:15:DG:C2'	2:4:16:DA:H5'	2.37	0.53
3:C:20:ASP:OD1	5:C:205:HOH:O	2.19	0.53
3:B:144:THR:H	3:B:147:THR:HG23	1.72	0.53
3:A:9:PHE:CZ	3:A:13:LEU:HD22	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:13:LEU:O	3:C:17:VAL:HG23	2.08	0.52
2:2:2:DG:H5"	3:A:116:LYS:CD	2.39	0.52
2:2:17:DC:C2'	2:2:18:DG:H5'	2.39	0.52
1:1:11:DG:H1	2:2:14:DC:H42	1.57	0.52
3:A:144:THR:H	3:A:147:THR:HG21	1.74	0.52
3:D:23:ILE:HD12	3:D:98:LYS:HB3	1.92	0.52
3:D:57:LYS:O	3:D:61:GLU:HG3	2.10	0.52
3:A:47:GLN:HE21	3:A:48:LYS:H	1.57	0.52
1:3:17:DC:OP1	3:D:138:SER:HB3	2.10	0.51
1:3:17:DC:H2"	1:3:18:DA:H5'	1.91	0.51
3:C:28:LYS:HE2	3:C:40:SER:HB2	1.92	0.51
3:C:80:GLU:HB3	3:C:83:PRO:CD	2.41	0.51
3:C:80:GLU:HB3	3:C:83:PRO:HD2	1.92	0.51
3:C:101:GLN:HB3	3:C:132:ILE:HG23	1.93	0.51
3:D:73:VAL:CG1	3:D:74:SER:N	2.74	0.51
3:A:57:LYS:O	3:A:61:GLU:HG3	2.11	0.51
3:B:101:GLN:HB3	3:B:132:ILE:HG23	1.93	0.50
3:B:80:GLU:HB3	3:B:83:PRO:CD	2.41	0.50
3:A:28:LYS:HE2	3:A:40:SER:HB2	1.93	0.50
3:D:91:LEU:C	3:D:93:PRO:HD2	2.31	0.50
3:D:123:LEU:HD11	3:D:149:ARG:CG	2.41	0.50
3:C:73:VAL:HG12	3:C:74:SER:N	2.27	0.50
3:C:104:LEU:HD13	3:C:132:ILE:HG12	1.94	0.50
3:A:96:LYS:HD3	3:B:12:TYR:CZ	2.46	0.50
3:D:124:GLU:O	3:D:127:THR:HB	2.12	0.50
3:A:123:LEU:HD11	3:A:149:ARG:CG	2.42	0.50
3:A:124:GLU:O	3:A:127:THR:HB	2.12	0.49
3:A:73:VAL:HG12	3:A:74:SER:N	2.25	0.49
1:1:12:DT:O3'	3:B:139:LYS:HE3	2.12	0.49
1:3:24:DG:H1	2:4:1:DC:H42	1.59	0.49
2:2:22:DT:H2"	2:2:23:DG:O4'	2.13	0.49
2:4:12:DC:O3'	3:D:139:LYS:HE3	2.12	0.49
3:D:28:LYS:HE2	3:D:40:SER:HB2	1.94	0.49
2:2:9:DT:H2"	2:2:10:DC:C5	2.48	0.49
3:A:107:LYS:HE2	3:A:128:TRP:CE2	2.48	0.49
3:B:80:GLU:HB3	3:B:83:PRO:HD2	1.95	0.49
1:1:6:DA:H2"	1:1:7:DC:O5'	2.13	0.49
1:3:24:DG:H1	2:4:1:DC:N4	2.10	0.49
3:A:148:VAL:HG12	3:A:148:VAL:O	2.13	0.49
2:4:22:DT:H2'	2:4:23:DG:C8	2.48	0.49
3:A:23:ILE:HD12	3:A:98:LYS:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:15:DG:H2"	1:3:16:DA:C5'	2.28	0.48
3:D:100:LYS:HB2	3:D:135:LEU:HD13	1.95	0.48
3:B:80:GLU:O	3:B:83:PRO:HD2	2.14	0.48
3:B:23:ILE:CG2	3:B:105:VAL:HG21	2.43	0.48
3:B:75:ASP:HB2	3:B:77:ILE:HD11	1.95	0.48
3:C:12:TYR:CZ	3:D:96:LYS:HD3	2.49	0.48
3:D:9:PHE:CZ	3:D:13:LEU:HD22	2.48	0.48
2:4:8:DG:H2"	2:4:9:DT:H5'	1.95	0.47
3:D:107:LYS:HE2	3:D:128:TRP:CE2	2.49	0.47
3:D:33:TYR:CZ	3:D:38:GLN:HB2	2.49	0.47
3:A:73:VAL:CG1	3:A:74:SER:N	2.78	0.47
3:A:91:LEU:C	3:A:93:PRO:HD2	2.34	0.47
3:B:144:THR:OG1	3:B:145:SER:N	2.48	0.47
3:B:125:VAL:C	3:B:127:THR:N	2.68	0.47
3:D:127:THR:HG22	3:D:128:TRP:CE3	2.50	0.47
1:1:1:DG:H1'	1:1:2:DC:O5'	2.15	0.47
1:1:14:DA:OP2	3:A:47:GLN:HA	2.14	0.47
2:2:19:DT:H72	3:B:28:LYS:HB3	1.97	0.47
1:3:5:DA:H2"	1:3:6:DA:C5'	2.43	0.47
1:3:15:DG:OP2	3:D:20:ASP:OD1	2.32	0.47
3:A:101:GLN:HB3	3:A:132:ILE:HG23	1.96	0.47
1:3:2:DC:H2'	3:C:33:TYR:CE2	2.50	0.47
2:4:19:DT:H72	3:C:28:LYS:HB3	1.97	0.47
3:B:28:LYS:HE2	3:B:40:SER:HB2	1.96	0.47
3:D:64:VAL:CG2	3:D:65:GLY:H	2.23	0.47
1:1:15:DG:C2'	1:1:16:DA:H5'	2.37	0.47
1:3:23:DC:H42	2:4:2:DG:H1	1.63	0.47
3:B:112:LEU:N	3:B:113:PRO:HD2	2.30	0.47
3:C:29:PRO:HA	3:C:37:HIS:HD2	1.79	0.47
3:B:104:LEU:HD13	3:B:132:ILE:HG12	1.96	0.46
3:C:29:PRO:HA	3:C:37:HIS:CD2	2.50	0.46
3:D:112:LEU:N	3:D:113:PRO:HD2	2.30	0.46
2:2:24:DC:H2"	3:D:53:TRP:HE1	1.74	0.46
3:B:129:VAL:HA	3:B:132:ILE:HG13	1.96	0.46
3:C:20:ASP:OD2	3:C:47:GLN:NE2	2.48	0.46
3:A:82:LYS:HA	3:A:82:LYS:HD2	1.69	0.46
3:A:127:THR:HG22	3:A:128:TRP:CE3	2.50	0.46
3:C:80:GLU:O	3:C:83:PRO:HD2	2.16	0.46
3:C:125:VAL:C	3:C:127:THR:N	2.68	0.46
3:D:148:VAL:HG12	3:D:148:VAL:O	2.14	0.46
2:4:19:DT:H73	3:C:28:LYS:HD2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:144:THR:N	3:D:147:THR:CG2	2.78	0.46
3:A:54:PHE:CD2	3:B:97:LEU:HD21	2.51	0.46
1:1:16:DA:H1'	1:1:17:DC:O4'	2.16	0.45
3:A:33:TYR:CZ	3:A:38:GLN:HB2	2.51	0.45
3:A:99:GLN:O	3:A:99:GLN:HG2	2.17	0.45
3:D:144:THR:H	3:D:147:THR:HG21	1.80	0.45
3:C:112:LEU:N	3:C:113:PRO:HD2	2.31	0.45
3:A:104:LEU:HD23	3:A:104:LEU:HA	1.78	0.45
3:A:144:THR:CG2	3:A:147:THR:HG22	2.47	0.45
3:A:148:VAL:O	3:A:151:VAL:HG23	2.17	0.45
3:C:115:ALA:HA	3:C:121:LYS:HB3	1.99	0.45
3:A:80:GLU:C	3:A:83:PRO:HD2	2.36	0.45
3:B:104:LEU:O	3:B:108:ILE:HG13	2.17	0.45
3:C:75:ASP:HB2	3:C:77:ILE:HD11	1.98	0.45
3:C:104:LEU:O	3:C:108:ILE:HG13	2.17	0.45
3:C:125:VAL:C	3:C:127:THR:H	2.19	0.45
3:D:55:LEU:O	3:D:58:LEU:HB2	2.16	0.44
2:2:19:DT:H1'	2:2:20:DT:H5'	1.99	0.44
3:A:58:LEU:HD22	3:A:62:ILE:CD1	2.47	0.44
1:1:13:DG:H2"	1:1:14:DA:OP2	2.17	0.44
3:C:23:ILE:CG2	3:C:105:VAL:HG21	2.48	0.44
3:D:144:THR:O	3:D:148:VAL:HG23	2.17	0.44
1:3:2:DC:H5	3:C:32:SER:OG	2.00	0.44
3:B:138:SER:C	3:B:139:LYS:HG2	2.37	0.44
3:C:52:ARG:O	3:C:55:LEU:N	2.48	0.44
3:D:64:VAL:CG2	3:D:65:GLY:N	2.80	0.44
3:A:144:THR:OG1	3:A:145:SER:N	2.50	0.44
3:A:144:THR:N	3:A:147:THR:CG2	2.76	0.44
3:D:101:GLN:HB3	3:D:132:ILE:HG23	2.00	0.44
3:D:144:THR:CG2	3:D:147:THR:HG22	2.47	0.44
3:D:148:VAL:O	3:D:151:VAL:HG23	2.18	0.44
3:C:46:THR:O	3:C:47:GLN:HG2	2.18	0.44
3:D:80:GLU:C	3:D:83:PRO:HD2	2.37	0.44
3:B:125:VAL:C	3:B:127:THR:H	2.21	0.44
3:A:58:LEU:HD22	3:A:62:ILE:HD11	1.99	0.44
3:A:127:THR:O	3:A:130:ASP:HB2	2.17	0.44
3:B:86:ASN:O	3:B:90:GLN:HG3	2.17	0.44
3:B:52:ARG:O	3:B:55:LEU:N	2.48	0.43
2:4:8:DG:H2"	2:4:9:DT:C5'	2.48	0.43
2:4:16:DA:H2"	2:4:17:DC:O5'	2.17	0.43
3:A:51:ARG:HH22	3:B:137:ASP:CG	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:112:LEU:N	3:A:113:PRO:HD2	2.33	0.43
3:D:92:GLN:HG3	3:D:103:ASN:CG	2.38	0.43
2:2:3:DA:H2"	2:2:4:DA:O5'	2.19	0.43
3:C:27:ILE:HG21	3:C:148:VAL:CG2	2.49	0.43
3:D:47:GLN:HE21	3:D:48:LYS:N	2.16	0.43
3:D:127:THR:O	3:D:130:ASP:HB2	2.18	0.43
1:1:17:DC:H2'	1:1:18:DA:C8	2.53	0.43
3:B:146:GLU:OE2	3:B:149:ARG:NH1	2.52	0.43
2:4:19:DT:C7	3:C:28:LYS:CD	2.92	0.43
3:B:29:PRO:HA	3:B:37:HIS:CD2	2.54	0.43
3:C:92:GLN:N	3:C:93:PRO:HD2	2.34	0.43
3:A:55:LEU:O	3:A:58:LEU:HB2	2.19	0.42
3:B:47:GLN:OE1	3:B:51:ARG:HD2	2.18	0.42
3:B:80:GLU:HB3	3:B:83:PRO:HG2	2.00	0.42
3:C:144:THR:OG1	3:C:145:SER:N	2.51	0.42
3:D:58:LEU:HD22	3:D:62:ILE:CD1	2.49	0.42
3:A:100:LYS:HB2	3:A:135:LEU:HD13	2.01	0.42
3:D:82:LYS:N	3:D:83:PRO:CD	2.82	0.42
3:D:92:GLN:HG3	3:D:103:ASN:ND2	2.34	0.42
3:A:51:ARG:NH2	3:B:137:ASP:OD1	2.53	0.42
3:A:144:THR:O	3:A:148:VAL:HG23	2.19	0.42
3:B:29:PRO:HA	3:B:37:HIS:HD2	1.85	0.42
3:B:144:THR:N	3:B:147:THR:HG23	2.35	0.42
3:C:33:TYR:CZ	3:C:38:GLN:HB2	2.55	0.42
3:D:58:LEU:HD22	3:D:62:ILE:HD11	2.01	0.42
3:B:92:GLN:N	3:B:93:PRO:HD2	2.35	0.42
3:C:130:ASP:OD1	3:C:141:ARG:NH2	2.52	0.42
3:A:92:GLN:N	3:A:93:PRO:HD2	2.35	0.42
3:B:64:VAL:HG13	3:B:65:GLY:N	2.34	0.42
3:C:146:GLU:OE2	3:C:149:ARG:NH1	2.53	0.42
3:B:115:ALA:HA	3:B:121:LYS:HB3	2.00	0.42
1:1:4:DA:H2"	1:1:5:DA:OP2	2.19	0.42
3:C:24:ILE:CG2	3:C:25:ALA:N	2.83	0.41
3:C:64:VAL:HG13	3:C:65:GLY:N	2.35	0.41
1:3:6:DA:H2"	1:3:7:DC:O5'	2.20	0.41
2:4:2:DG:H2'	2:4:3:DA:C8	2.55	0.41
3:A:82:LYS:N	3:A:83:PRO:CD	2.83	0.41
3:B:24:ILE:CG2	3:B:25:ALA:N	2.82	0.41
3:C:138:SER:C	3:C:139:LYS:HG2	2.39	0.41
3:D:99:GLN:O	3:D:99:GLN:HG2	2.19	0.41
1:1:13:DG:H2"	1:1:14:DA:H5"	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:1:DG:H1'	1:3:2:DC:H5'	2.02	0.41
3:B:144:THR:H	3:B:147:THR:HG21	1.83	0.41
3:D:104:LEU:HD23	3:D:104:LEU:HA	1.77	0.41
2:4:19:DT:H73	3:C:28:LYS:CD	2.51	0.41
3:B:52:ARG:HA	3:B:55:LEU:HD22	2.03	0.41
3:C:144:THR:N	3:C:147:THR:HG23	2.35	0.41
1:1:14:DA:N6	2:2:10:DC:N4	2.68	0.41
1:3:24:DG:N2	2:4:1:DC:N3	2.68	0.41
3:A:51:ARG:NH2	3:B:137:ASP:CG	2.73	0.41
3:B:27:ILE:HG21	3:B:148:VAL:CG2	2.50	0.41
1:3:15:DG:C2'	1:3:16:DA:H5'	2.29	0.41
2:4:2:DG:OP1	3:D:116:LYS:HG2	2.20	0.41
3:C:6:ASN:HB3	3:C:9:PHE:HB3	2.02	0.41
1:1:1:DG:H1'	1:1:2:DC:C5'	2.51	0.41
5:1:203:HOH:O	2:2:15:DG:P	2.78	0.41
2:4:18:DG:H5"	3:C:142:LYS:HB2	2.02	0.41
2:4:23:DG:H2"	2:4:24:DC:C5'	2.50	0.41
3:A:80:GLU:HB3	3:A:83:PRO:HG2	2.02	0.41
3:B:6:ASN:HD22	3:B:8:GLU:H	1.69	0.41
3:D:144:THR:OG1	3:D:145:SER:N	2.52	0.41
3:B:128:TRP:O	3:B:131:GLN:HB2	2.21	0.41
3:C:144:THR:H	3:C:147:THR:HG21	1.83	0.41
3:C:51:ARG:NH2	3:D:137:ASP:OD1	2.54	0.40
3:B:112:LEU:N	3:B:113:PRO:CD	2.84	0.40
3:A:96:LYS:HD3	3:B:12:TYR:CE2	2.56	0.40
3:D:70:ARG:HG3	3:D:70:ARG:O	2.21	0.40
3:B:130:ASP:OD1	3:B:141:ARG:NH2	2.54	0.40
3:C:112:LEU:N	3:C:113:PRO:CD	2.84	0.40
3:D:82:LYS:HA	3:D:82:LYS:HD2	1.71	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	
3	A	150/152 (99%)	136 (91%)	14 (9%)	0	100	100
3	B	150/152 (99%)	136 (91%)	13 (9%)	1 (1%)	22	60
3	C	150/152 (99%)	136 (91%)	12 (8%)	2 (1%)	12	45
3	D	150/152 (99%)	134 (89%)	16 (11%)	0	100	100
All	All	600/608 (99%)	542 (90%)	55 (9%)	3 (0%)	29	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	139	LYS
3	C	139	LYS
3	C	53	TRP

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	
3	A	139/139 (100%)	100 (72%)	39 (28%)	0	2
3	B	139/139 (100%)	99 (71%)	40 (29%)	0	2
3	C	139/139 (100%)	101 (73%)	38 (27%)	0	2
3	D	139/139 (100%)	98 (70%)	41 (30%)	0	1
All	All	556/556 (100%)	398 (72%)	158 (28%)	0	2

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	3	THR
3	A	7	LYS
3	A	28	LYS
3	A	34	LYS
3	A	36	LYS
3	A	40	SER
3	A	42	THR
3	A	44	GLN

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Mol	Chain	Res	Type
3	A	46	THR
3	A	47	GLN
3	A	50	GLN
3	A	55	LEU
3	A	57	LYS
3	A	68	ARG
3	A	69	ASP
3	A	72	SER
3	A	78	LEU
3	A	82	LYS
3	A	89	THR
3	A	96	LYS
3	A	101	GLN
3	A	106	LEU
3	A	110	GLU
3	A	116	LYS
3	A	117	GLU
3	A	120	ASP
3	A	121	LYS
3	A	123	LEU
3	A	124	GLU
3	A	126	CYS
3	A	127	THR
3	A	128	TRP
3	A	138	SER
3	A	139	LYS
3	A	141	ARG
3	A	142	LYS
3	A	144	THR
3	A	145	SER
3	A	147	THR
3	B	3	THR
3	B	7	LYS
3	B	28	LYS
3	B	34	LYS
3	B	36	LYS
3	B	42	THR
3	B	44	GLN
3	B	46	THR
3	B	48	LYS
3	B	50	GLN
3	B	55	LEU

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Mol	Chain	Res	Type
3	B	57	LYS
3	B	64	VAL
3	B	68	ARG
3	B	69	ASP
3	B	72	SER
3	B	74	SER
3	B	78	LEU
3	B	79	SER
3	B	82	LYS
3	B	89	THR
3	B	96	LYS
3	B	101	GLN
3	B	106	LEU
3	B	110	GLU
3	B	112	LEU
3	B	114	SER
3	B	116	LYS
3	B	123	LEU
3	B	124	GLU
3	B	127	THR
3	B	128	TRP
3	B	138	SER
3	B	139	LYS
3	B	140	THR
3	B	142	LYS
3	B	143	THR
3	B	144	THR
3	B	145	SER
3	B	147	THR
3	C	3	THR
3	C	7	LYS
3	C	28	LYS
3	C	34	LYS
3	C	36	LYS
3	C	42	THR
3	C	44	GLN
3	C	46	THR
3	C	48	LYS
3	C	55	LEU
3	C	57	LYS
3	C	64	VAL
3	C	68	ARG

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Mol	Chain	Res	Type
3	C	69	ASP
3	C	72	SER
3	C	74	SER
3	C	78	LEU
3	C	79	SER
3	C	82	LYS
3	C	89	THR
3	C	96	LYS
3	C	101	GLN
3	C	106	LEU
3	C	110	GLU
3	C	112	LEU
3	C	114	SER
3	C	116	LYS
3	C	123	LEU
3	C	124	GLU
3	C	127	THR
3	C	128	TRP
3	C	138	SER
3	C	139	LYS
3	C	140	THR
3	C	142	LYS
3	C	143	THR
3	C	144	THR
3	C	147	THR
3	D	3	THR
3	D	7	LYS
3	D	28	LYS
3	D	32	SER
3	D	34	LYS
3	D	36	LYS
3	D	40	SER
3	D	42	THR
3	D	44	GLN
3	D	46	THR
3	D	47	GLN
3	D	50	GLN
3	D	55	LEU
3	D	57	LYS
3	D	68	ARG
3	D	69	ASP
3	D	72	SER

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Mol	Chain	Res	Type
3	D	78	LEU
3	D	82	LYS
3	D	89	THR
3	D	96	LYS
3	D	101	GLN
3	D	103	ASN
3	D	106	LEU
3	D	110	GLU
3	D	116	LYS
3	D	117	GLU
3	D	120	ASP
3	D	121	LYS
3	D	123	LEU
3	D	124	GLU
3	D	126	CYS
3	D	127	THR
3	D	128	TRP
3	D	130	ASP
3	D	138	SER
3	D	139	LYS
3	D	142	LYS
3	D	144	THR
3	D	145	SER
3	D	147	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	6	ASN
3	A	26	GLN
3	A	37	HIS
3	A	44	GLN
3	A	47	GLN
3	B	6	ASN
3	B	26	GLN
3	B	37	HIS
3	B	44	GLN
3	B	90	GLN
3	B	103	ASN
3	C	6	ASN
3	C	37	HIS
3	C	44	GLN

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Mol	Chain	Res	Type
3	C	90	GLN
3	C	103	ASN
3	D	6	ASN
3	D	37	HIS
3	D	44	GLN
3	D	47	GLN
3	D	50	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.