Full wwPDB X-ray Structure Validation Report (i)

May 28, 2020 – 08:12 pm BST

PDB ID	:	1P8K
Title	:	The structure and DNA recognition of a bifunctional homing endonuclease and group I intron splicing factor
Authors	:	Stoddard, B.L.; Bolduc, J.M.
Deposited on	:	2003-05-07
Resolution	:	2.60 Å(reported)

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

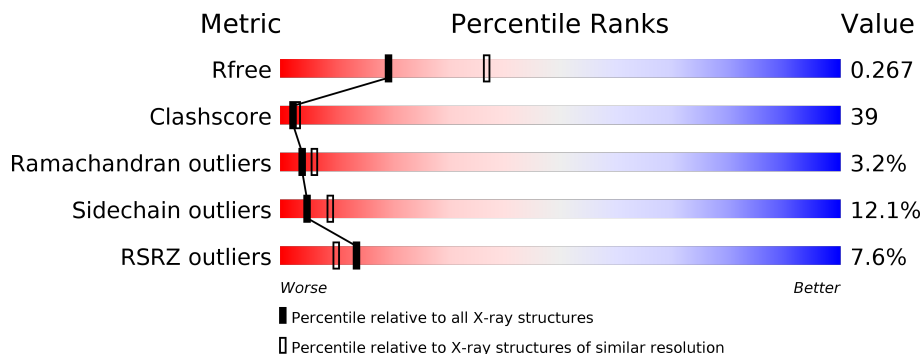|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.60 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	Percentile Ranks	Value
Rfree		0.267
Clashscore		39
Ramachandran outliers		3.2%
Sidechain outliers		12.1%
RSRZ outliers		7.6%

Worse ———— *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	18	6% / 44% 50% 6%
2	B	13	8% / 92% 8%
3	C	16	13% / 38% 56% 6%
4	D	15	13% / 47% 47% 7%
5	Z	254	7% / 46% 44% 9% •

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 3362 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 5'-D(P*GP*CP*GP*CP*GP*CP*TP*GP*AP*GP*GP* AP*GP*GP*TP*TP*TP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	18	375	176	70	111	18	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	13	268	127	50	78	13	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	16	332	157	65	94	16	0	0	0

- Molecule 4 is a DNA chain called 5'-D(P*CP*CP*TP*CP*CP*TP*CP*AP*GP*CP*GP*C P*GP*CP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	D	15	300	142	50	93	15	0	0	0

- Molecule 5 is a protein called Intron-encoded endonuclease I-AniI.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
5	Z	254	2085	1363	339	379	2	2	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	1	GLY	-	CLONING ARTIFACT	UNP P03880
Z	2	SER	-	CLONING ARTIFACT	UNP P03880
Z	61	ARG	ILE	SEE REMARK 999	UNP P03880
Z	66	MSE	MET	MODIFIED RESIDUE	UNP P03880
Z	90	MSE	MET	MODIFIED RESIDUE	UNP P03880

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

| Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Mg 1 1	0	0
6	Z	1	Total Mg 1 1	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
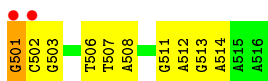
• Molecule 1: 5'-D(P*GP*CP*GP*CP*GP*CP*TP*GP*AP*GP*GP*AP*GP*GP*TP*TP*TP* C)-3'

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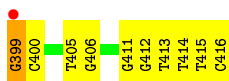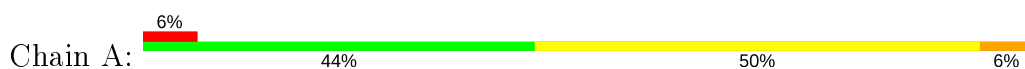
• Molecule 2: 5'-D(P*TP*CP*TP*GP*TP*AP*AP*AP*GP*CP*GP*CP*A)-3'

Chain B:
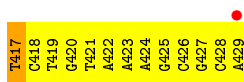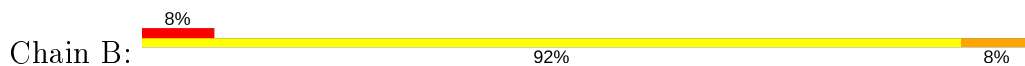
• Molecule 3: 5'-D(P*GP*CP*GP*CP*TP*TP*TP*AP*CP*AP*GP*AP*GP*AP*AP*A)-3'
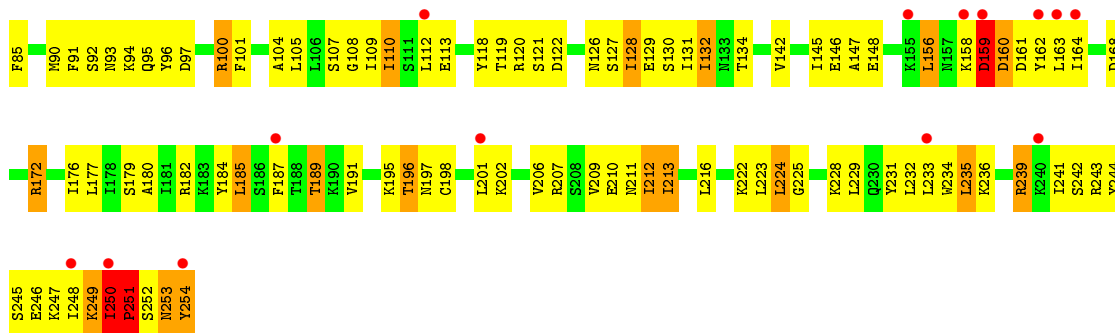
Chain C:

• Molecule 4: 5'-D(P*CP*CP*TP*CP*CP*TP*CP*AP*GP*CP*GP*CP*GP*CP*T)-3'

Chain D:

• Molecule 5: Intron-encoded endonuclease I-AniI

Chain Z:

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	60.46Å 72.84Å 65.23Å 90.00° 108.21° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 47.20 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.60) 88.5 (47.20-2.60)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.67 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.239 , 0.264 0.243 , 0.267	Depositor DCC
R_{free} test set	2799 reflections (9.50%)	wwPDB-VP
Wilson B-factor (Å^2)	37.2	Xtriage
Anisotropy	0.855	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 54.3	EDS
L-test for twinning[2]	$<|L|> = 0.49$, $<L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3362	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.90% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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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: 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	A	0.99	2/420 (0.5%)	0.86	0/646
2	B	1.06	2/300 (0.7%)	0.85	0/459
3	C	0.98	3/373 (0.8%)	0.82	0/572
4	D	1.11	2/333 (0.6%)	0.93	0/508
5	Z	0.67	1/2124 (0.0%)	1.04	11/2854 (0.4%)
All	All	0.84	10/3550 (0.3%)	0.97	11/5039 (0.2%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	517	DC	P-O5'	6.94	1.66	1.59
1	A	399	DG	P-O5'	6.53	1.66	1.59
3	C	501	DG	P-O5'	6.28	1.66	1.59
2	B	417	DT	P-O5'	6.06	1.65	1.59
2	B	417	DT	OP3-P	-5.72	1.54	1.61
5	Z	251	PRO	CB-CG	5.64	1.78	1.50
3	C	501	DG	P-OP1	5.37	1.58	1.49
1	A	399	DG	P-OP1	5.36	1.58	1.49
3	C	501	DG	P-OP2	5.21	1.57	1.49
4	D	517	DC	P-OP1	5.02	1.57	1.49

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Z	251	PRO	N-CA-C	10.90	140.44	112.10
5	Z	62	ASN	N-CA-C	9.82	137.53	111.00
5	Z	250	ILE	N-CA-C	8.20	133.15	111.00
5	Z	249	LYS	CB-CG-CD	-7.76	91.42	111.60
5	Z	250	ILE	CB-CA-C	-7.33	96.94	111.60
5	Z	61	ARG	N-CA-C	-7.05	91.97	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	Z	62	ASN	C-N-CA	-6.22	106.15	121.70
5	Z	62	ASN	N-CA-CB	-5.85	100.08	110.60
5	Z	249	LYS	CD-CE-NZ	-5.73	98.52	111.70
5	Z	3	ASP	N-CA-C	-5.21	96.94	111.00
5	Z	254	TYR	N-CA-C	5.11	124.79	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	375	0	203	14	1
2	B	268	0	147	22	0
3	C	332	0	180	17	1
4	D	300	0	169	18	0
5	Z	2085	0	2164	178	0
6	B	1	0	0	0	0
6	Z	1	0	0	0	0
All	All	3362	0	2863	239	1

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 39.

All (239) 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:Z:251:PRO:CG	5:Z:251:PRO:CB	1.78	1.52
5:Z:222:LYS:HA	5:Z:254:TYR:CE1	1.61	1.36
5:Z:222:LYS:CA	5:Z:254:TYR:HE1	1.41	1.32
2:B:425:DG:H2"	2:B:426:DC:H5'	1.36	1.08
5:Z:231:TYR:CD2	5:Z:254:TYR:O	2.09	1.04
4:D:529:DG:H2"	4:D:530:DC:H5"	1.35	1.04
5:Z:231:TYR:HD2	5:Z:254:TYR:O	1.41	1.02
5:Z:249:LYS:O	5:Z:250:ILE:HG13	1.60	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:530:DC:H2"	4:D:531:DT:OP1	1.61	1.01
1:A:415:DT:H2"	1:A:416:DC:H5"	1.45	0.98
5:Z:222:LYS:HA	5:Z:254:TYR:HE1	0.81	0.97
4:D:524:DA:H2"	4:D:525:DG:H5'	1.46	0.95
5:Z:223:LEU:N	5:Z:254:TYR:CE1	2.34	0.95
5:Z:142:VAL:CG1	5:Z:254:TYR:OH	2.18	0.92
2:B:419:DT:H2"	2:B:420:DG:H5"	1.51	0.91
5:Z:239:ARG:NH2	5:Z:251:PRO:CG	2.34	0.90
5:Z:210:GLU:HB2	5:Z:248:ILE:HD11	1.51	0.89
5:Z:127:SER:HA	5:Z:176:ILE:HG21	1.54	0.88
3:C:501:DG:H4'	3:C:502:DC:H5'	1.51	0.88
5:Z:222:LYS:CA	5:Z:254:TYR:CE1	2.34	0.86
5:Z:216:LEU:HD22	5:Z:254:TYR:HE2	1.40	0.86
5:Z:223:LEU:HG	5:Z:254:TYR:CE2	2.13	0.83
5:Z:247:LYS:O	5:Z:248:ILE:HG13	1.78	0.82
5:Z:142:VAL:HG11	5:Z:254:TYR:OH	1.79	0.82
5:Z:235:LEU:HG	5:Z:250:ILE:HG21	1.62	0.80
5:Z:38:ILE:O	5:Z:41:VAL:HG23	1.81	0.79
4:D:529:DG:C2'	4:D:530:DC:H5"	2.11	0.79
5:Z:110:ILE:H	5:Z:110:ILE:HD13	1.49	0.78
5:Z:235:LEU:HG	5:Z:250:ILE:CG2	2.13	0.77
5:Z:210:GLU:HA	5:Z:248:ILE:HD13	1.66	0.77
4:D:528:DC:H2"	4:D:529:DG:C8	2.20	0.77
4:D:524:DA:C2'	4:D:525:DG:H5'	2.15	0.76
3:C:501:DG:H1'	3:C:502:DC:C6	2.19	0.76
5:Z:142:VAL:HG13	5:Z:254:TYR:OH	1.84	0.76
4:D:530:DC:H2'	4:D:531:DT:H72	1.67	0.75
5:Z:130:SER:O	5:Z:134:THR:HG23	1.87	0.75
5:Z:223:LEU:HG	5:Z:254:TYR:CZ	2.21	0.75
2:B:420:DG:H2'	2:B:421:DT:H72	1.69	0.75
5:Z:6:TYR:CD2	5:Z:84:ILE:HD12	2.22	0.75
5:Z:60:LYS:O	5:Z:61:ARG:C	2.25	0.74
5:Z:248:ILE:HG22	5:Z:249:LYS:N	2.02	0.74
2:B:420:DG:H2'	2:B:421:DT:C7	2.18	0.74
5:Z:231:TYR:CE2	5:Z:254:TYR:O	2.40	0.74
5:Z:239:ARG:NH2	5:Z:251:PRO:HG2	2.01	0.74
1:A:412:DG:H2"	1:A:413:DT:OP2	1.88	0.73
5:Z:239:ARG:NH2	5:Z:251:PRO:HG3	2.04	0.71
3:C:513:DG:H2"	3:C:514:DA:N7	2.05	0.71
3:C:513:DG:H2"	3:C:514:DA:C8	2.26	0.71
5:Z:100:ARG:HH11	5:Z:100:ARG:CG	2.04	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Z:54:GLY:HA3	5:Z:69:LEU:HD11	1.72	0.71
5:Z:100:ARG:HG3	5:Z:100:ARG:HH11	1.56	0.70
5:Z:222:LYS:HG2	5:Z:254:TYR:CD1	2.27	0.70
3:C:506:DT:OP1	5:Z:206:VAL:HG23	1.92	0.70
5:Z:210:GLU:HB2	5:Z:248:ILE:CD1	2.20	0.70
1:A:412:DG:O6	5:Z:61:ARG:NH1	2.25	0.69
5:Z:172:ARG:HE	5:Z:196:THR:HG22	1.58	0.68
5:Z:163:LEU:HD12	5:Z:241:ILE:HG12	1.74	0.68
1:A:415:DT:C2'	1:A:416:DC:H5"	2.23	0.68
3:C:512:DA:C3'	3:C:513:DG:H5"	2.25	0.67
5:Z:46:LYS:O	5:Z:50:ILE:HG12	1.95	0.67
5:Z:2:SER:N	5:Z:5:THR:OG1	2.23	0.67
4:D:530:DC:C2'	4:D:531:DT:OP1	2.42	0.66
5:Z:104:ALA:HA	5:Z:109:ILE:HD12	1.76	0.66
1:A:406:DG:O6	5:Z:24:LYS:HE2	1.96	0.66
5:Z:60:LYS:O	5:Z:61:ARG:O	2.13	0.66
5:Z:222:LYS:NZ	5:Z:253:ASN:HB3	2.11	0.65
5:Z:249:LYS:C	5:Z:250:ILE:HG13	2.17	0.65
5:Z:223:LEU:HD12	5:Z:254:TYR:OXT	1.96	0.65
2:B:427:DG:OP1	2:B:427:DG:H4'	1.97	0.65
5:Z:118:TYR:OH	5:Z:120:ARG:HG2	1.96	0.64
5:Z:216:LEU:HD22	5:Z:254:TYR:CE2	2.28	0.64
2:B:421:DT:H2"	2:B:422:DA:C8	2.30	0.64
5:Z:127:SER:HA	5:Z:176:ILE:CG2	2.27	0.64
5:Z:110:ILE:H	5:Z:110:ILE:CD1	2.10	0.64
2:B:428:DC:H2"	2:B:429:DA:C5	2.32	0.64
2:B:425:DG:C2'	2:B:426:DC:H5'	2.23	0.64
5:Z:43:LEU:HD13	5:Z:224:LEU:HD12	1.80	0.63
5:Z:162:TYR:CZ	5:Z:243:ARG:NH2	2.66	0.63
5:Z:222:LYS:CB	5:Z:254:TYR:CE1	2.81	0.63
5:Z:250:ILE:HB	5:Z:251:PRO:HD3	1.79	0.63
5:Z:228:LYS:HE3	5:Z:253:ASN:OD1	1.99	0.62
5:Z:222:LYS:HA	5:Z:254:TYR:CZ	2.29	0.62
5:Z:222:LYS:CG	5:Z:254:TYR:CD1	2.83	0.61
5:Z:92:SER:C	5:Z:94:LYS:H	2.01	0.61
4:D:529:DG:H2"	4:D:530:DC:C5'	2.21	0.61
4:D:517:DC:OP3	5:Z:94:LYS:HE3	1.99	0.61
2:B:423:DA:C2	2:B:424:DA:C4	2.89	0.61
3:C:512:DA:C2'	3:C:513:DG:H5"	2.30	0.61
5:Z:196:THR:HG22	5:Z:197:ASN:H	1.65	0.61
2:B:420:DG:O6	5:Z:202:LYS:HE3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Z:239:ARG:HH21	5:Z:251:PRO:HG2	1.66	0.60
3:C:512:DA:H2"	3:C:513:DG:O4'	2.01	0.60
5:Z:212:ILE:HD13	5:Z:212:ILE:H	1.66	0.60
5:Z:239:ARG:CZ	5:Z:251:PRO:HG3	2.30	0.60
4:D:530:DC:H2"	4:D:531:DT:C6	2.36	0.60
5:Z:82:LEU:N	5:Z:83:PRO:HD2	2.16	0.60
5:Z:156:LEU:HD12	5:Z:156:LEU:O	2.01	0.60
3:C:501:DG:H1'	3:C:502:DC:C5	2.37	0.59
5:Z:60:LYS:O	5:Z:64:ILE:O	2.20	0.59
2:B:417:DT:OP1	5:Z:147:ALA:O	2.20	0.59
5:Z:126:ASN:HB2	5:Z:131:ILE:HD11	1.85	0.59
5:Z:5:THR:O	5:Z:8:TYR:HB3	2.04	0.58
3:C:512:DA:H2"	3:C:513:DG:H5"	1.85	0.57
5:Z:212:ILE:HD13	5:Z:212:ILE:N	2.18	0.57
5:Z:248:ILE:HG22	5:Z:249:LYS:H	1.67	0.57
1:A:414:DT:H2"	1:A:415:DT:C7	2.34	0.57
2:B:419:DT:C2'	2:B:420:DG:H5"	2.27	0.57
5:Z:248:ILE:CG2	5:Z:249:LYS:N	2.68	0.57
5:Z:58:PHE:CE2	5:Z:67:VAL:HG13	2.40	0.57
1:A:411:DG:H2"	1:A:412:DG:O5'	2.04	0.56
5:Z:156:LEU:HD22	5:Z:164:ILE:HD11	1.87	0.56
5:Z:82:LEU:HB2	5:Z:83:PRO:CD	2.35	0.56
3:C:507:DT:H2"	3:C:508:DA:C8	2.40	0.56
5:Z:231:TYR:CE1	5:Z:235:LEU:HD13	2.41	0.56
3:C:502:DC:H2"	3:C:503:DG:OP2	2.07	0.56
5:Z:210:GLU:CA	5:Z:248:ILE:HD13	2.37	0.55
4:D:531:DT:OP1	4:D:531:DT:O4'	2.25	0.55
1:A:399:DG:H1'	1:A:400:DC:C6	2.41	0.55
5:Z:210:GLU:CB	5:Z:248:ILE:CD1	2.85	0.55
5:Z:222:LYS:HG2	5:Z:254:TYR:CE1	2.41	0.54
4:D:531:DT:OP1	4:D:531:DT:C6	2.60	0.54
5:Z:222:LYS:C	5:Z:254:TYR:HE1	2.06	0.54
5:Z:108:GLY:O	5:Z:110:ILE:HG23	2.08	0.54
5:Z:74:LYS:HA	5:Z:77:LEU:HD12	1.89	0.54
5:Z:247:LYS:C	5:Z:248:ILE:HG13	2.28	0.54
5:Z:96:TYR:CE1	5:Z:121:SER:HB3	2.43	0.53
5:Z:236:LYS:HA	5:Z:239:ARG:HH11	1.73	0.53
5:Z:235:LEU:CG	5:Z:250:ILE:HG21	2.35	0.53
5:Z:225:GLY:O	5:Z:228:LYS:HB3	2.09	0.53
5:Z:241:ILE:CG2	5:Z:244:TYR:HD2	2.20	0.53
1:A:405:DT:H2"	1:A:406:DG:C8	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Z:250:ILE:HB	5:Z:251:PRO:CD	2.39	0.53
5:Z:92:SER:O	5:Z:94:LYS:N	2.42	0.53
1:A:399:DG:H1'	1:A:400:DC:O5'	2.09	0.52
5:Z:91:PHE:HB3	5:Z:131:ILE:HD12	1.91	0.52
5:Z:92:SER:C	5:Z:94:LYS:N	2.61	0.52
5:Z:110:ILE:CD1	5:Z:110:ILE:N	2.71	0.52
5:Z:248:ILE:CG2	5:Z:249:LYS:H	2.23	0.52
5:Z:159:ASP:OD2	5:Z:159:ASP:N	2.43	0.51
2:B:426:DC:H2"	2:B:427:DG:C8	2.45	0.51
5:Z:235:LEU:HG	5:Z:250:ILE:HG22	1.91	0.51
1:A:412:DG:C6	5:Z:61:ARG:NH1	2.79	0.51
5:Z:13:PHE:CE2	5:Z:34:ILE:HG12	2.45	0.51
5:Z:248:ILE:HG22	5:Z:249:LYS:O	2.09	0.51
5:Z:38:ILE:HD12	5:Z:67:VAL:HG22	1.92	0.51
5:Z:80:PHE:O	5:Z:83:PRO:HG2	2.09	0.51
5:Z:179:SER:O	5:Z:182:ARG:HB3	2.10	0.51
5:Z:132:ILE:HD11	5:Z:180:ALA:O	2.11	0.50
2:B:427:DG:H2'	2:B:428:DC:C5	2.47	0.50
5:Z:228:LYS:HD2	5:Z:254:TYR:OXT	2.12	0.50
5:Z:216:LEU:HB3	5:Z:254:TYR:CD2	2.47	0.50
5:Z:247:LYS:O	5:Z:248:ILE:CG1	2.58	0.50
5:Z:129:GLU:OE1	5:Z:129:GLU:HA	2.11	0.49
5:Z:245:SER:C	5:Z:247:LYS:H	2.16	0.49
5:Z:184:TYR:HD2	5:Z:185:LEU:HD13	1.77	0.49
5:Z:172:ARG:HA	5:Z:198:CYS:HA	1.95	0.49
5:Z:189:THR:HG21	5:Z:202:LYS:O	2.12	0.49
5:Z:210:GLU:CB	5:Z:248:ILE:HD11	2.34	0.49
5:Z:128:ILE:HD12	5:Z:180:ALA:HA	1.95	0.48
5:Z:229:LEU:O	5:Z:229:LEU:HD12	2.13	0.48
1:A:411:DG:H1'	1:A:412:DG:H5'	1.95	0.48
2:B:423:DA:H2"	2:B:424:DA:H8	1.78	0.48
5:Z:184:TYR:HD2	5:Z:185:LEU:CD1	2.26	0.48
5:Z:85:PHE:CD2	5:Z:90:MSE:HE2	2.49	0.48
5:Z:96:TYR:O	5:Z:100:ARG:HB3	2.14	0.47
5:Z:160:ASP:OD1	5:Z:161:ASP:N	2.47	0.47
5:Z:228:LYS:CE	5:Z:253:ASN:OD1	2.62	0.47
3:C:503:DG:OP2	3:C:503:DG:H8	1.96	0.47
5:Z:234:TRP:O	5:Z:235:LEU:C	2.52	0.47
5:Z:43:LEU:HD22	5:Z:225:GLY:HA3	1.96	0.47
5:Z:112:LEU:HB3	5:Z:113:GLU:OE1	2.13	0.47
3:C:501:DG:H4'	3:C:502:DC:C5'	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:531:DT:OP1	4:D:531:DT:H6	1.97	0.47
1:A:412:DG:N7	5:Z:61:ARG:NH1	2.46	0.47
4:D:530:DC:H2'	4:D:531:DT:C7	2.42	0.47
5:Z:172:ARG:NE	5:Z:196:THR:HG22	2.28	0.47
5:Z:235:LEU:CD1	5:Z:250:ILE:HG21	2.45	0.47
5:Z:241:ILE:HG21	5:Z:244:TYR:CD2	2.50	0.46
5:Z:21:ILE:HD11	5:Z:101:PHE:HA	1.96	0.46
5:Z:92:SER:HB3	5:Z:177:LEU:HD22	1.97	0.46
5:Z:142:VAL:HG11	5:Z:254:TYR:HH	1.77	0.46
5:Z:163:LEU:HD12	5:Z:241:ILE:CG1	2.43	0.45
5:Z:222:LYS:HZ3	5:Z:253:ASN:HB3	1.80	0.45
5:Z:182:ARG:HD2	5:Z:191:VAL:HG23	1.98	0.45
2:B:427:DG:H2'	2:B:428:DC:C6	2.52	0.45
1:A:399:DG:C1'	1:A:400:DC:O5'	2.64	0.45
5:Z:64:ILE:H	5:Z:64:ILE:HD12	1.82	0.45
5:Z:222:LYS:HZ2	5:Z:253:ASN:HB3	1.82	0.45
5:Z:209:VAL:HG13	5:Z:234:TRP:CH2	2.51	0.44
5:Z:164:ILE:O	5:Z:244:TYR:OH	2.25	0.44
5:Z:81:ILE:O	5:Z:82:LEU:C	2.54	0.44
4:D:517:DC:H3'	5:Z:18:TYR:HB3	1.98	0.44
5:Z:100:ARG:CG	5:Z:100:ARG:NH1	2.71	0.44
5:Z:65:GLU:C	5:Z:66:MSE:HG2	2.38	0.44
5:Z:127:SER:O	5:Z:128:ILE:C	2.55	0.44
5:Z:145:ILE:O	5:Z:146:GLU:C	2.56	0.44
5:Z:64:ILE:N	5:Z:64:ILE:HD12	2.32	0.44
5:Z:162:TYR:OH	5:Z:243:ARG:NH2	2.51	0.44
5:Z:222:LYS:CG	5:Z:254:TYR:CE1	3.00	0.44
5:Z:95:GLN:HB2	5:Z:95:GLN:HE21	1.69	0.43
5:Z:128:ILE:HD12	5:Z:180:ALA:CA	2.49	0.43
5:Z:229:LEU:O	5:Z:233:LEU:HG	2.18	0.43
3:C:512:DA:H2"	3:C:513:DG:C8	2.53	0.43
5:Z:245:SER:C	5:Z:247:LYS:N	2.71	0.43
5:Z:235:LEU:CG	5:Z:250:ILE:CG2	2.91	0.43
3:C:511:DG:H2"	3:C:512:DA:OP2	2.18	0.43
5:Z:216:LEU:HB3	5:Z:254:TYR:HD2	1.84	0.43
5:Z:222:LYS:CB	5:Z:254:TYR:CD1	3.01	0.42
5:Z:107:SER:HB2	5:Z:109:ILE:HG13	2.02	0.42
5:Z:35:GLU:HG3	5:Z:68:ALA:HB2	2.01	0.42
4:D:530:DC:H1'	4:D:531:DT:OP2	2.20	0.42
5:Z:222:LYS:HD3	5:Z:254:TYR:HD1	1.84	0.42
5:Z:80:PHE:O	5:Z:84:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Z:43:LEU:CD1	5:Z:224:LEU:HD12	2.48	0.42
5:Z:241:ILE:CG2	5:Z:244:TYR:CD2	3.01	0.42
5:Z:164:ILE:HA	5:Z:243:ARG:HH12	1.85	0.42
5:Z:128:ILE:HD11	5:Z:179:SER:HB2	2.02	0.42
5:Z:182:ARG:HB2	5:Z:201:LEU:HD22	2.02	0.42
5:Z:211:ASN:HD22	5:Z:211:ASN:HA	1.68	0.42
2:B:420:DG:H2"	2:B:421:DT:C6	2.55	0.41
2:B:420:DG:C8	2:B:421:DT:H72	2.55	0.41
5:Z:66:MSE:HE3	5:Z:66:MSE:HB3	1.91	0.41
2:B:423:DA:C4	2:B:424:DA:C8	3.08	0.41
5:Z:210:GLU:CA	5:Z:248:ILE:CD1	2.98	0.41
5:Z:187:PHE:HZ	5:Z:212:ILE:HD12	1.85	0.41
4:D:527:DG:H1'	4:D:528:DC:H5"	2.03	0.41
5:Z:213:ILE:HG23	5:Z:231:TYR:OH	2.21	0.41
5:Z:242:SER:O	5:Z:243:ARG:C	2.59	0.41
5:Z:56:VAL:HA	5:Z:68:ALA:O	2.21	0.41
2:B:424:DA:C2	2:B:425:DG:C5	3.09	0.41
2:B:427:DG:C2'	2:B:428:DC:C6	3.04	0.41
2:B:418:DC:H5	5:Z:168:ASP:OD2	2.04	0.40
5:Z:82:LEU:HD11	5:Z:105:LEU:HD23	2.04	0.40
5:Z:239:ARG:HA	5:Z:245:SER:OG	2.21	0.40
5:Z:232:LEU:HD23	5:Z:232:LEU:HA	1.88	0.40
5:Z:97:ASP:OD1	5:Z:120:ARG:CG	2.70	0.40
3:C:503:DG:OP2	3:C:503:DG:C8	2.74	0.40
5:Z:9:LEU:HD23	5:Z:9:LEU:HA	1.82	0.40
5:Z:6:TYR:CD2	5:Z:84:ILE:CD1	2.99	0.40

All (1) 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)
1:A:399:DG:OP3	3:C:501:DG:N2[1_456]	2.19	0.01

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	Z	252/254 (99%)	215 (85%)	29 (12%)	8 (3%)	4 6

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	Z	62	ASN
5	Z	128	ILE
5	Z	159	ASP
5	Z	93	ASN
5	Z	250	ILE
5	Z	158	LYS
5	Z	251	PRO
5	Z	132	ILE

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	Z	232/230 (101%)	204 (88%)	28 (12%)	5 9

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	Z	26	LYS
5	Z	34	ILE
5	Z	40	ASP
5	Z	59	ARG
5	Z	67	VAL
5	Z	100	ARG
5	Z	110	ILE
5	Z	119	THR
5	Z	122	ASP
5	Z	148	GLU
5	Z	156	LEU

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Mol	Chain	Res	Type
5	Z	159	ASP
5	Z	160	ASP
5	Z	172	ARG
5	Z	185	LEU
5	Z	189	THR
5	Z	195	LYS
5	Z	196	THR
5	Z	207	ARG
5	Z	212	ILE
5	Z	213	ILE
5	Z	224	LEU
5	Z	235	LEU
5	Z	239	ARG
5	Z	246	GLU
5	Z	251	PRO
5	Z	252	SER
5	Z	253	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
5	Z	95	GLN
5	Z	133	ASN
5	Z	171	GLN
5	Z	211	ASN
5	Z	230	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 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)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	18/18 (100%)	0.01	1 (5%)	24	19	60, 72, 100, 105	0
2	B	13/13 (100%)	0.49	1 (7%)	13	10	70, 88, 95, 99	0
3	C	16/16 (100%)	0.32	2 (12%)	3	2	62, 78, 104, 108	0
4	D	15/15 (100%)	0.41	2 (13%)	3	2	64, 76, 97, 99	0
5	Z	252/254 (99%)	0.70	18 (7%)	16	11	46, 63, 88, 106	0
All	All	314/316 (99%)	0.62	24 (7%)	13	10	46, 65, 93, 108	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	Z	254	TYR	9.8
5	Z	1	GLY	5.0
5	Z	164	ILE	5.0
4	D	531	DT	4.0
5	Z	187	PHE	3.9
5	Z	163	LEU	3.7
5	Z	162	TYR	3.6
3	C	501	DG	3.5
5	Z	158	LYS	3.4
5	Z	240	LYS	3.4
1	A	399	DG	3.2
5	Z	248	ILE	2.7
4	D	530	DC	2.5
5	Z	159	ASP	2.5
5	Z	80	PHE	2.5
5	Z	155	LYS	2.5
3	C	502	DC	2.4
5	Z	112	LEU	2.4
5	Z	41	VAL	2.3
5	Z	233	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
5	Z	250	ILE	2.2
5	Z	4	LEU	2.1
2	B	429	DA	2.1
5	Z	201	LEU	2.1

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MG	Z	601	1/1	0.75	0.18	60,60,60,60	0
6	MG	B	602	1/1	0.89	0.18	77,77,77,77	0

6.5 Other polymers (i)

There are no such residues in this entry.