Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:37 AM GMT

PDB ID	:	2HVR
Title	:	Structure of T4 RNA Ligase 2 with Nicked 5'-Adenylated nucleic acid duplex containing a 3'-deoxyribonucleotide at the nick
Authors	:	Nandakumar, J.; Lima, C.D.
Deposited on	:	2006-07-30
Resolution	:	2.45 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

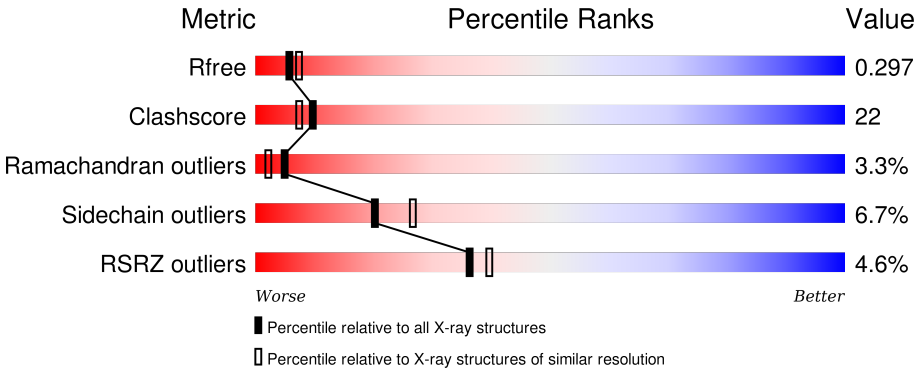
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.45 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))
R_{free}	91344	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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	24	8% 25% 71% .
1	F	24	13% 25% 71% .
2	D	12	8% 17% 67% 17%
2	G	12	25% 58% 17%
3	E	13	23% 77%

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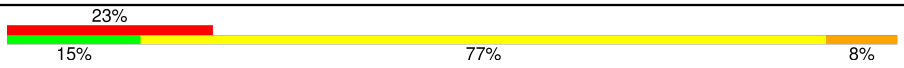
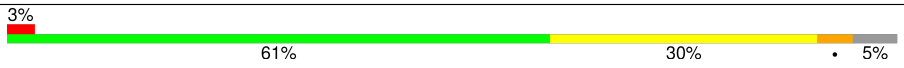
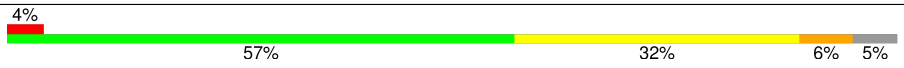
Mol	Chain	Length	Quality of chain
3	H	13	
4	A	335	
4	B	335	

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
5	BTB	A	335	-	-	-	X
5	BTB	C	201	-	-	-	X
5	BTB	F	202	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7219 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(*AP*TP*TP*CP*CP*GP*AP*TP*AP*GP*TP*GP*GP*GP*TP*CP*GP*CP*AP*AP*TP*TP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	24	Total	C	N	O	P	0	0	0
			494	236	91	144	23			
1	F	24	Total	C	N	O	P	0	0	0
			494	236	91	144	23			

- Molecule 2 is DNA/RNA hybrid called 5'-D(*CP*AP*AP*TP*TP*GP*CP*GP*AP*C)-R(P*(OMC)P*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	12	Total	C	N	O	P	0	0	0
			241	116	44	70	11			
2	G	12	Total	C	N	O	P	0	0	0
			241	116	44	70	11			

- Molecule 3 is DNA/RNA hybrid called 5'-R(P*A)-D(P*CP*AP*CP*TP*AP*TP*CP*GP*GP*AP*AP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	13	Total	C	N	O	P	0	0	0
			268	127	50	78	13			
3	H	13	Total	C	N	O	P	0	0	0
			268	127	50	78	13			

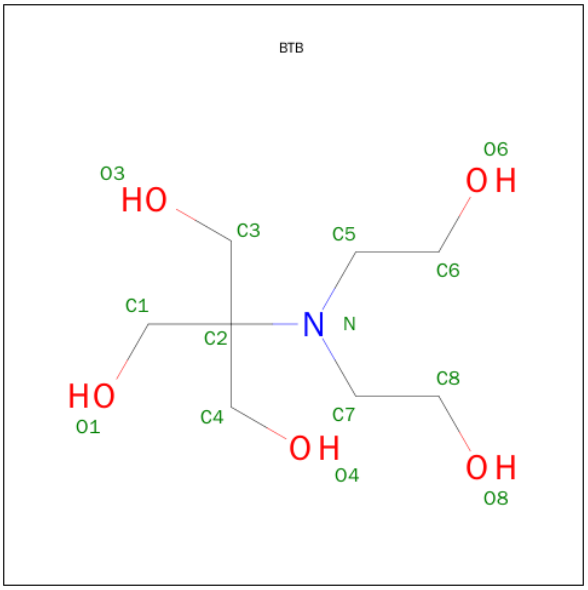
- Molecule 4 is a protein called T4 RNA ligase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	319	Total	C	N	O	S	0	0	0
			2521	1617	409	482	13			
4	B	319	Total	C	N	O	S	0	0	0
			2521	1617	409	482	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	CLONING ARTIFACT	UNP P32277
A	112	GLY	CYS	SEE REMARK 999	UNP P32277
B	0	SER	-	CLONING ARTIFACT	UNP P32277
B	112	GLY	CYS	SEE REMARK 999	UNP P32277

- Molecule 5 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: BTB) (formula: $C_8H_{19}NO_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C N O 14 8 1 5	0	0
5	F	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	76	Total O 76 76	0	0
6	B	40	Total O 40 40	0	0
6	C	7	Total O 7 7	0	0

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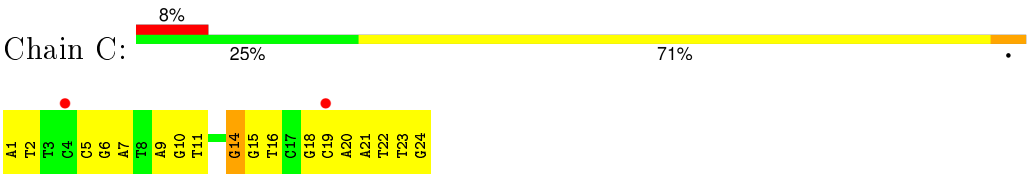
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	2	Total O 2 2	0	0
6	G	2	Total O 2 2	0	0
6	H	2	Total O 2 2	0	0

3 Residue-property plots (i)

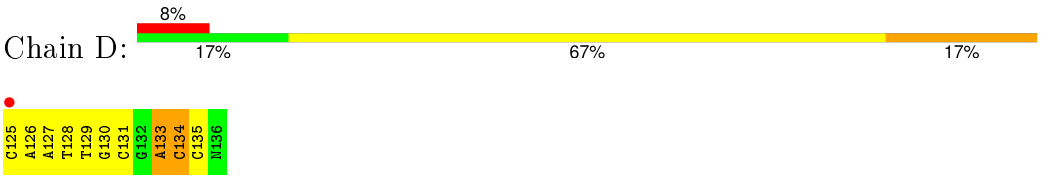
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: 5'-D(*AP*TP*TP*CP*CP*GP*AP*TP*AP*GP*TP*GP*GP*GP*GP*TP*CP*GP*CP*AP*AP*TP*TP*G)-3'



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

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

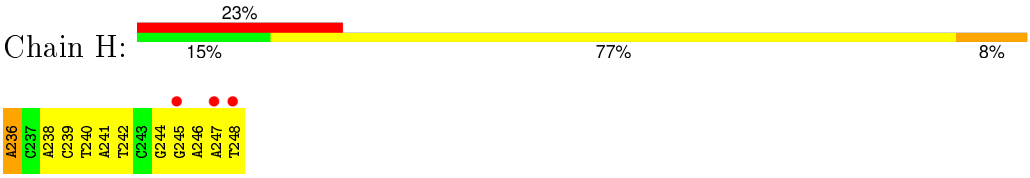


• Molecule 2: 5'-D(*CP*AP*AP*TP*TP*GP*CP*GP*AP*C)-R(P*(OMC)P*C)-3'

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

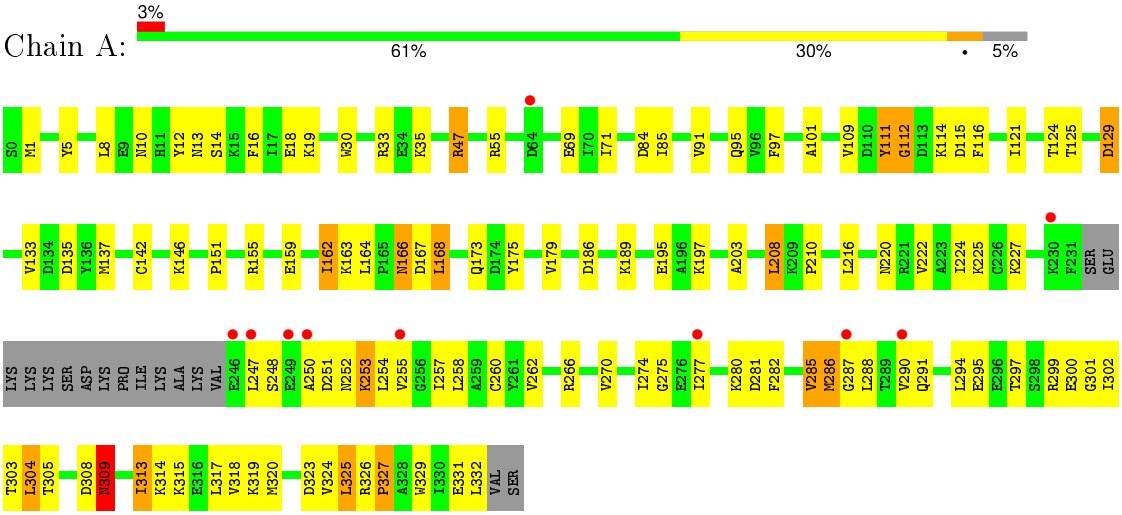
• Molecule 3: 5'-R(P*A)-D(P*CP*AP*CP*TP*AP*TP*CP*GP*GP*AP*AP*T)-3'

Chain H:



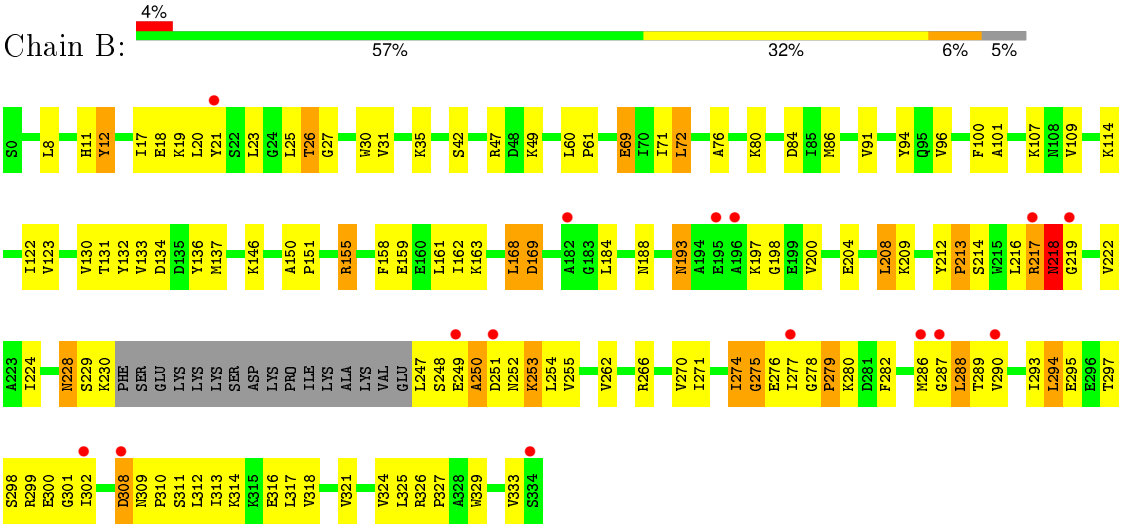
• Molecule 4: T4 RNA ligase 2

Chain A:



• Molecule 4: T4 RNA ligase 2

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	83.57Å 106.16Å 125.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.92 – 2.45 19.92 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.0 (19.92-2.45) 99.0 (19.92-2.45)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.82 (at 2.44Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.236 , 0.295 0.238 , 0.297	Depositor DCC
R_{free} test set	2056 reflections (4.99%)	DCC
Wilson B-factor (Å^2)	48.9	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 54.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 41177 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7219	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.68% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, O2C, BTB

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	0.33	0/554	0.74	0/855
1	F	0.35	0/554	0.73	0/855
2	D	0.30	0/225	0.72	0/345
2	G	0.32	0/225	0.75	0/345
3	E	1.14	4/299 (1.3%)	1.76	8/455 (1.8%)
3	H	1.20	5/299 (1.7%)	1.75	8/455 (1.8%)
4	A	0.42	0/2570	0.64	1/3472 (0.0%)
4	B	0.40	0/2570	0.64	1/3471 (0.0%)
All	All	0.50	9/7296 (0.1%)	0.82	18/10253 (0.2%)

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	1
1	F	0	2
2	D	0	2
2	G	0	2
All	All	0	7

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	236	A	N3-C4	10.31	1.41	1.34
3	E	236	A	N3-C4	9.10	1.40	1.34
3	H	236	A	C2-N3	7.27	1.40	1.33
3	E	236	A	C2-N3	6.97	1.39	1.33
3	H	236	A	N1-C2	6.86	1.40	1.34
3	E	236	A	N7-C5	-6.40	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	236	A	N1-C2	5.89	1.39	1.34
3	H	236	A	C6-N1	5.17	1.39	1.35
3	H	236	A	N7-C5	-5.00	1.36	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	236	A	C2-N3-C4	19.72	120.46	110.60
3	H	236	A	C2-N3-C4	19.56	120.38	110.60
3	E	236	A	N1-C2-N3	-16.95	120.83	129.30
3	H	236	A	N1-C2-N3	-16.68	120.96	129.30
3	E	236	A	N3-C4-C5	-11.19	118.97	126.80
3	H	236	A	N3-C4-C5	-11.16	118.99	126.80
3	H	236	A	C5-N7-C8	10.38	109.09	103.90
3	E	236	A	C5-N7-C8	9.71	108.75	103.90
3	H	236	A	N3-C4-N9	7.96	133.77	127.40
3	H	236	A	N7-C8-N9	-7.71	109.95	113.80
3	E	236	A	N3-C4-N9	7.59	133.47	127.40
3	E	236	A	N7-C8-N9	-7.37	110.11	113.80
3	H	236	A	C4-C5-N7	-6.81	107.29	110.70
3	E	236	A	C4-C5-N7	-6.80	107.30	110.70
3	H	236	A	C4-C5-C6	6.56	120.28	117.00
3	E	236	A	C4-C5-C6	6.21	120.10	117.00
4	A	111	TYR	N-CA-C	-5.32	96.63	111.00
4	B	150	ALA	N-CA-C	-5.17	97.03	111.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	14	DG	Sidechain
2	D	133	DA	Sidechain
2	D	134	DC	Sidechain
1	F	14	DG	Sidechain
1	F	15	DG	Sidechain
2	G	133	DA	Sidechain
2	G	134	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	494	0	273	25	0
1	F	494	0	273	27	0
2	D	241	0	138	12	0
2	G	241	0	138	10	0
3	E	268	0	148	12	0
3	H	268	0	148	16	0
4	A	2521	0	2511	92	0
4	B	2521	0	2517	111	0
5	A	14	0	19	0	0
5	C	14	0	19	4	0
5	F	14	0	19	4	0
6	A	76	0	0	1	0
6	B	40	0	0	1	0
6	C	7	0	0	0	0
6	F	2	0	0	0	0
6	G	2	0	0	0	0
6	H	2	0	0	1	0
All	All	7219	0	6203	296	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 22.

All (296) 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)
1:C:9:DA:H2"	1:C:10:DG:H5"	1.28	1.14
2:G:133:DA:H2"	2:G:134:DC:H5"	1.21	1.13
4:A:251:ASP:HB2	4:A:308:ASP:HB3	1.33	1.10
2:D:133:DA:H2"	2:D:134:DC:H5"	1.16	1.08
3:H:241:DA:H2"	3:H:242:DT:H5'	1.42	1.01
1:C:10:DG:H2"	1:C:11:DT:H5'	1.44	0.99
1:C:21:DA:H2"	1:C:22:DT:H5"	1.46	0.97
2:D:133:DA:C2'	2:D:134:DC:H5"	1.96	0.96
4:A:133:VAL:HG12	4:A:137:MET:HB3	1.50	0.94
2:G:133:DA:C2'	2:G:134:DC:H5"	2.00	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:274:ILE:HD11	4:B:288:LEU:HD13	1.52	0.91
4:B:133:VAL:HG13	4:B:137:MET:HB3	1.54	0.89
1:C:9:DA:C2'	1:C:10:DG:H5"	2.04	0.87
4:A:287:GLY:O	4:A:291:GLN:HG2	1.74	0.87
4:B:290:VAL:HG13	4:B:317:LEU:HD12	1.59	0.84
2:D:126:DA:H2"	2:D:127:DA:H5'	1.60	0.84
4:B:250:ALA:HA	4:B:253:LYS:HG2	1.59	0.83
4:B:326:ARG:HB2	4:B:327:PRO:HD3	1.61	0.82
3:H:238:DA:H2"	3:H:239:DC:H5"	1.62	0.82
2:D:133:DA:H2"	2:D:134:DC:C5'	2.06	0.81
5:F:202:BTB:H82	2:G:135:OMC:HN42	1.45	0.81
6:H:48:HOH:O	4:B:209:LYS:HE3	1.81	0.80
4:A:315:LYS:O	4:A:318:VAL:HG22	1.81	0.80
4:A:30:TRP:HE3	4:A:208:LEU:HD22	1.47	0.79
2:G:133:DA:H2"	2:G:134:DC:C5'	2.10	0.79
1:F:7:DA:H2"	1:F:8:DT:H5'	1.64	0.78
4:A:274:ILE:HG22	4:A:275:GLY:H	1.48	0.77
4:B:286:MET:HE1	4:B:318:VAL:HG13	1.65	0.77
4:A:326:ARG:HB3	4:A:327:PRO:HD3	1.67	0.77
4:A:286:MET:HB3	4:A:325:LEU:HD12	1.68	0.76
4:A:35:LYS:HE3	4:A:227:LYS:HD3	1.67	0.76
4:A:16:PHE:HA	4:A:19:LYS:HD3	1.67	0.76
1:C:21:DA:C2'	1:C:22:DT:H5"	2.17	0.75
5:C:201:BTB:C8	2:D:135:OMC:HN42	2.01	0.74
3:H:246:DA:H2"	3:H:247:DA:H5'	1.68	0.74
4:A:162:ILE:O	4:A:162:ILE:HD13	1.88	0.73
3:H:238:DA:H2"	3:H:239:DC:C5'	2.19	0.73
3:H:241:DA:H2"	3:H:242:DT:C5'	2.17	0.73
1:F:15:DG:H2'	1:F:16:DT:C7	2.20	0.72
4:A:133:VAL:CG1	4:A:137:MET:HG2	2.20	0.72
5:C:201:BTB:H82	2:D:135:OMC:HN42	1.55	0.71
1:C:9:DA:H2"	1:C:10:DG:C5'	2.14	0.71
1:F:15:DG:H2'	1:F:16:DT:H72	1.71	0.70
4:A:331:GLU:O	4:A:332:LEU:HG	1.92	0.70
4:A:166:ASN:HD22	4:A:167:ASP:N	1.89	0.69
4:A:30:TRP:CE3	4:A:208:LEU:HD22	2.27	0.69
4:B:159:GLU:CD	4:B:159:GLU:H	1.95	0.69
4:B:279:PRO:HA	4:B:333:VAL:HG11	1.75	0.69
4:B:290:VAL:HG22	4:B:321:VAL:HG21	1.75	0.69
4:A:253:LYS:HG3	4:A:254:LEU:HD22	1.75	0.68
4:A:266:ARG:O	4:A:270:VAL:HG23	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:242:DT:H2"	3:E:243:DC:C5	2.29	0.68
4:A:168:LEU:HD13	4:A:203:ALA:HB3	1.75	0.68
1:C:23:DT:H2"	1:C:24:DG:H5'	1.77	0.67
1:F:9:DA:H2"	1:F:10:DG:H5'	1.77	0.67
1:C:23:DT:H2"	1:C:24:DG:C5'	2.25	0.67
4:A:274:ILE:HG22	4:A:275:GLY:N	2.10	0.66
3:H:238:DA:C2'	3:H:239:DC:H5"	2.25	0.66
4:A:166:ASN:C	4:A:166:ASN:HD22	1.98	0.66
2:D:130:DG:H1'	2:D:131:DC:H5'	1.77	0.65
1:C:1:DA:H5"	4:B:318:VAL:HG11	1.79	0.65
4:A:257:ILE:O	4:A:260:CYS:HB2	1.98	0.64
1:F:9:DA:H2"	1:F:10:DG:C5'	2.27	0.64
4:B:286:MET:CE	4:B:318:VAL:HG13	2.27	0.64
4:B:286:MET:HG3	4:B:287:GLY:N	2.13	0.64
1:F:4:DC:H2"	1:F:5:DC:O5'	1.99	0.63
1:F:18:DG:OP1	1:F:18:DG:H4'	1.99	0.63
4:A:47:ARG:NH1	4:A:91:VAL:O	2.31	0.63
4:A:309:ASN:O	4:A:313:ILE:HG12	1.99	0.63
4:A:304:LEU:HD13	4:A:304:LEU:H	1.63	0.62
4:A:274:ILE:HD11	4:A:288:LEU:HD13	1.81	0.62
1:C:15:DG:H2'	1:C:16:DT:H72	1.81	0.62
4:B:295:GLU:O	4:B:299:ARG:HB2	1.99	0.62
4:B:133:VAL:CG1	4:B:137:MET:HB3	2.28	0.62
4:B:20:LEU:HD23	4:B:25:LEU:HD12	1.81	0.62
4:A:253:LYS:HG3	4:A:254:LEU:N	2.15	0.61
4:B:80:LYS:HE3	4:B:84:ASP:OD2	2.00	0.61
4:B:248:SER:OG	4:B:251:ASP:HB2	1.99	0.60
4:A:133:VAL:HG12	4:A:137:MET:CB	2.27	0.60
4:A:112:GLY:HA3	6:A:362:HOH:O	2.00	0.60
4:A:10:ASN:OD1	4:A:225:LYS:HE3	2.02	0.60
4:B:297:THR:HG23	4:B:298:SER:N	2.15	0.60
1:C:10:DG:C2'	1:C:11:DT:H5'	2.25	0.60
4:A:14:SER:O	4:A:18:GLU:HG2	2.02	0.60
1:F:7:DA:C2'	1:F:8:DT:H5'	2.30	0.59
4:B:193:ASN:HD22	4:B:193:ASN:N	2.00	0.59
3:E:241:DA:H1'	3:E:242:DT:H5'	1.85	0.59
4:A:304:LEU:HB2	4:A:314:LYS:HZ3	1.68	0.59
4:B:262:VAL:HG12	4:B:324:VAL:HG21	1.85	0.59
4:B:184:LEU:HG	4:B:188:ASN:ND2	2.18	0.59
4:B:279:PRO:CA	4:B:333:VAL:HG11	2.33	0.58
4:A:262:VAL:HG12	4:A:324:VAL:HG21	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:304:LEU:N	4:A:304:LEU:HD13	2.19	0.58
4:B:290:VAL:O	4:B:294:LEU:HD22	2.04	0.57
1:C:15:DG:H2'	1:C:16:DT:C7	2.34	0.57
1:F:8:DT:H2"	1:F:9:DA:N7	2.20	0.57
4:B:251:ASP:HA	4:B:308:ASP:OD1	2.05	0.57
2:G:129:DT:H2"	2:G:130:DG:O5'	2.05	0.56
4:B:289:THR:O	4:B:293:ILE:HG13	2.06	0.56
5:F:202:BTB:H82	2:G:135:OMC:N4	2.18	0.56
4:B:229:SER:O	4:B:230:LYS:HB3	2.06	0.56
1:F:7:DA:H1'	1:F:8:DT:C5'	2.36	0.56
4:B:282:PHE:HA	4:B:329:TRP:CZ3	2.40	0.56
4:B:42:SER:HA	4:B:96:VAL:O	2.05	0.56
1:F:6:DG:H2"	1:F:7:DA:H5'	1.88	0.56
4:B:158:PHE:HB3	4:B:159:GLU:OE2	2.06	0.56
4:B:169:ASP:HB3	4:B:200:VAL:HG22	1.88	0.56
4:B:297:THR:CG2	4:B:298:SER:N	2.68	0.55
4:B:94:TYR:CE2	4:B:123:VAL:HG22	2.41	0.55
4:A:308:ASP:O	4:A:309:ASN:HB2	2.05	0.55
4:A:121:ILE:O	4:A:133:VAL:HG23	2.05	0.55
4:A:168:LEU:HD12	4:A:168:LEU:H	1.72	0.55
4:B:30:TRP:HE3	4:B:208:LEU:HD22	1.71	0.55
3:H:241:DA:OP2	3:H:241:DA:H8	1.90	0.55
4:B:23:LEU:HD12	4:B:23:LEU:N	2.22	0.55
4:A:159:GLU:CD	4:A:159:GLU:H	2.09	0.54
4:A:314:LYS:H	4:A:314:LYS:HD2	1.72	0.54
5:C:201:BTB:H81	2:D:135:OMC:HN42	1.70	0.54
4:A:299:ARG:HH11	4:A:299:ARG:HG3	1.72	0.54
4:A:85:ILE:HD12	4:A:85:ILE:C	2.28	0.54
4:A:251:ASP:CB	4:A:308:ASP:HB3	2.22	0.54
4:B:169:ASP:HB3	4:B:200:VAL:CG2	2.38	0.54
4:B:266:ARG:O	4:B:270:VAL:HG23	2.08	0.53
4:B:282:PHE:N	4:B:329:TRP:CH2	2.76	0.53
4:B:134:ASP:OD2	4:B:136:TYR:HB2	2.09	0.53
4:A:166:ASN:C	4:A:166:ASN:ND2	2.61	0.53
4:A:71:ILE:HD13	4:A:116:PHE:HB2	1.90	0.53
4:B:17:ILE:O	4:B:20:LEU:HB2	2.09	0.53
4:B:25:LEU:O	4:B:27:GLY:N	2.42	0.53
4:B:229:SER:O	4:B:230:LYS:CB	2.55	0.53
4:A:251:ASP:OD1	4:A:313:ILE:HD11	2.08	0.53
1:F:7:DA:H1'	1:F:8:DT:H5'	1.89	0.53
4:B:302:ILE:HD12	4:B:302:ILE:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:239:DC:H2'	3:H:240:DT:H72	1.91	0.52
4:B:193:ASN:H	4:B:193:ASN:HD22	1.55	0.52
2:G:127:DA:H1'	2:G:128:DT:H5'	1.91	0.52
3:E:243:DC:H2"	3:E:244:DG:C8	2.45	0.52
4:B:309:ASN:OD1	4:B:312:LEU:HB3	2.10	0.52
1:F:18:DG:H2'	1:F:19:DC:C6	2.45	0.52
3:H:239:DC:H2"	3:H:240:DT:C6	2.44	0.52
4:A:8:LEU:HB2	4:A:225:LYS:HD3	1.92	0.52
4:A:124:THR:HA	4:A:129:ASP:O	2.09	0.52
4:A:95:GLN:HG2	4:A:97:PHE:CE1	2.44	0.52
4:A:133:VAL:CG1	4:A:137:MET:HB3	2.30	0.52
4:B:314:LYS:O	4:B:318:VAL:HG23	2.10	0.52
1:F:12:DG:H2"	1:F:13:DG:O5'	2.10	0.51
4:B:132:TYR:O	4:B:213:PRO:HG3	2.11	0.51
1:F:1:DA:N1	3:H:248:DT:O2	2.42	0.51
2:D:125:DC:H2"	2:D:126:DA:O5'	2.11	0.51
4:B:217:ARG:HB3	4:B:217:ARG:NH1	2.25	0.51
1:C:14:DG:H2"	1:C:15:DG:O5'	2.10	0.51
4:B:19:LYS:O	4:B:23:LEU:HD13	2.10	0.51
4:B:217:ARG:C	4:B:219:GLY:H	2.14	0.51
4:B:155:ARG:O	4:B:155:ARG:HG2	2.11	0.50
4:A:291:GLN:O	4:A:295:GLU:HG3	2.12	0.50
4:B:301:GLY:C	4:B:302:ILE:HD12	2.32	0.50
1:F:10:DG:H2"	1:F:11:DT:O5'	2.11	0.50
1:C:1:DA:H2"	1:C:2:DT:O5'	2.12	0.50
3:E:237:DC:H2"	3:E:238:DA:H5'	1.94	0.50
4:A:248:SER:OG	4:A:251:ASP:HB3	2.11	0.50
1:C:1:DA:C8	4:B:318:VAL:HG21	2.47	0.50
3:E:248:DT:H71	4:B:314:LYS:NZ	2.27	0.50
4:B:193:ASN:ND2	4:B:193:ASN:H	2.09	0.50
4:B:294:LEU:HA	4:B:297:THR:HG22	1.94	0.50
4:B:254:LEU:HD13	4:B:254:LEU:O	2.11	0.49
2:G:125:DC:H2"	2:G:126:DA:O5'	2.11	0.49
4:B:249:GLU:O	4:B:250:ALA:HB2	2.12	0.49
1:C:6:DG:H2"	1:C:7:DA:C8	2.48	0.49
1:C:9:DA:C3'	1:C:10:DG:H5"	2.39	0.49
4:B:247:LEU:N	4:B:247:LEU:HD23	2.28	0.48
1:F:2:DT:H2"	1:F:3:DT:O5'	2.13	0.48
4:B:302:ILE:HG22	4:B:302:ILE:O	2.13	0.48
4:A:257:ILE:HG22	4:A:258:LEU:N	2.28	0.48
4:A:216:LEU:HD12	4:A:220:ASN:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:130:DG:H2"	2:D:131:DC:O5'	2.14	0.48
4:A:304:LEU:HD22	4:A:305:THR:N	2.29	0.48
5:F:202:BTB:C8	2:G:135:OMC:HN42	2.22	0.48
4:B:309:ASN:C	4:B:311:SER:H	2.17	0.48
4:B:123:VAL:HG23	4:B:133:VAL:HG23	1.96	0.48
4:A:251:ASP:C	4:A:253:LYS:H	2.16	0.48
1:F:1:DA:H61	3:H:248:DT:H3	1.61	0.48
2:G:134:DC:H2"	2:G:135:OMC:H6	1.79	0.47
4:A:275:GLY:O	4:A:277:ILE:HG13	2.14	0.47
4:B:168:LEU:HD12	4:B:168:LEU:N	2.30	0.47
4:A:133:VAL:HG13	4:A:137:MET:HG2	1.95	0.47
4:A:168:LEU:N	4:A:168:LEU:HD12	2.29	0.47
4:B:252:ASN:O	4:B:255:VAL:HB	2.15	0.47
4:A:186:ASP:OD1	4:A:189:LYS:NZ	2.48	0.47
4:B:313:ILE:HG22	4:B:314:LYS:N	2.30	0.47
4:B:25:LEU:C	4:B:27:GLY:H	2.18	0.47
4:A:294:LEU:O	4:A:297:THR:HG22	2.14	0.47
4:B:12:TYR:CD1	4:B:12:TYR:C	2.88	0.47
4:B:72:LEU:O	4:B:76:ALA:HB2	2.14	0.47
1:C:18:DG:H2"	1:C:19:DC:O5'	2.15	0.47
1:F:6:DG:H2"	1:F:7:DA:C5'	2.45	0.47
3:H:244:DG:H2"	3:H:245:DG:C8	2.50	0.47
4:A:175:TYR:O	4:A:179:VAL:HG23	2.14	0.47
4:A:254:LEU:O	4:A:257:ILE:N	2.48	0.47
1:C:21:DA:H2"	1:C:22:DT:C5'	2.31	0.47
1:F:7:DA:H2"	1:F:8:DT:OP2	2.15	0.46
4:A:286:MET:HG3	4:A:287:GLY:N	2.30	0.46
4:B:254:LEU:C	4:B:254:LEU:HD13	2.35	0.46
1:F:10:DG:H1	3:H:239:DC:H42	1.62	0.46
3:E:242:DT:H2"	3:E:243:DC:C6	2.50	0.46
4:A:282:PHE:CE1	4:A:325:LEU:HD13	2.51	0.46
4:A:12:TYR:O	4:A:14:SER:N	2.49	0.46
1:C:19:DC:H2"	1:C:20:DA:OP2	2.16	0.46
4:B:20:LEU:CD2	4:B:25:LEU:HD12	2.45	0.46
4:B:18:GLU:HA	4:B:21:TYR:HD1	1.79	0.46
4:B:274:ILE:O	4:B:276:GLU:N	2.49	0.46
4:B:298:SER:C	4:B:300:GLU:H	2.19	0.46
4:B:146:LYS:HA	4:B:184:LEU:CD2	2.46	0.46
4:B:193:ASN:ND2	4:B:193:ASN:N	2.64	0.45
3:H:236:A:H5"	4:B:8:LEU:HD12	1.98	0.45
4:A:320:MET:O	4:A:324:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:216:LEU:O	4:B:218:ASN:N	2.50	0.45
4:B:130:VAL:O	4:B:131:THR:HB	2.17	0.45
4:B:286:MET:HG3	4:B:287:GLY:H	1.79	0.45
4:A:248:SER:O	4:A:252:ASN:HB2	2.17	0.45
4:B:161:LEU:C	4:B:163:LYS:H	2.19	0.45
4:A:281:ASP:O	4:A:285:VAL:HG23	2.15	0.45
2:D:134:DC:H2"	2:D:135:OMC:H6	1.82	0.45
4:B:71:ILE:HD11	4:B:100:PHE:CD1	2.52	0.45
4:B:107:LYS:O	4:B:109:VAL:HG22	2.16	0.45
4:B:271:ILE:HG23	4:B:277:ILE:CD1	2.46	0.45
4:B:31:VAL:O	4:B:208:LEU:HD23	2.17	0.44
2:D:128:DT:H2"	2:D:129:DT:O5'	2.16	0.44
1:F:9:DA:H1'	1:F:10:DG:H5"	1.98	0.44
4:A:133:VAL:CG1	4:A:137:MET:CG	2.94	0.44
4:B:298:SER:C	4:B:300:GLU:N	2.70	0.44
3:E:237:DC:C2'	3:E:238:DA:H5'	2.47	0.44
4:A:285:VAL:HG21	4:A:329:TRP:CZ3	2.53	0.44
1:F:7:DA:C1'	1:F:8:DT:H5'	2.47	0.44
3:E:239:DC:C2'	3:E:240:DT:H71	2.48	0.44
4:A:257:ILE:O	4:A:260:CYS:CB	2.64	0.44
4:A:247:LEU:HD22	4:A:252:ASN:OD1	2.18	0.43
4:A:319:LYS:HG2	4:A:323:ASP:OD2	2.17	0.43
4:A:111:TYR:O	4:A:112:GLY:O	2.37	0.43
4:A:30:TRP:O	4:A:155:ARG:HA	2.18	0.43
4:B:274:ILE:HG22	4:B:274:ILE:O	2.18	0.43
4:A:308:ASP:O	4:A:309:ASN:CB	2.66	0.43
4:A:125:THR:OG1	4:A:129:ASP:HB2	2.19	0.43
4:B:214:SER:OG	4:B:222:VAL:HG21	2.17	0.43
1:F:7:DA:H1'	1:F:8:DT:H5"	2.01	0.43
4:B:228:ASN:HD22	4:B:230:LYS:N	2.17	0.43
4:B:122:ILE:HD11	4:B:132:TYR:CZ	2.55	0.42
4:B:25:LEU:C	4:B:27:GLY:N	2.72	0.42
4:A:101:ALA:O	4:A:114:LYS:HA	2.19	0.42
1:F:8:DT:H2"	1:F:9:DA:C8	2.54	0.42
1:C:22:DT:H2'	1:C:23:DT:H72	1.99	0.42
4:B:101:ALA:O	4:B:114:LYS:HA	2.19	0.42
4:B:35:LYS:HG2	4:B:204:GLU:OE1	2.20	0.42
1:C:5:DC:H42	3:E:244:DG:H1	1.68	0.42
4:A:5:TYR:HB2	4:A:97:PHE:CE2	2.54	0.42
4:B:86:MET:N	6:B:344:HOH:O	2.52	0.42
4:B:11:HIS:HA	4:B:224:ILE:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:251:ASP:C	4:A:253:LYS:N	2.73	0.42
4:A:142:CYS:O	4:A:146:LYS:N	2.53	0.42
4:A:301:GLY:O	4:A:303:THR:N	2.53	0.42
3:H:239:DC:H2"	3:H:240:DT:H6	1.84	0.41
4:B:298:SER:HA	4:B:302:ILE:O	2.20	0.41
3:E:241:DA:H2"	3:E:242:DT:O5'	2.20	0.41
4:B:60:LEU:HA	4:B:61:PRO:HD3	1.95	0.41
4:B:69:GLU:H	4:B:69:GLU:CD	2.21	0.41
1:C:14:DG:O6	5:C:201:BTB:H62	2.21	0.41
1:C:23:DT:H2"	1:C:24:DG:H5"	1.99	0.41
4:B:286:MET:HB3	4:B:325:LEU:HD12	2.03	0.41
4:A:308:ASP:CG	4:A:308:ASP:O	2.59	0.41
4:B:20:LEU:HB3	4:B:26:THR:HG23	2.03	0.41
4:A:224:ILE:HG22	4:A:225:LYS:N	2.35	0.41
4:A:33:ARG:HH11	4:A:135:ASP:CG	2.24	0.41
4:B:274:ILE:O	4:B:275:GLY:C	2.59	0.41
4:A:195:GLU:OE1	4:A:197:LYS:HE3	2.21	0.41
3:H:240:DT:H2"	3:H:241:DA:OP2	2.21	0.41
4:A:163:LYS:O	4:A:164:LEU:C	2.59	0.41
1:F:1:DA:H2"	1:F:2:DT:OP2	2.20	0.41
3:E:243:DC:H2"	3:E:244:DG:OP2	2.20	0.41
4:B:217:ARG:C	4:B:219:GLY:N	2.74	0.41
4:B:217:ARG:CZ	4:B:217:ARG:HB3	2.51	0.41
4:B:161:LEU:C	4:B:163:LYS:N	2.73	0.41
4:B:316:GLU:OE1	4:B:316:GLU:HA	2.20	0.41
4:B:297:THR:CG2	4:B:298:SER:H	2.34	0.41
4:B:326:ARG:HB2	4:B:327:PRO:CD	2.41	0.41
4:A:35:LYS:CE	4:A:227:LYS:HD3	2.45	0.41
3:E:239:DC:H2"	3:E:240:DT:H71	2.02	0.41
4:A:1:MET:HB3	4:A:1:MET:HE2	1.72	0.41
1:C:2:DT:H5'	4:B:287:GLY:HA3	2.03	0.41
4:A:290:VAL:O	4:A:294:LEU:HD23	2.21	0.40
4:A:210:PRO:HD3	4:A:222:VAL:O	2.21	0.40
4:B:212:TYR:HA	4:B:213:PRO:HD2	1.75	0.40
4:B:278:GLY:C	4:B:280:LYS:H	2.24	0.40
4:A:254:LEU:O	4:A:255:VAL:C	2.60	0.40
4:A:220:ASN:HA	4:A:220:ASN:HD22	1.65	0.40
1:F:13:DG:N7	5:F:202:BTB:H51	2.36	0.40
4:B:91:VAL:HG13	4:B:123:VAL:HG13	2.04	0.40
4:B:298:SER:HA	4:B:302:ILE:C	2.41	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	
4	A	315/335 (94%)	277 (88%)	29 (9%)	9 (3%)	6	3
4	B	315/335 (94%)	272 (86%)	31 (10%)	12 (4%)	4	1
All	All	630/670 (94%)	549 (87%)	60 (10%)	21 (3%)	5	2

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	309	ASN
4	B	250	ALA
4	B	275	GLY
4	A	13	ASN
4	A	112	GLY
4	A	302	ILE
4	B	26	THR
4	B	213	PRO
4	B	217	ARG
4	A	250	ALA
4	B	197	LYS
4	B	198	GLY
4	B	218	ASN
4	B	308	ASP
4	B	310	PRO
4	A	285	VAL
4	B	274	ILE
4	A	151	PRO
4	A	313	ILE
4	A	327	PRO
4	B	279	PRO

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
4	A	277/293 (94%)	257 (93%)	20 (7%)	18 24
4	B	278/293 (95%)	261 (94%)	17 (6%)	23 32
All	All	555/586 (95%)	518 (93%)	37 (7%)	20 27

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	47	ARG
4	A	55	ARG
4	A	69	GLU
4	A	84	ASP
4	A	109	VAL
4	A	115	ASP
4	A	129	ASP
4	A	162	ILE
4	A	166	ASN
4	A	168	LEU
4	A	173	GLN
4	A	208	LEU
4	A	253	LYS
4	A	280	LYS
4	A	286	MET
4	A	300	GLU
4	A	304	LEU
4	A	309	ASN
4	A	317	LEU
4	A	325	LEU
4	B	12	TYR
4	B	47	ARG
4	B	49	LYS
4	B	69	GLU
4	B	72	LEU
4	B	151	PRO
4	B	155	ARG

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Mol	Chain	Res	Type
4	B	162	ILE
4	B	168	LEU
4	B	169	ASP
4	B	193	ASN
4	B	208	LEU
4	B	218	ASN
4	B	228	ASN
4	B	253	LYS
4	B	288	LEU
4	B	294	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	166	ASN
4	A	173	GLN
4	A	193	ASN
4	A	220	ASN
4	A	228	ASN
4	A	268	ASN
4	A	322	GLN
4	B	173	GLN
4	B	193	ASN
4	B	220	ASN
4	B	228	ASN
4	B	268	ASN
4	B	322	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
2	OMC	D	135	1,2	13,22,23	0.83	0	20,31,34	1.23	2 (10%)
2	O2C	D	136	2	12,20,21	0.78	0	12,28,31	1.04	1 (8%)
2	OMC	G	135	1,2	13,22,23	0.89	1 (7%)	20,31,34	1.08	1 (5%)
2	O2C	G	136	2	12,20,21	0.78	0	12,28,31	1.08	1 (8%)

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
2	OMC	D	135	1,2	-	0/5/27/28	0/2/2/2
2	O2C	D	136	2	-	0/3/21/22	0/2/2/2
2	OMC	G	135	1,2	-	0/5/27/28	0/2/2/2
2	O2C	G	136	2	-	0/3/21/22	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	135	OMC	C6-C5	-2.11	1.33	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	135	OMC	CM2-O2'-C2'	-2.89	106.43	114.59
2	G	135	OMC	C2-N3-C4	3.05	119.92	115.61
2	D	135	OMC	C2-N3-C4	3.06	119.93	115.61
2	D	136	O2C	C2-N3-C4	3.11	119.99	115.61
2	G	136	O2C	C2-N3-C4	3.15	120.05	115.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	135	OMC	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	135	OMC	4	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

3 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	$\#\|Z\| > 2$
5	BTB	A	335	-	12,13,13	1.77	1 (8%)	8,16,16	2.27	2 (25%)
5	BTB	C	201	-	12,13,13	1.78	2 (16%)	8,16,16	2.18	2 (25%)
5	BTB	F	202	-	12,13,13	1.76	1 (8%)	8,16,16	2.13	2 (25%)

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
5	BTB	A	335	-	-	0/21/21/21	0/0/0/0
5	BTB	C	201	-	-	0/21/21/21	0/0/0/0
5	BTB	F	202	-	-	0/21/21/21	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	201	BTB	C7-N	2.18	1.51	1.48
5	F	202	BTB	C5-N	5.29	1.56	1.48
5	A	335	BTB	C5-N	5.33	1.56	1.48
5	C	201	BTB	C5-N	5.34	1.56	1.48

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	335	BTB	O3-C3-C2	-2.61	104.83	111.12
5	C	201	BTB	O3-C3-C2	-2.31	105.56	111.12
5	F	202	BTB	O3-C3-C2	-2.00	106.29	111.12
5	C	201	BTB	C7-N-C2	4.97	128.21	113.86
5	F	202	BTB	C7-N-C2	4.98	128.25	113.86
5	A	335	BTB	C7-N-C2	5.07	128.51	113.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	201	BTB	4	0
5	F	202	BTB	4	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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(Å^2)	Q<0.9
1	C	24/24 (100%)	0.61	2 (8%) 14 14	52, 91, 124, 130	0
1	F	24/24 (100%)	0.49	3 (12%) 5 5	48, 74, 150, 161	0
2	D	10/12 (83%)	0.79	1 (10%) 9 9	60, 101, 121, 123	0
2	G	10/12 (83%)	0.31	0 100 100	63, 74, 90, 93	0
3	E	13/13 (100%)	0.64	0 100 100	38, 91, 118, 126	0
3	H	13/13 (100%)	0.97	3 (23%) 1 1	38, 94, 141, 146	0
4	A	319/335 (95%)	0.02	10 (3%) 52 56	18, 47, 103, 122	0
4	B	319/335 (95%)	0.19	15 (4%) 35 38	23, 52, 110, 127	0
All	All	732/768 (95%)	0.17	34 (4%) 36 40	18, 54, 114, 161	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	219	GLY	4.4
4	B	334	SER	3.7
4	B	290	VAL	3.6
4	B	277	ILE	3.4
4	B	308	ASP	3.4
4	B	21	TYR	3.4
3	H	248	DT	3.3
4	B	286	MET	3.3
4	B	249	GLU	3.2
1	C	19	DC	3.1
4	A	230	LYS	3.0
4	B	217	ARG	3.0
4	B	251	ASP	2.8
4	A	246	GLU	2.8
4	A	249	GLU	2.8
4	A	250	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
3	H	245	DG	2.7
4	B	287	GLY	2.7
4	A	290	VAL	2.5
4	A	64	ASP	2.5
1	C	4	DC	2.5
2	D	125	DC	2.4
4	A	277	ILE	2.3
4	B	196	ALA	2.3
4	B	182	ALA	2.3
4	B	195	GLU	2.2
4	B	302	ILE	2.2
4	A	287	GLY	2.2
1	F	1	DA	2.2
4	A	247	LEU	2.2
4	A	255	VAL	2.1
3	H	247	DA	2.1
1	F	3	DT	2.0
1	F	4	DC	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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
2	OMC	G	135	21/22	0.96	0.13	-	24,40,48,55	0
2	OMC	D	135	21/22	0.97	0.16	-	32,41,46,49	0
2	O2C	G	136	19/20	0.98	0.10	-	34,38,46,47	0
2	O2C	D	136	19/20	0.97	0.12	-	23,36,46,48	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

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, 95^{th} 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
5	BTB	F	202	14/14	0.80	0.31	6.00	60,81,84,90	0
5	BTB	C	201	14/14	0.83	0.23	2.58	74,81,92,96	0
5	BTB	A	335	14/14	0.85	0.31	2.01	110,114,117,119	0

6.5 Other polymers

There are no such residues in this entry.