



Full wwPDB X-ray Structure Validation Report

May 26, 2020 – 09:15 pm BST

PDB ID : 4Q44
Title : Polymerase-Damaged DNA Complex
Authors : Nair, D.T.; Kottur, J.; Sharma, A.
Deposited on : 2014-04-13
Resolution : 2.71 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the  symbol.

The following versions of software and data (see [references](#) ) 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
buster-report : 1.1.7 (2018)
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

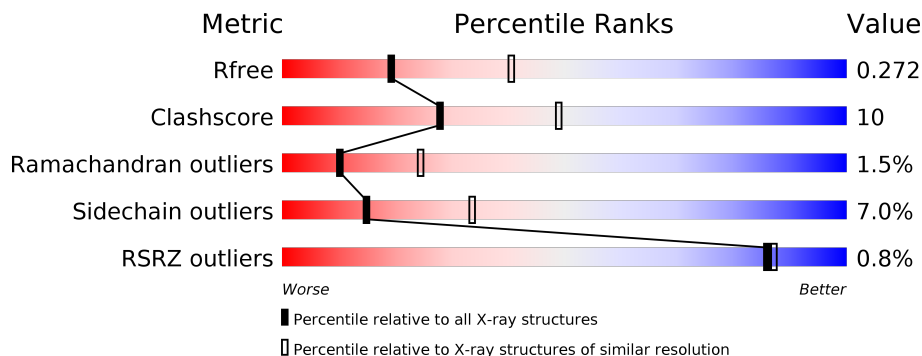
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION







The reported resolution of this entry is 2.71 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}	130704	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	342	 6% 75% 22%
1	F	342	 73% 24%
2	B	18	 50% 50%
2	C	18	 6% 78% 17% 6%
2	G	18	 6% 78% 22%
2	H	18	 67% 11% 22%

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 6904 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 protein called DNA polymerase IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	342	2684	1692	493	485	14	0	0	0
1	F	342	2688	1695	494	485	14	0	0	0

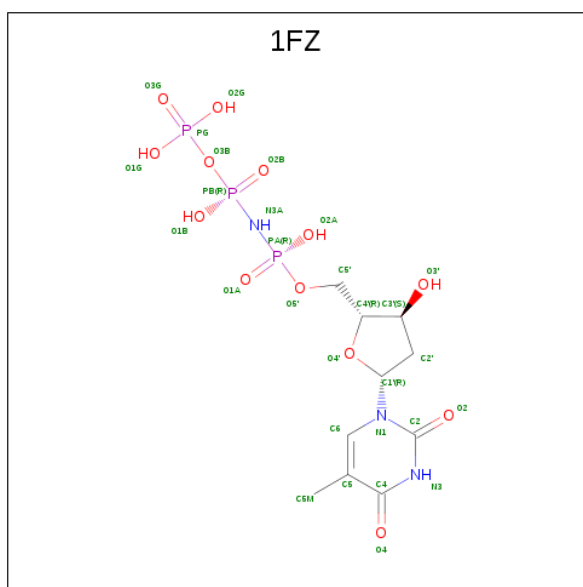
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	EXPRESSION TAG	UNP Q47155
A	1	SER	-	EXPRESSION TAG	UNP Q47155
A	64	ALA	LYS	CONFLICT	UNP Q47155
A	205	ALA	LYS	CONFLICT	UNP Q47155
F	0	GLY	-	EXPRESSION TAG	UNP Q47155
F	1	SER	-	EXPRESSION TAG	UNP Q47155
F	64	ALA	LYS	CONFLICT	UNP Q47155
F	205	ALA	LYS	CONFLICT	UNP Q47155

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	18	370	179	66	108	17	0	0	0
2	C	17	350	169	64	101	16	0	0	0
2	G	18	370	179	66	108	17	0	0	0
2	H	14	293	140	54	85	14	0	0	0

- Molecule 3 is 5'-O-[(R)-hydroxy{[(R)-hydroxy(phosphonoxy)phosphoryl]amino}phosphoryl]thymidine (three-letter code: 1FZ) (formula: C₁₀H₁₈N₃O₁₃P₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	A	1	Total	C	N	O	P	0	0
			29	10	3	13	3		
3	F	1	Total	C	N	O	P	0	0
			29	10	3	13	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		
4	F	2	Total	Mg	0	0
			2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	18	Total	O	0	0
			18	18		
5	F	40	Total	O	0	0
			40	40		
5	B	4	Total	O	0	0
			4	4		
5	C	6	Total	O	0	0
			6	6		
5	G	11	Total	O	0	0
			11	11		

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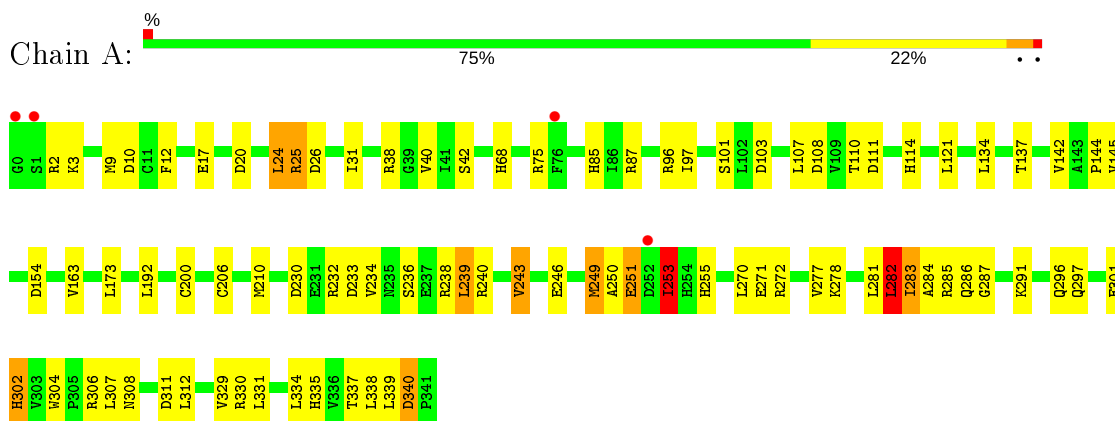
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	8	Total	O	0	0
			8	8		

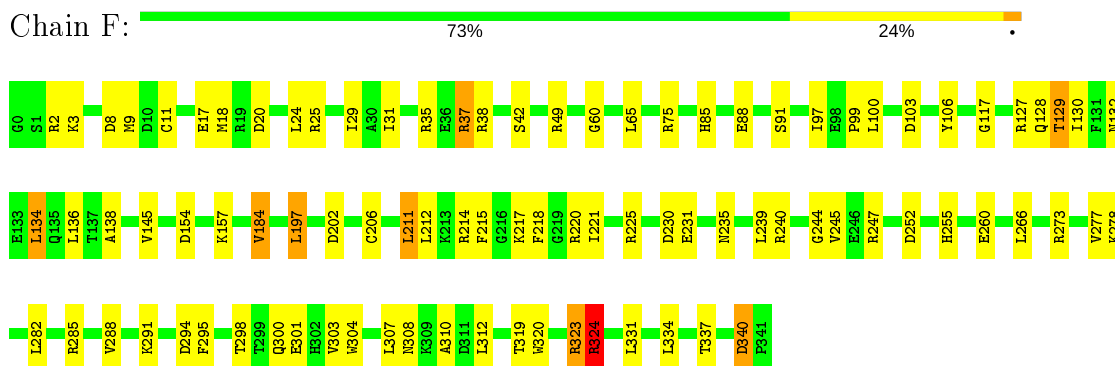
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: DNA polymerase IV



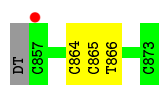
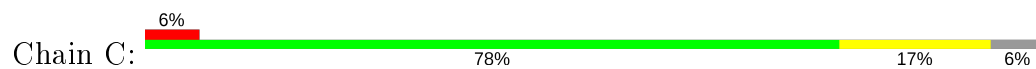
- Molecule 1: DNA polymerase IV



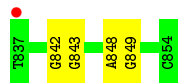
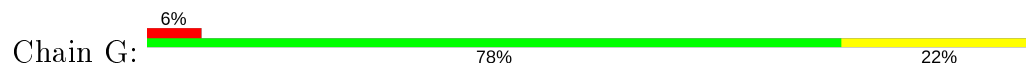
- Molecule 2: DNA (5'-D(*TP*CP*TP*AP*(RDG)P*GP*GP*TP*CP*CP*TP*AP*GP*GP*A P*CP*CP*C)-3')



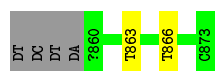
- Molecule 2: DNA (5'-D(*TP*CP*TP*AP*(RDG)P*GP*GP*TP*CP*CP*TP*AP*GP*GP*A P*CP*CP*C)-3')



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.66Å 56.93Å 110.40Å 90.00° 94.66° 90.00°	Depositor
Resolution (Å)	48.21 – 2.71 48.21 – 2.71	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.21-2.71) 99.6 (48.21-2.71)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.69Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8_1069)	Depositor
R, R_{free}	0.225 , 0.270 0.227 , 0.272	Depositor DCC
R_{free} test set	1501 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	47.7	Xtrriage
Anisotropy	0.291	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 29.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6904	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: RDG, MG, 1FZ

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	0.24	0/2735	0.47	1/3695 (0.0%)
1	F	0.23	0/2739	0.44	0/3699
2	B	0.41	0/381	0.99	0/583
2	C	0.42	0/359	1.05	0/549
2	G	0.41	0/381	1.04	0/583
2	H	0.40	0/296	0.96	0/454
All	All	0.28	0/6891	0.63	1/9563 (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	F	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	282	LEU	CB-CG-CD1	-5.63	101.42	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	340	ASP	Peptide

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	2684	0	2734	63	0
1	F	2688	0	2745	51	0
2	B	370	0	208	7	0
2	C	350	0	196	4	0
2	G	370	0	208	5	0
2	H	293	0	161	2	0
3	A	29	0	14	3	0
3	F	29	0	14	2	0
4	A	2	0	0	0	0
4	F	2	0	0	0	0
5	A	18	0	0	5	0
5	B	4	0	0	0	0
5	C	6	0	0	0	0
5	F	40	0	0	9	0
5	G	11	0	0	2	0
5	H	8	0	0	1	0
All	All	6904	0	6280	126	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 10.

All (126) 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:F:235:ASN:O	5:F:520:HOH:O	1.81	0.99
2:H:863:DT:O4	5:H:907:HOH:O	1.83	0.97
3:F:401:1FZ:O1G	5:F:524:HOH:O	1.90	0.90
1:A:3:LYS:H	1:A:110:THR:HG22	1.44	0.82
1:A:154:ASP:OD2	5:A:504:HOH:O	1.98	0.79
2:G:849:DG:O6	5:G:903:HOH:O	2.05	0.73
1:F:11:CYS:HB3	1:F:49:ARG:HH12	1.52	0.73
1:F:230:ASP:O	5:F:501:HOH:O	2.07	0.72
1:F:291:LYS:HB3	1:F:331:LEU:HB3	1.72	0.72
1:F:298:THR:OG1	1:F:323:ARG:NH1	2.25	0.70
1:F:285:ARG:NH1	2:H:866:DT:OP2	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:MET:HB2	1:A:103:ASP:HB2	1.77	0.67
1:F:129:THR:HA	1:F:132:ASN:HB2	1.78	0.66
1:A:110:THR:OG1	1:A:111:ASP:N	2.30	0.65
1:F:255:HIS:ND1	5:F:503:HOH:O	2.28	0.65
1:A:96:ARG:NH1	1:A:234:VAL:O	2.27	0.65
1:A:38:ARG:NH2	1:A:251:GLU:OE1	2.26	0.65
1:A:286:GLN:HE21	1:A:307:LEU:HD12	1.64	0.63
1:A:302:HIS:NE2	1:A:311:ASP:OD2	2.32	0.63
1:F:20:ASP:OD2	1:F:75:ARG:NH2	2.30	0.63
1:F:8:ASP:OD2	5:F:522:HOH:O	2.15	0.63
1:A:20:ASP:OD2	1:A:75:ARG:NH2	2.32	0.62
1:F:245:VAL:HG22	1:F:273:ARG:HH11	1.65	0.62
1:A:286:GLN:HE22	1:A:308:ASN:H	1.48	0.62
1:A:249:MET:SD	1:A:250:ALA:N	2.67	0.62
1:A:145:VAL:HB	1:A:230:ASP:HB3	1.82	0.61
1:A:304:TRP:NE1	1:A:308:ASN:OD1	2.26	0.61
1:F:2:ARG:NH2	5:F:501:HOH:O	2.32	0.61
1:A:25:ARG:NH1	1:A:26:ASP:OD1	2.34	0.61
1:F:301:GLU:OE2	5:F:523:HOH:O	2.16	0.61
3:A:401:1FZ:O2A	5:A:507:HOH:O	2.16	0.60
1:A:282:LEU:HD12	1:A:283:ILE:H	1.66	0.59
1:A:278:LYS:CB	1:A:282:LEU:HD23	2.33	0.58
2:C:864:DC:H2''	2:C:865:DC:H5''	1.86	0.58
1:A:240:ARG:HH21	1:A:243:VAL:HB	1.70	0.57
1:F:300:GLN:NE2	1:F:319:THR:OG1	2.38	0.57
1:F:240:ARG:NH1	2:G:843:DG:OP1	2.37	0.56
1:A:291:LYS:HG3	1:A:297:GLN:HB3	1.88	0.56
2:B:851:DA:H2''	2:B:852:DC:H5''	1.86	0.56
1:F:3:LYS:NZ	1:F:117:GLY:O	2.35	0.56
1:A:278:LYS:HB2	1:A:282:LEU:HD23	1.88	0.56
1:A:87:ARG:NH2	1:A:101:SER:O	2.36	0.55
1:A:287:GLY:HA3	1:A:301:GLU:HG2	1.87	0.55
1:F:85:HIS:HB3	1:F:134:LEU:HD21	1.87	0.55
1:F:285:ARG:HB2	1:F:337:THR:HB	1.89	0.55
1:F:212:LEU:HD21	1:F:220:ARG:HB2	1.88	0.54
1:F:9:MET:HB2	1:F:103:ASP:HB2	1.89	0.54
1:F:145:VAL:HB	1:F:230:ASP:HB3	1.89	0.54
1:A:24:LEU:O	1:A:26:ASP:N	2.40	0.54
1:A:286:GLN:HG2	1:A:312:LEU:HD21	1.90	0.53
1:F:197:LEU:HD12	1:F:202:ASP:HB3	1.91	0.53
1:A:312:LEU:HD13	1:A:334:LEU:HD22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:ASP:OD1	1:A:340:ASP:N	2.42	0.52
1:F:184:VAL:O	5:F:506:HOH:O	2.19	0.52
1:F:310:ALA:N	5:F:521:HOH:O	2.41	0.52
1:A:142:VAL:HB	1:A:163:VAL:HG22	1.92	0.52
1:F:154:ASP:HA	1:F:157:LYS:HD2	1.93	0.51
1:F:273:ARG:HH12	2:G:842:DG:H5'	1.75	0.51
1:A:282:LEU:HD21	1:A:338:LEU:HG	1.93	0.50
1:A:240:ARG:NH2	2:B:843:DG:OP1	2.45	0.50
1:A:96:ARG:NH2	1:A:233:ASP:OD1	2.41	0.49
1:A:278:LYS:HG2	1:A:282:LEU:HB3	1.94	0.49
1:F:35:ARG:HD3	1:F:60:GLY:HA2	1.95	0.49
1:F:273:ARG:NH2	2:G:843:DG:OP1	2.46	0.49
1:A:38:ARG:NH1	1:A:249:MET:O	2.38	0.48
1:A:285:ARG:HD3	1:A:337:THR:HG21	1.95	0.48
1:A:282:LEU:HD11	1:A:339:LEU:H	1.78	0.48
1:A:282:LEU:HD11	1:A:338:LEU:HA	1.96	0.48
1:A:285:ARG:NH2	2:C:866:DT:OP2	2.47	0.48
1:F:240:ARG:HH21	1:F:277:VAL:HG21	1.78	0.47
1:A:286:GLN:NE2	1:A:308:ASN:H	2.11	0.47
1:A:282:LEU:CG	1:A:283:ILE:H	2.27	0.47
1:A:306:ARG:NH2	5:A:511:HOH:O	2.47	0.47
1:F:17:GLU:HG3	1:F:31:ILE:HD11	1.97	0.47
1:A:283:ILE:HG22	1:A:304:TRP:O	2.15	0.47
1:A:285:ARG:HH12	2:C:865:DC:H3'	1.81	0.46
1:F:312:LEU:HD13	1:F:334:LEU:HD22	1.97	0.46
1:A:291:LYS:HB3	1:A:331:LEU:HB3	1.98	0.46
1:A:253:ILE:HG12	1:A:329:VAL:HB	1.98	0.46
1:F:97:ILE:O	1:F:99:PRO:HD3	2.15	0.46
1:F:18:MET:HE3	1:F:25:ARG:HD3	1.98	0.45
1:A:282:LEU:CD1	1:A:283:ILE:H	2.28	0.45
1:F:278:LYS:HZ1	1:F:282:LEU:HB2	1.82	0.45
1:A:173:LEU:O	1:A:200:CYS:HB2	2.15	0.45
1:F:304:TRP:HE1	1:F:308:ASN:HB2	1.82	0.45
1:A:97:ILE:HG12	1:A:107:LEU:HD22	1.98	0.45
2:B:843:DG:H2'	2:B:844:DT:C6	2.51	0.45
1:A:2:ARG:O	1:A:144:PRO:HA	2.17	0.45
1:F:197:LEU:HD11	1:F:206:CYS:SG	2.57	0.44
1:F:221:ILE:O	1:F:225:ARG:HG2	2.18	0.44
1:A:270:LEU:HD22	1:A:334:LEU:HB3	1.99	0.44
1:F:244:GLY:O	1:F:273:ARG:NH1	2.50	0.44
1:F:24:LEU:HB3	1:F:29:ILE:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:ASN:HD21	1:A:311:ASP:HB2	1.82	0.44
1:A:251:GLU:HG3	1:A:330:ARG:HA	1.99	0.44
1:F:130:ILE:O	1:F:134:LEU:HB2	2.17	0.44
1:F:100:LEU:HD11	1:F:106:TYR:CE1	2.53	0.44
1:F:288:VAL:HG12	1:F:334:LEU:HD23	1.99	0.44
1:A:2:ARG:NH2	1:A:232:ARG:O	2.51	0.44
1:A:10:ASP:HB2	1:A:137:THR:HG23	1.99	0.43
1:A:255:HIS:ND1	1:F:294:ASP:O	2.52	0.43
3:F:401:1FZ:O5'	3:F:401:1FZ:H1	2.18	0.43
1:F:215:PHE:HB3	1:F:218:PHE:HD2	1.83	0.43
1:F:38:ARG:NH1	1:F:252:ASP:OD1	2.43	0.43
1:A:85:HIS:HB3	1:A:134:LEU:HD21	1.99	0.42
1:A:17:GLU:HG3	1:A:31:ILE:HD11	2.01	0.42
1:A:12:PHE:HB3	3:A:401:1FZ:O3'	2.19	0.42
1:F:128:GLN:O	1:F:129:THR:HB	2.19	0.42
1:F:88:GLU:O	1:F:91:SER:OG	2.29	0.42
1:A:285:ARG:HH22	2:C:866:DT:P	2.43	0.42
1:A:239:LEU:HD12	1:A:239:LEU:HA	1.91	0.42
2:B:848:DA:H2''	2:B:849:DG:C8	2.54	0.42
3:A:401:1FZ:H1	3:A:401:1FZ:O5'	2.19	0.42
1:A:68:HIS:O	5:A:505:HOH:O	2.21	0.42
1:F:127:ARG:HD2	1:F:138:ALA:O	2.20	0.41
1:A:284:ALA:HB2	1:A:339:LEU:HD23	2.02	0.41
1:F:211:LEU:HD12	1:F:211:LEU:HA	1.83	0.41
1:F:320:TRP:O	1:F:324:ARG:HG2	2.20	0.41
1:A:108:ASP:OD1	1:A:110:THR:HG23	2.20	0.41
1:A:246:GLU:HG2	2:B:842:DG:OP2	2.21	0.41
1:A:301:GLU:OE2	1:A:335:HIS:ND1	2.44	0.40
1:F:37:ARG:NH1	5:G:901:HOH:O	2.53	0.40
1:A:282:LEU:HD11	1:A:339:LEU:N	2.36	0.40
5:A:501:HOH:O	2:B:841:RDG:H12	2.22	0.40
2:B:850:DG:H2''	2:B:851:DA:C8	2.56	0.40
2:G:848:DA:H2''	2:G:849:DG:C8	2.56	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	
1	A	340/342 (99%)	316 (93%)	18 (5%)	6 (2%)	8	20
1	F	340/342 (99%)	318 (94%)	18 (5%)	4 (1%)	13	30
All	All	680/684 (99%)	634 (93%)	36 (5%)	10 (2%)	10	24

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	251	GLU
1	A	282	LEU
1	F	340	ASP
1	A	24	LEU
1	A	253	ILE
1	A	25	ARG
1	A	283	ILE
1	F	324	ARG
1	F	129	THR
1	F	307	LEU

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	
1	A	285/286 (100%)	264 (93%)	21 (7%)	13	31
1	F	286/286 (100%)	267 (93%)	19 (7%)	16	36
All	All	571/572 (100%)	531 (93%)	40 (7%)	15	34

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	VAL
1	A	42	SER
1	A	114	HIS
1	A	121	LEU
1	A	192	LEU
1	A	206	CYS
1	A	210	MET
1	A	236	SER
1	A	238	ARG
1	A	239	LEU
1	A	243	VAL
1	A	249	MET
1	A	253	ILE
1	A	271	GLU
1	A	272	ARG
1	A	277	VAL
1	A	281	LEU
1	A	282	LEU
1	A	296	GLN
1	A	302	HIS
1	A	340	ASP
1	F	37	ARG
1	F	42	SER
1	F	65	LEU
1	F	134	LEU
1	F	136	LEU
1	F	184	VAL
1	F	197	LEU
1	F	211	LEU
1	F	214	ARG
1	F	217	LYS
1	F	231	GLU
1	F	239	LEU
1	F	247	ARG
1	F	260	GLU
1	F	266	LEU
1	F	295	PHE
1	F	303	VAL
1	F	323	ARG
1	F	324	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	286	GLN
1	F	300	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](#)

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	RDG	C	860	2	22,31,32	2.90	12 (54%)	24,44,47	2.01	10 (41%)
2	RDG	G	841	2	22,31,32	2.89	12 (54%)	24,44,47	2.07	11 (45%)
2	RDG	B	841	2	22,31,32	2.91	12 (54%)	24,44,47	1.95	9 (37%)
2	RDG	H	860	2	22,31,32	2.91	12 (54%)	24,44,47	1.97	10 (41%)

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	RDG	C	860	2	-	0/6/26/27	0/4/4/4
2	RDG	G	841	2	-	3/6/26/27	0/4/4/4
2	RDG	B	841	2	-	2/6/26/27	0/4/4/4
2	RDG	H	860	2	-	3/6/26/27	0/4/4/4

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	841	RDG	O6-C6	7.56	1.43	1.24
2	G	841	RDG	O6-C6	7.55	1.43	1.24
2	C	860	RDG	O6-C6	7.54	1.43	1.24
2	H	860	RDG	O6-C6	7.54	1.43	1.24
2	B	841	RDG	C2-N2	7.38	1.45	1.34
2	C	860	RDG	C2-N2	7.34	1.45	1.34
2	H	860	RDG	C2-N2	7.32	1.45	1.34
2	G	841	RDG	C2-N2	7.21	1.45	1.34
2	G	841	RDG	O3'-C3'	-3.67	1.35	1.43
2	C	860	RDG	O3'-C3'	-3.66	1.35	1.43
2	H	860	RDG	O3'-C3'	-3.65	1.35	1.43
2	B	841	RDG	O3'-C3'	-3.64	1.35	1.43
2	G	841	RDG	C5'-C4'	-2.97	1.42	1.51
2	H	860	RDG	C5'-C4'	-2.93	1.42	1.51
2	B	841	RDG	C5'-C4'	-2.90	1.42	1.51
2	C	860	RDG	C5'-C4'	-2.85	1.42	1.51
2	B	841	RDG	C2'-C3'	-2.79	1.45	1.52
2	H	860	RDG	C2'-C3'	-2.78	1.45	1.52
2	G	841	RDG	C6-N1	2.76	1.37	1.33
2	G	841	RDG	C2'-C3'	-2.72	1.45	1.52
2	C	860	RDG	C6-N1	2.72	1.37	1.33
2	H	860	RDG	C6-N1	2.67	1.37	1.33
2	C	860	RDG	C2'-C3'	-2.65	1.45	1.52
2	B	841	RDG	C6-N1	2.57	1.37	1.33
2	C	860	RDG	C4-N3	2.53	1.39	1.35
2	B	841	RDG	C4-N3	2.47	1.39	1.35
2	H	860	RDG	C4-N3	2.45	1.39	1.35
2	G	841	RDG	C8-N7	2.45	1.39	1.34
2	B	841	RDG	C8-N7	2.33	1.38	1.34
2	H	860	RDG	C8-N7	2.32	1.38	1.34
2	B	841	RDG	C9-C10	2.31	1.42	1.39
2	C	860	RDG	C8-N7	2.29	1.38	1.34
2	C	860	RDG	C9-C10	2.27	1.42	1.39
2	H	860	RDG	C9-C10	2.26	1.42	1.39
2	G	841	RDG	C9-C10	2.21	1.42	1.39
2	C	860	RDG	C1'-N9	-2.20	1.42	1.49
2	G	841	RDG	C1'-N9	-2.18	1.42	1.49
2	C	860	RDG	C3'-C4'	-2.18	1.47	1.53
2	G	841	RDG	C4-N3	2.18	1.39	1.35
2	H	860	RDG	C1'-N9	-2.18	1.42	1.49
2	B	841	RDG	C1'-N9	-2.17	1.43	1.49
2	G	841	RDG	C3'-C4'	-2.12	1.47	1.53
2	H	860	RDG	C6-C5	2.11	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	841	RDG	C6-C5	2.07	1.44	1.41
2	H	860	RDG	C3'-C4'	-2.05	1.47	1.53
2	C	860	RDG	C6-C5	2.02	1.44	1.41
2	B	841	RDG	C3'-C4'	-2.01	1.47	1.53
2	B	841	RDG	C6-C5	2.00	1.44	1.41

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	841	RDG	C2-N3-C4	4.27	120.13	115.28
2	C	860	RDG	C2-N3-C4	4.22	120.07	115.28
2	H	860	RDG	C2-N3-C4	4.22	120.07	115.28
2	B	841	RDG	C2-N3-C4	4.01	119.83	115.28
2	G	841	RDG	C11-N2-C2	-3.64	118.18	123.28
2	B	841	RDG	C5-C6-N1	-3.20	119.06	123.43
2	B	841	RDG	C6-N1-C2	3.18	120.88	115.18
2	H	860	RDG	C5-C6-N1	-3.10	119.19	123.43
2	G	841	RDG	C5-C6-N1	-3.10	119.19	123.43
2	C	860	RDG	C5-C6-N1	-3.09	119.21	123.43
2	C	860	RDG	O5'-C5'-C4'	3.05	119.37	108.99
2	C	860	RDG	C6-N1-C2	3.03	120.61	115.18
2	H	860	RDG	C6-N1-C2	2.97	120.49	115.18
2	G	841	RDG	C6-N1-C2	2.90	120.37	115.18
2	B	841	RDG	N3-C2-N1	-2.83	121.76	126.23
2	B	841	RDG	C6-C5-C4	-2.82	118.11	120.80
2	C	860	RDG	N3-C2-N1	-2.81	121.79	126.23
2	G	841	RDG	C6-C5-C4	-2.79	118.14	120.80
2	H	860	RDG	N3-C2-N1	-2.75	121.89	126.23
2	G	841	RDG	N3-C2-N1	-2.73	121.92	126.23
2	C	860	RDG	C6-C5-C4	-2.68	118.24	120.80
2	G	841	RDG	C4-C5-N7	-2.61	106.67	109.40
2	H	860	RDG	C6-C5-C4	-2.60	118.32	120.80
2	H	860	RDG	O5'-C5'-C4'	2.45	117.33	108.99
2	G	841	RDG	C11-C10-C9	-2.45	124.95	129.01
2	H	860	RDG	C11-N2-C2	-2.45	119.86	123.28
2	C	860	RDG	C11-C10-C9	-2.42	125.00	129.01
2	H	860	RDG	C11-C10-C9	-2.37	125.08	129.01
2	C	860	RDG	C11-N2-C2	-2.36	119.98	123.28
2	H	860	RDG	C4-C5-N7	-2.36	106.94	109.40
2	B	841	RDG	C10-C11-N2	2.35	117.80	112.71
2	C	860	RDG	C10-C11-N2	2.35	117.80	112.71
2	B	841	RDG	O5'-C5'-C4'	2.35	116.99	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	841	RDG	C10-C11-N2	2.35	117.79	112.71
2	B	841	RDG	C11-C10-C9	-2.32	125.17	129.01
2	C	860	RDG	C4-C5-N7	-2.27	107.04	109.40
2	B	841	RDG	C4-C5-N7	-2.26	107.04	109.40
2	G	841	RDG	O5'-C5'-C4'	2.24	116.62	108.99
2	H	860	RDG	C10-C11-N2	2.23	117.54	112.71
2	G	841	RDG	N2-C2-N1	2.11	120.84	117.19

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	841	RDG	C3'-C4'-C5'-O5'
2	H	860	RDG	O4'-C4'-C5'-O5'
2	H	860	RDG	C3'-C4'-C5'-O5'
2	G	841	RDG	O4'-C4'-C5'-O5'
2	B	841	RDG	O4'-C4'-C5'-O5'
2	G	841	RDG	C3'-C4'-C5'-O5'
2	H	860	RDG	C4'-C5'-O5'-P
2	G	841	RDG	C10-C11-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	841	RDG	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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	1FZ	A	401	4	26,30,30	1.45	3 (11%)	32,47,47	1.67	5 (15%)
3	1FZ	F	401	4	26,30,30	1.44	3 (11%)	32,47,47	1.73	3 (9%)

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	1FZ	A	401	4	-	3/16/34/34	0/2/2/2
3	1FZ	F	401	4	-	5/16/34/34	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	401	1FZ	C4-C5	3.39	1.48	1.41
3	F	401	1FZ	PA-O1A	3.37	1.51	1.46
3	A	401	1FZ	PA-O1A	3.37	1.51	1.46
3	A	401	1FZ	C4-C5	3.35	1.48	1.41
3	A	401	1FZ	PB-O2B	3.32	1.51	1.46
3	F	401	1FZ	PB-O2B	3.31	1.51	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	401	1FZ	C4-N3-C2	6.69	120.79	115.14
3	A	401	1FZ	C4-N3-C2	6.57	120.69	115.14
3	F	401	1FZ	PG-O3B-PB	-3.79	119.27	132.62
3	A	401	1FZ	PG-O3B-PB	-3.22	121.26	132.62
3	A	401	1FZ	C5-C6-N1	-2.62	119.37	122.19
3	A	401	1FZ	C2'-C1'-N1	-2.56	108.36	114.27
3	F	401	1FZ	C5-C6-N1	-2.51	119.49	122.19
3	A	401	1FZ	O3B-PB-N3A	-2.11	100.74	106.59

There are no chirality outliers.

All (8) torsion outliers are listed below:

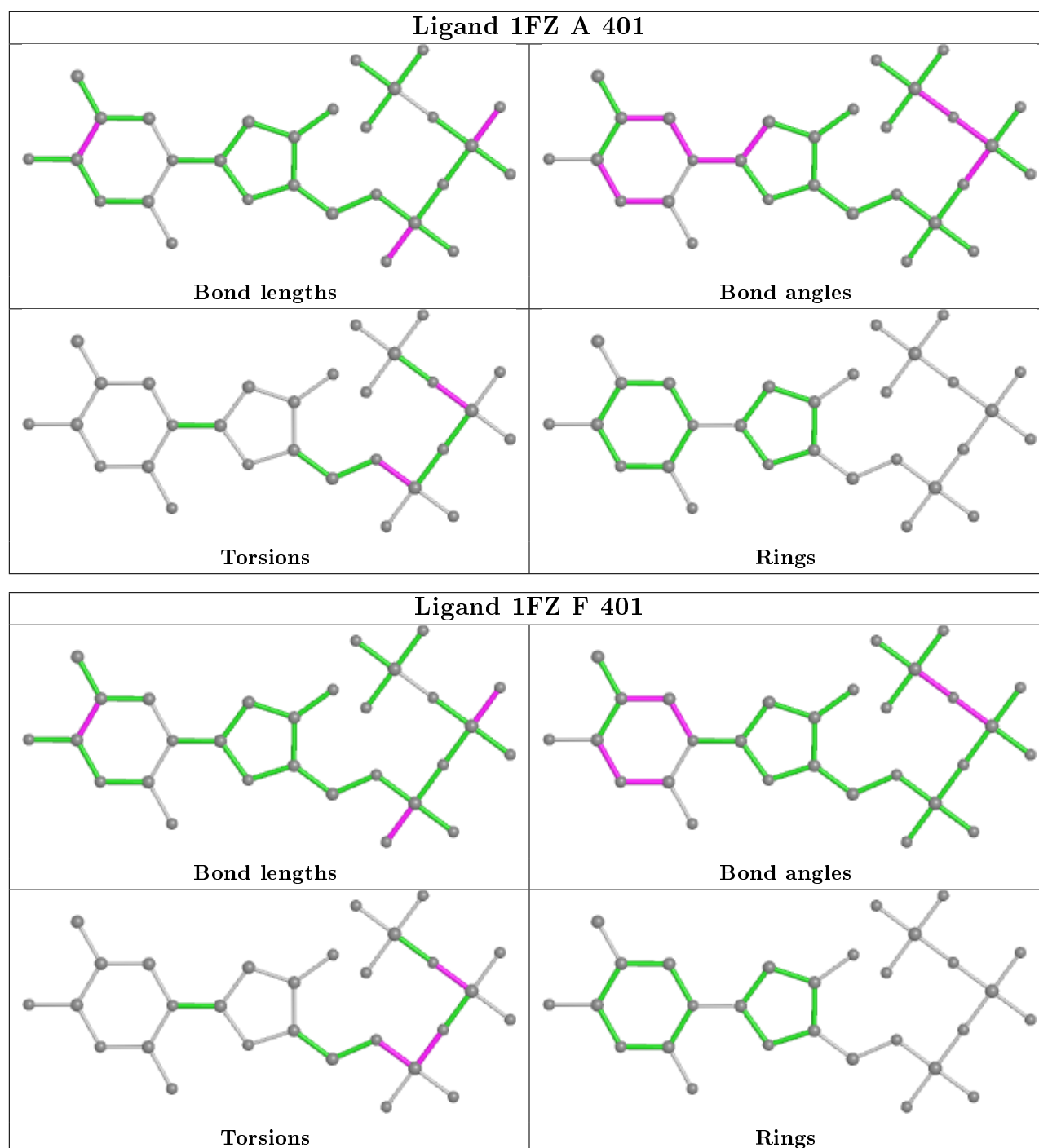
Mol	Chain	Res	Type	Atoms
3	A	401	1FZ	C5'-O5'-PA-O2A
3	A	401	1FZ	PG-O3B-PB-O1B
3	A	401	1FZ	PG-O3B-PB-O2B
3	F	401	1FZ	C5'-O5'-PA-O2A
3	F	401	1FZ	PB-N3A-PA-O1A
3	F	401	1FZ	PG-O3B-PB-O1B
3	F	401	1FZ	PG-O3B-PB-O2B
3	F	401	1FZ	C5'-O5'-PA-O1A

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	1FZ	3	0
3	F	401	1FZ	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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(Å ²)	Q<0.9
1	A	342/342 (100%)	0.15	4 (1%) 79 80	49, 64, 81, 101	0
1	F	342/342 (100%)	-0.04	0 100 100	44, 57, 72, 83	0
2	B	17/18 (94%)	-0.20	0 100 100	51, 66, 87, 90	0
2	C	16/18 (88%)	-0.11	1 (6%) 20 19	51, 67, 91, 116	0
2	G	17/18 (94%)	-0.10	1 (5%) 22 21	47, 62, 85, 93	0
2	H	13/18 (72%)	-0.43	0 100 100	49, 59, 73, 78	0
All	All	747/756 (98%)	0.04	6 (0%) 86 87	44, 60, 79, 116	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	0	GLY	5.9
2	C	857	DC	4.5
1	A	252	ASP	3.6
2	G	837	DT	3.2
1	A	1	SER	2.9
1	A	76	PHE	2.6

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. 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
2	RDG	H	860	28/29	0.86	0.16	64,77,95,95	0
2	RDG	G	841	28/29	0.94	0.20	43,50,87,95	0
2	RDG	C	860	28/29	0.94	0.18	63,68,73,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	RDG	B	841	28/29	0.95	0.18	46,52,59,61	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

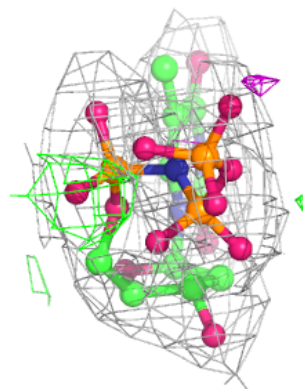
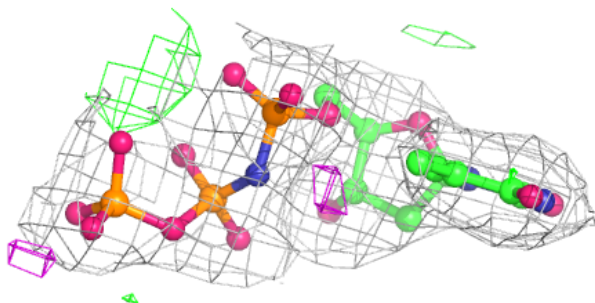
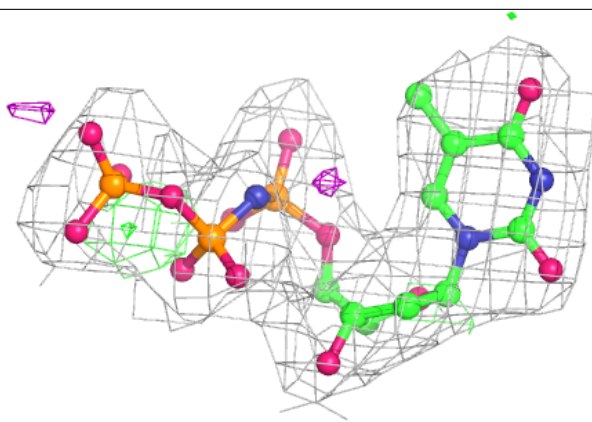
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MG	F	402	1/1	0.64	0.19	39,39,39,39	0
4	MG	F	403	1/1	0.81	0.19	63,63,63,63	0
4	MG	A	403	1/1	0.93	0.09	60,60,60,60	0
4	MG	A	402	1/1	0.95	0.17	46,46,46,46	0
3	1FZ	F	401	29/29	0.96	0.14	39,51,61,63	0
3	1FZ	A	401	29/29	0.97	0.15	47,54,63,67	0

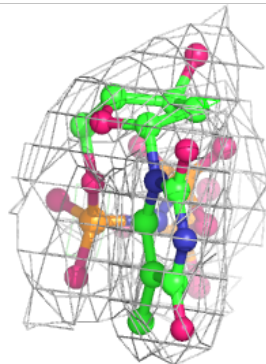
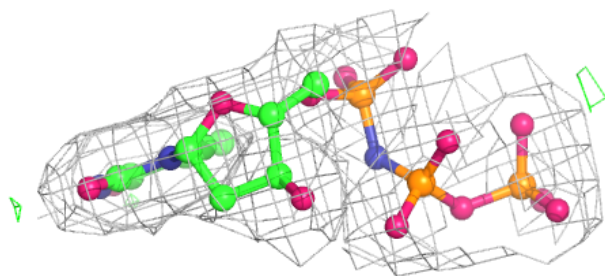
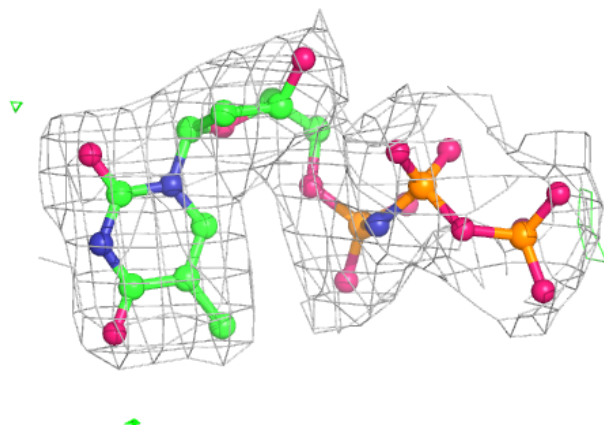
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 1FZ F 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around 1FZ A 401:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers

There are no such residues in this entry.