Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:57 PM GMT

PDB ID	:	1DC1
Title	:	RESTRICTION ENZYME BSOBI/DNA COMPLEX STRUCTURE: ENCIR-CLEMENT OF THE DNA AND HISTIDINE-CATALYZED HYDROLYSIS WITHIN A CANONICAL RESTRICTION ENZYME FOLD
Authors	:	van der Woerd, M.J.; Pelletier, J.J.; Xu, S.-Y.; Friedman, A.M.
Deposited on	:	1999-11-04
Resolution	:	1.70 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	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 1.70 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.
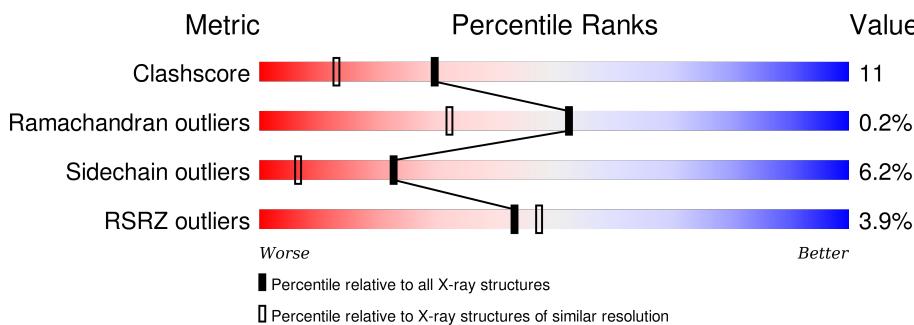
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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. 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	C	13	54% 15% 31%
1	W	13	8% · 31% 31% 31% 8%
2	A	323	4% · 76% 18% · ·
2	B	323	3% · 72% 22% · ·
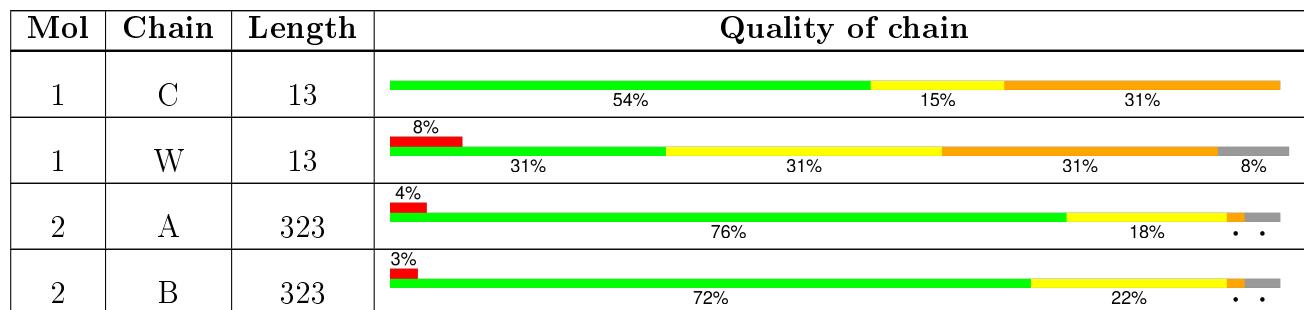
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DIO	A	1000	-	-	-	X
3	DIO	A	1008	-	-	-	X
3	DIO	B	1003	-	-	-	X
3	DIO	B	1005	-	-	-	X
3	DIO	B	1006	-	-	X	X
3	DIO	B	1009	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6020 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(*T*AP*TP*AP*CP*TP*CP*GP*AP*GP*T P*AP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	W	12	Total 243	C 118	N 44	O 70	P 11	0	0	0
1	C	13	Total 247	C 118	N 44	O 73	P 12	0	0	0

- Molecule 2 is a protein called BSOBI RESTRICTION ENDONUCLEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	310	Total 2488	C 1583	N 416	O 482	S 7	0	6	0
2	B	311	Total 2508	C 1595	N 424	O 481	S 8	0	9	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	205	SER	PRO	CONFLICT	UNP P70985
B	205	SER	PRO	CONFLICT	UNP P70985

- Molecule 3 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: $C_4H_8O_2$).
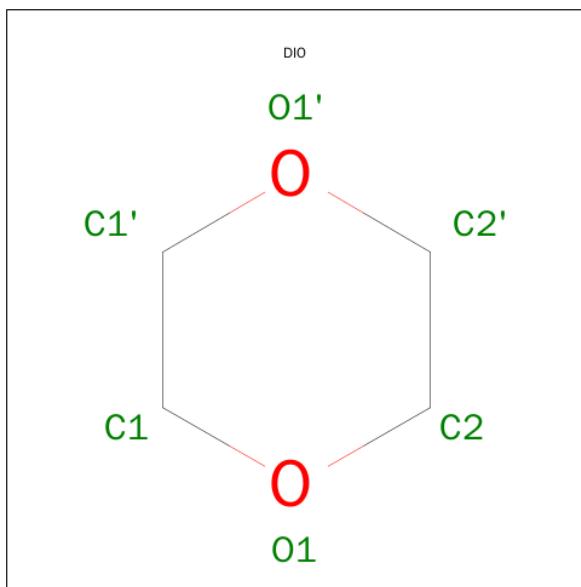
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 6	C 4	O 2	0	0
3	B	1	Total 6	C 4	O 2	0	0
3	A	1	Total 6	C 4	O 2	0	0
3	B	1	Total 6	C 4	O 2	0	0
3	A	1	Total 6	C 4	O 2	0	0
3	B	1	Total 6	C 4	O 2	0	0
3	B	1	Total 6	C 4	O 2	0	0
3	A	1	Total 6	C 4	O 2	0	0
3	A	1	Total 6	C 4	O 2	0	0
3	B	1	Total 6	C 4	O 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	209	Total 209	O 209	0	0
4	B	198	Total 198	O 198	0	0

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| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	39	Total 39	O 39	0	0
4	W	28	Total 28	O 28	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 errors 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: DNA (5'-D(*T*AP*TP*AP*CP*TP*CP*GP*AP*GP*TP*AP*T)-3')
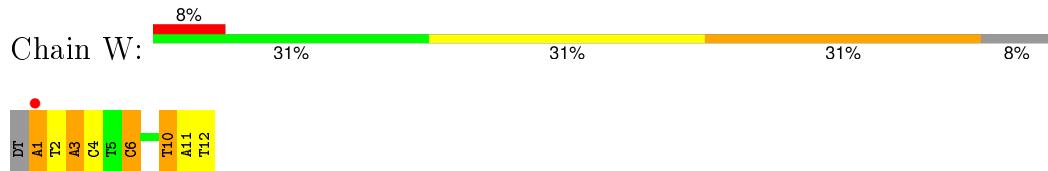

• Molecule 1: DNA (5'-D(*T*AP*TP*AP*CP*TP*CP*GP*AP*GP*TP*AP*T)-3')

• Molecule 2: BSOBI RESTRICTION ENDONUCLEASE

• Molecule 2: BSOBI RESTRICTION ENDONUCLEASE

H253 I264 R265 K271 G272 L273 S274 P275 K276 F279 S300 N303 L316 C317 I320 I321 N322 I323
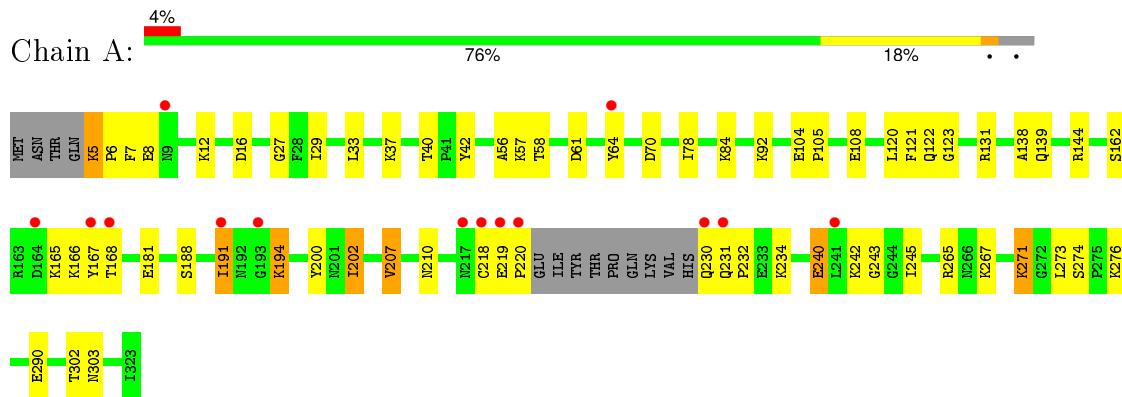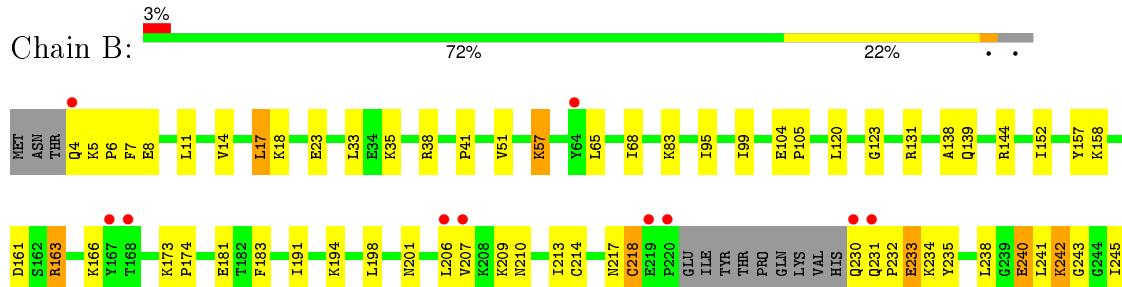
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	80.29Å 87.82Å 99.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 1.70 29.43 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (8.00-1.70) 99.4 (29.43-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 1.70Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.190 , 0.253 0.187 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	18.9	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 72.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \lvert L \rvert > = 0.48, < L^2 > = 0.31$	Xtriage
Outliers	0 of 77445 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6020	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% 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 $< \lvert L \rvert >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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: DIO

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	C	1.07	0/276	1.11	2/425 (0.5%)
1	W	1.16	0/272	1.05	0/418
2	A	0.82	0/2565	0.84	0/3461
2	B	0.80	1/2606 (0.0%)	0.82	0/3516
All	All	0.84	1/5719 (0.0%)	0.86	2/7820 (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	C	0	2
1	W	0	4
2	A	0	1
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	157	TYR	CE2-CZ	5.11	1.45	1.38

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	3	DT	C1'-O4'-C4'	-6.10	104.00	110.10
1	C	11	DT	O5'-P-OP2	-6.08	100.23	105.70

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	64	TYR	Sidechain
1	C	4	DA	Sidechain
1	C	7	DC	Sidechain
1	W	1	DA	Sidechain
1	W	10	DT	Sidechain
1	W	3	DA	Sidechain
1	W	6	DC	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	C	247	0	137	8	0
1	W	243	0	138	12	0
2	A	2488	0	2491	52	0
2	B	2508	0	2508	59	0
3	A	30	0	40	4	0
3	B	30	0	40	10	0
4	A	209	0	0	15	0
4	B	198	0	0	13	0
4	C	39	0	0	3	0
4	W	28	0	0	2	0
All	All	6020	0	5354	123	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 11.

All (123) 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:B:241:LEU:HD23	3:B:1006:DIO:H2'1	1.28	1.12
2:B:201:ASN:HD21	3:B:1006:DIO:H1'2	1.32	0.91
2:A:242:LYS:HE3	4:A:1173:HOH:O	1.71	0.88
1:W:4:DC:H4'	2:B:210[B]:ASN:OD1	1.74	0.86
2:A:27:GLY:HA3	2:A:245:ILE:HG12	1.56	0.85
2:A:84:LYS:HB3	3:A:1007:DIO:H1'2	1.58	0.85
2:A:108:GLU:OE1	2:A:108:GLU:HA	1.77	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:191:ILE:O	2:A:194:LYS:HG3	1.83	0.78
2:B:163:ARG:HD2	2:B:183:PHE:CD1	2.20	0.75
2:B:99:ILE:O	2:B:104:GLU:HG3	1.87	0.75
2:B:241:LEU:HD23	3:B:1006:DIO:C2'	2.14	0.72
2:B:217:ASN:O	2:B:218:CYS:HB3	1.91	0.70
2:B:201:ASN:ND2	3:B:1006:DIO:H1'2	2.04	0.68
2:B:245:ILE:HG22	4:B:1121:HOH:O	1.93	0.67
2:B:210[B]:ASN:OD1	4:B:1193:HOH:O	2.11	0.67
2:A:122:GLN:HB3	4:A:1141:HOH:O	1.95	0.67
2:A:210:ASN:OD1	4:A:1132:HOH:O	2.13	0.67
1:C:11:DT:H2"	1:C:12:DA:H5'	1.78	0.66
1:W:11:DA:N7	4:W:410:HOH:O	2.28	0.65
1:W:1:DA:H5"	1:W:2:DT:C7	2.27	0.64
2:A:33:LEU:HD12	4:A:1026:HOH:O	1.96	0.64
2:B:232:PRO:HB2	2:B:273:LEU:CD1	2.27	0.64
1:W:12:DT:OP2	4:W:482:HOH:O	2.14	0.64
2:A:200:TYR:O	2:A:202:ILE:HD13	1.96	0.64
2:A:5:LYS:HE2	4:A:1197:HOH:O	1.99	0.62
1:W:1:DA:H5"	1:W:2:DT:H72	1.80	0.62
2:A:84:LYS:HB3	3:A:1007:DIO:C1'	2.29	0.62
2:B:161:ASP:OD1	2:B:163:ARG:HD3	1.99	0.62
2:A:188:SER:OG	2:A:220:PRO:HD3	2.01	0.61
2:A:191:ILE:HG22	4:A:1088:HOH:O	1.99	0.61
2:A:207:VAL:HG13	2:A:267:LYS:HG3	1.83	0.61
2:B:242:LYS:NZ	4:B:1195:HOH:O	2.31	0.60
2:B:231:GLN:HB2	2:B:234:LYS:HG2	1.83	0.59
2:B:5:LYS:HB3	2:B:7:PHE:CE1	2.36	0.59
1:W:6:DC:C5	2:B:253:HIS:CE1	2.91	0.59
1:W:6:DC:O2	2:B:131:ARG:HD3	2.03	0.58
2:B:104:GLU:HB2	2:B:105:PRO:HD3	1.86	0.58
2:A:231:GLN:N	2:A:232:PRO:HD3	2.20	0.56
1:W:1:DA:N6	1:C:12:DA:C2	2.73	0.56
2:A:78:ILE:HD11	3:A:1008:DIO:H21	1.88	0.55
2:B:233:GLU:CD	2:B:233:GLU:H	2.08	0.54
2:B:158:LYS:CE	4:B:1168:HOH:O	2.56	0.54
1:W:1:DA:C5'	1:W:2:DT:H72	2.39	0.53
2:A:276:LYS:NZ	4:A:1115:HOH:O	2.40	0.52
2:A:138:ALA:HB2	2:A:243:GLY:HA3	1.91	0.52
2:A:42:TYR:HD2	4:A:1141:HOH:O	1.92	0.51
2:A:276:LYS:HD3	2:A:302:THR:HG21	1.91	0.51
2:B:217:ASN:C	2:B:217:ASN:OD1	2.48	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:139:GLN:HB2	3:B:1006:DIO:H2'2	1.92	0.51
2:B:207:VAL:HG11	2:B:264:ILE:HA	1.91	0.51
1:W:10:DT:H2"	1:W:11:DA:H5'	1.92	0.51
2:A:162:SER:HA	2:A:167:TYR:HE1	1.77	0.50
2:A:29:ILE:HG23	3:B:1005:DIO:H2'2	1.92	0.50
2:A:265:ARG:HD2	4:A:1140:HOH:O	2.10	0.50
2:B:214[A]:CYS:SG	2:B:235:TYR:CD2	3.05	0.50
1:C:7:DC:O2	2:A:131:ARG:HD3	2.11	0.50
2:B:210[B]:ASN:ND2	4:B:1193:HOH:O	2.43	0.49
2:B:57:LYS:HD2	2:B:57:LYS:N	2.26	0.49
2:B:138:ALA:HB2	2:B:243:GLY:HA3	1.95	0.48
2:A:165:LYS:HD3	2:A:165:LYS:N	2.28	0.48
2:B:242:LYS:HG3	2:B:279:PHE:CZ	2.49	0.48
2:B:8:GLU:HG2	4:B:1146:HOH:O	2.14	0.48
2:A:121:PHE:CE1	2:B:35:LYS:HE3	2.49	0.48
2:B:316[B]:LEU:CD1	2:B:320:ILE:HD12	2.44	0.47
2:A:139:GLN:NE2	3:A:1002:DIO:H22	2.29	0.47
2:A:191:ILE:CG2	4:A:1088:HOH:O	2.58	0.47
2:B:51:VAL:HA	4:B:1084:HOH:O	2.14	0.47
2:A:56:ALA:HB1	2:A:61:ASP:HB2	1.96	0.47
2:B:198:LEU:HD11	2:B:213:ILE:HG23	1.97	0.47
2:B:265[B]:ARG:NH1	4:B:1117:HOH:O	2.03	0.46
2:A:144:ARG:HD2	2:A:181:GLU:CD	2.36	0.46
2:B:95:ILE:CD1	3:B:1001:DIO:H2'2	2.46	0.46
1:C:4:DA:H4'	1:C:5:DC:OP1	2.14	0.46
2:B:95:ILE:HD12	3:B:1001:DIO:H2'2	1.98	0.45
2:B:11:LEU:HD21	2:B:17:LEU:HD13	1.98	0.45
2:B:144:ARG:HD2	2:B:181:GLU:CD	2.36	0.45
2:B:214[A]:CYS:SG	2:B:235:TYR:CE2	3.10	0.45
2:A:207:VAL:CG1	2:A:267:LYS:HG3	2.46	0.45
2:A:120:LEU:O	2:B:123:GLY:HA3	2.17	0.44
2:A:58:THR:O	2:A:61:ASP:HB2	2.17	0.44
2:A:12:LYS:HE2	2:A:16:ASP:OD2	2.17	0.44
3:B:1006:DIO:H21	4:B:1184:HOH:O	2.18	0.44
1:W:3:DA:OP1	2:B:209:LYS:NZ	2.48	0.43
2:A:123:GLY:HA3	2:B:120:LEU:O	2.17	0.43
2:A:5:LYS:HB2	2:A:8:GLU:OE1	2.17	0.43
1:C:12:DA:P	4:C:396:HOH:O	2.76	0.43
2:A:6:PRO:HB2	2:A:303:ASN:ND2	2.33	0.43
2:A:188:SER:CB	2:A:220:PRO:HG3	2.49	0.43
2:A:271:LYS:HD2	2:A:271:LYS:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:5:LYS:HB3	2:A:7:PHE:CE2	2.54	0.43
2:A:5:LYS:HA	2:A:6:PRO:HD2	1.70	0.42
4:A:1119:HOH:O	3:B:1005:DIO:H1'1	2.19	0.42
2:B:276:LYS:HE2	2:B:323:ILE:HG23	1.99	0.42
2:A:165:LYS:N	2:A:165:LYS:CD	2.82	0.42
2:A:219:GLU:H	2:A:219:GLU:CD	2.19	0.42
1:C:11:DT:H2'	1:C:12:DA:C8	2.55	0.42
1:C:12:DA:H5"	4:C:396:HOH:O	2.19	0.42
2:B:194:LYS:HE2	4:B:1180:HOH:O	2.19	0.42
2:B:242:LYS:HG3	2:B:279:PHE:CE1	2.55	0.42
2:B:238:LEU:HD12	2:B:275:PRO:HB2	2.01	0.42
2:B:242:LYS:CE	4:B:1195:HOH:O	2.66	0.42
1:C:3:DT:H5"	4:C:258:HOH:O	2.20	0.42
2:A:240:GLU:CD	4:A:1172:HOH:O	2.58	0.42
2:B:65:LEU:O	2:B:68:ILE:HG12	2.20	0.42
2:A:33:LEU:HG	2:A:37:LYS:HE3	2.02	0.42
2:A:232:PRO:HB2	2:A:273:LEU:HD11	2.02	0.42
2:B:173:LYS:HG2	2:B:174:PRO:O	2.20	0.41
2:A:40:THR:HG23	4:A:1130:HOH:O	2.20	0.41
2:B:6:PRO:HB2	2:B:303:ASN:ND2	2.35	0.41
2:B:242:LYS:HE3	4:B:1195:HOH:O	2.19	0.41
2:B:161:ASP:OD2	2:B:163:ARG:NH1	2.54	0.41
1:W:3:DA:H4'	1:W:4:DC:OP1	2.21	0.41
2:A:33:LEU:CD1	4:A:1026:HOH:O	2.63	0.41
2:A:234:LYS:HD3	2:A:234:LYS:HA	1.74	0.41
2:B:240:GLU:HG3	4:B:1183:HOH:O	2.20	0.40
2:B:38:ARG:O	2:B:41:PRO:HD2	2.22	0.40
2:A:70:ASP:HB2	4:A:1149:HOH:O	2.21	0.40
2:B:317:CYS:O	2:B:321:ILE:HD12	2.21	0.40
2:A:121:PHE:CD1	2:B:35:LYS:HE3	2.56	0.40
2:A:104:GLU:HB2	2:A:105:PRO:HD3	2.04	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	
2	A	312/323 (97%)	303 (97%)	9 (3%)	0	100	100
2	B	316/323 (98%)	312 (99%)	3 (1%)	1 (0%)	46	26
All	All	628/646 (97%)	615 (98%)	12 (2%)	1 (0%)	52	32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	218	CYS

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	
2	A	272/279 (98%)	257 (94%)	15 (6%)	27	9
2	B	276/279 (99%)	257 (93%)	19 (7%)	19	5
All	All	548/558 (98%)	514 (94%)	34 (6%)	23	6

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	5	LYS
2	A	57	LYS
2	A	92	LYS
2	A	166	LYS
2	A	168	THR
2	A	191	ILE
2	A	194	LYS
2	A	202	ILE
2	A	207	VAL
2	A	218	CYS
2	A	230	GLN
2	A	240	GLU

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Mol	Chain	Res	Type
2	A	271	LYS
2	A	274	SER
2	A	290	GLU
2	B	4	GLN
2	B	14[A]	VAL
2	B	14[B]	VAL
2	B	17	LEU
2	B	18	LYS
2	B	23	GLU
2	B	33	LEU
2	B	57	LYS
2	B	83	LYS
2	B	163	ARG
2	B	166	LYS
2	B	191	ILE
2	B	206	LEU
2	B	230	GLN
2	B	233	GLU
2	B	240	GLU
2	B	242	LYS
2	B	271	LYS
2	B	300	SER

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

Mol	Chain	Res	Type
2	A	122	GLN
2	A	192	ASN
2	A	210	ASN
2	B	122	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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)

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
3	DIO	A	1000	-	6,6,6	0.68	0	6,6,6	0.38	0
3	DIO	A	1002	-	6,6,6	0.77	0	6,6,6	0.36	0
3	DIO	A	1004	-	6,6,6	0.77	0	6,6,6	0.40	0
3	DIO	A	1007	-	6,6,6	0.61	0	6,6,6	0.35	0
3	DIO	A	1008	-	6,6,6	0.84	0	6,6,6	0.31	0
3	DIO	B	1001	-	6,6,6	0.64	0	6,6,6	0.45	0
3	DIO	B	1003	-	6,6,6	0.57	0	6,6,6	0.39	0
3	DIO	B	1005	-	6,6,6	0.82	0	6,6,6	0.43	0
3	DIO	B	1006	-	6,6,6	0.56	0	6,6,6	0.44	0
3	DIO	B	1009	-	6,6,6	0.94	0	6,6,6	0.33	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DIO	A	1000	-	-	0/0/6/6	0/1/1/1
3	DIO	A	1002	-	-	0/0/6/6	0/1/1/1
3	DIO	A	1004	-	-	0/0/6/6	0/1/1/1
3	DIO	A	1007	-	-	0/0/6/6	0/1/1/1
3	DIO	A	1008	-	-	0/0/6/6	0/1/1/1
3	DIO	B	1001	-	-	0/0/6/6	0/1/1/1
3	DIO	B	1003	-	-	0/0/6/6	0/1/1/1
3	DIO	B	1005	-	-	0/0/6/6	0/1/1/1
3	DIO	B	1006	-	-	0/0/6/6	0/1/1/1
3	DIO	B	1009	-	-	0/0/6/6	0/1/1/1

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.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1002	DIO	1	0
3	A	1007	DIO	2	0
3	A	1008	DIO	1	0
3	B	1001	DIO	2	0
3	B	1005	DIO	2	0
3	B	1006	DIO	6	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	C	13/13 (100%)	-0.07	0	100	100	12, 16, 38, 77	0
1	W	12/13 (92%)	-0.21	1 (8%)	14	16	13, 14, 49, 76	0
2	A	310/323 (95%)	0.15	14 (4%)	37	41	11, 19, 45, 80	1 (0%)
2	B	311/323 (96%)	0.03	10 (3%)	51	55	11, 18, 38, 73	1 (0%)
All	All	646/672 (96%)	0.09	25 (3%)	43	47	11, 18, 42, 80	2 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	191	ILE	4.3
2	A	64	TYR	4.3
2	A	219	GLU	4.1
2	B	64	TYR	3.8
2	A	220	PRO	3.8
2	A	218	CYS	3.7
2	B	230	GLN	3.7
2	A	167	TYR	3.6
2	A	193	GLY	3.6
2	B	4	GLN	3.6
2	A	164	ASP	3.3
2	A	231	GLN	3.3
2	B	231	GLN	3.2
2	A	241	LEU	3.0
2	B	168	THR	2.9
2	A	217	ASN	2.8
2	B	167	TYR	2.6
2	A	230	GLN	2.5
2	B	219	GLU	2.5
2	A	168	THR	2.3
2	B	220	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	206	LEU	2.3
2	B	207	VAL	2.3
2	A	9[A]	ASN	2.2
1	W	1	DA	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
3	DIO	B	1009	6/6	0.66	0.34	11.74	63,68,70,70	0
3	DIO	B	1006	6/6	0.62	0.29	9.43	55,58,58,62	0
3	DIO	B	1005	6/6	0.73	0.21	6.31	55,60,64,64	0
3	DIO	A	1008	6/6	0.89	0.22	5.42	36,39,43,44	0
3	DIO	A	1000	6/6	0.81	0.15	4.96	59,61,63,63	0
3	DIO	B	1003	6/6	0.93	0.14	2.10	37,44,47,48	0
3	DIO	A	1004	6/6	0.85	0.18	1.25	52,53,55,56	0
3	DIO	A	1002	6/6	0.87	0.12	1.21	51,54,55,58	0
3	DIO	B	1001	6/6	0.94	0.10	0.74	20,24,28,31	0
3	DIO	A	1007	6/6	0.63	0.45	-	73,73,76,77	0

6.5 Other polymers (i)

There are no such residues in this entry.