



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:59 PM UTC

PDB ID : 4Q45 / pdb_00004q45
Title : DNA Polymerase- damaged DNA complex
Authors : Kottur, J.; Sharma, A.; Nair, D.T.
Deposited on : 2014-04-13
Resolution : 2.18 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

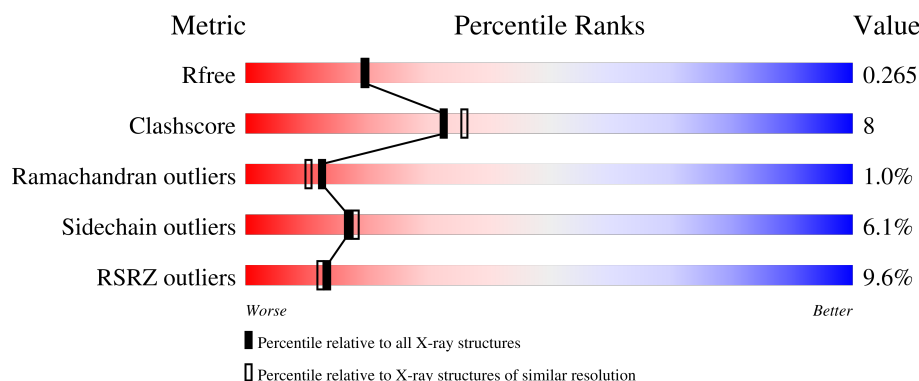
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 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}	180053	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	13% 75% 23% .
1	F	342	8% 80% 18% .
2	B	18	94% 6%
2	G	18	6% 72% 22% 6%
3	C	18	6% 78% 17% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	H	18	 A horizontal bar chart showing the quality of chain H. The bar is divided into three segments: a green segment representing 61%, a yellow segment representing 17%, and a grey segment representing 22%. The percentages are labeled below each segment.

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7230 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
1	F	342	Total	C	N	O	S	0	0	0
			2688	1695	494	485	14			
1	A	342	Total	C	N	O	S	0	0	0
			2688	1695	494	485	14			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	18	Total	C	N	O	P	0	0	0
			370	179	66	108	17			
2	B	18	Total	C	N	O	P	0	0	0
			370	179	66	108	17			

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

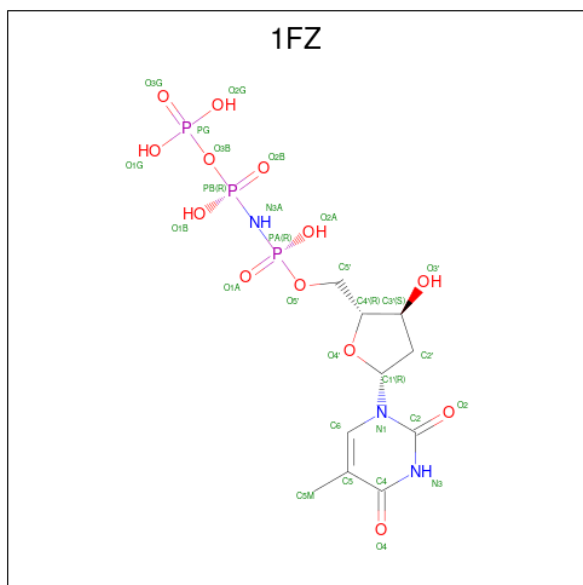
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	14	Total	C	N	O	P	0	0	0
			284	135	54	82	13			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	17	Total	C	N	O	P	0	0	0
			344	164	64	100	16			

- Molecule 4 is 5'-O-[(R)-hydroxy{[(R)-hydroxy(phosphonooxy)phosphoryl]amino}phosphoryl]thymidine (CCD ID: 1FZ) (formula: C₁₀H₁₈N₃O₁₃P₃).



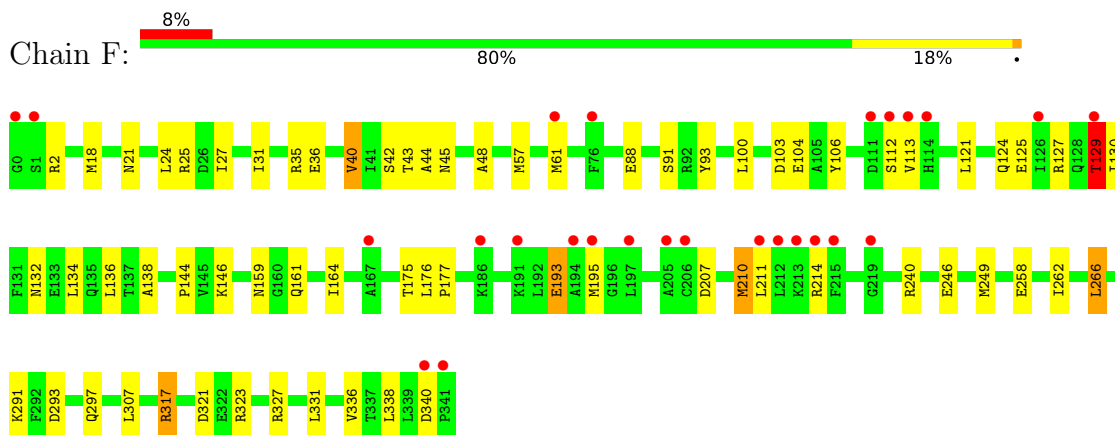
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	112	Total 112	O 112	0	0
6	G	38	Total 38	O 38	0	0
6	H	30	Total 30	O 30	0	0
6	B	28	Total 28	O 28	0	0
6	C	34	Total 34	O 34	0	0

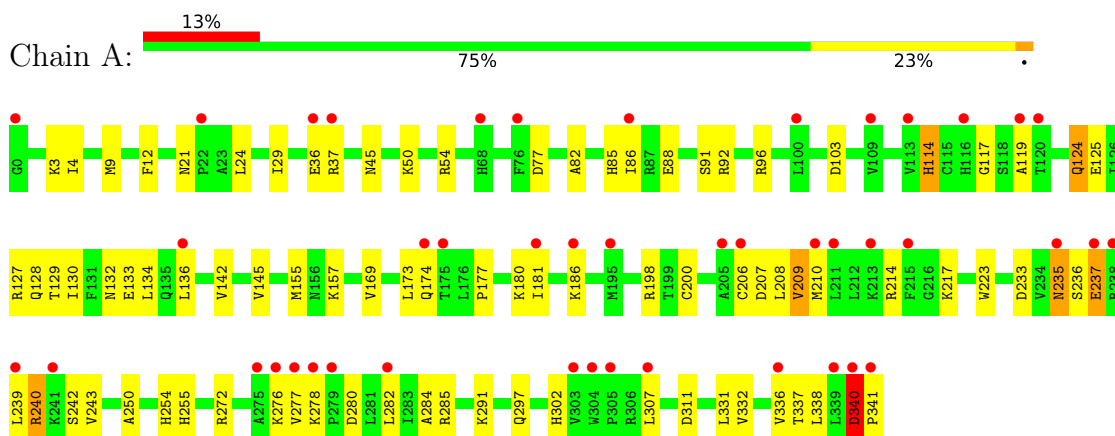
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

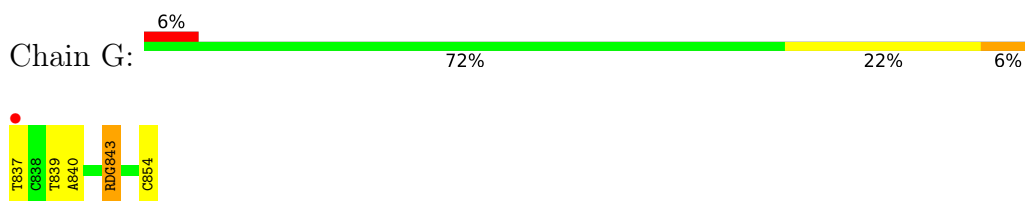
• Molecule 1: DNA polymerase IV



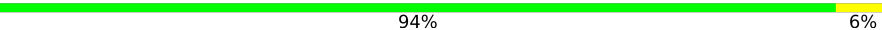
• Molecule 1: DNA polymerase IV

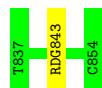


• Molecule 2: DNA (5'-D(*TP*CP*TP*AP*GP*GP*(RDG)P*TP*CP*CP*TP*AP*GP*GP*A P*CP*CP*C)-3')



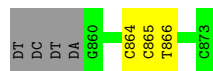
- Molecule 2: DNA (5'-D(*TP*CP*TP*AP*GP*GP*(RDG)P*TP*CP*CP*TP*AP*GP*GP*AP*CP*CP*C)-3')

Chain B:  94% 6%



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

Chain H:  61% 17% 22%



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

Chain C:  6% 78% 17% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.50Å 57.90Å 111.04Å 90.00° 90.44° 90.00°	Depositor
Resolution (Å)	51.34 – 2.18 51.34 – 2.18	Depositor EDS
% Data completeness (in resolution range)	90.0 (51.34-2.18) 98.3 (51.34-2.18)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.40 (at 2.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.212 , 0.257 0.221 , 0.265	Depositor DCC
R_{free} test set	2865 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	31.8	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 34.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7230	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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: 1FZ, RDG, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.38	0/2739	0.82	6/3699 (0.2%)
1	F	0.38	0/2739	0.78	3/3699 (0.1%)
2	B	0.21	0/381	0.89	0/583
2	G	0.17	0/381	0.72	0/583
3	C	0.19	0/385	0.75	0/592
3	H	0.17	0/318	0.70	0/489
All	All	0.35	0/6943	0.80	9/9645 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	ASN	CA-C-N	6.18	126.64	119.47
1	A	21	ASN	C-N-CA	6.18	126.64	119.47
1	A	128	GLN	N-CA-C	-6.16	101.17	110.28
1	A	155	MET	N-CA-C	5.93	117.41	111.07
1	F	340	ASP	N-CA-C	5.47	120.37	113.25
1	A	278	LYS	CA-C-N	5.37	125.03	119.56
1	A	278	LYS	C-N-CA	5.37	125.03	119.56
1	F	21	ASN	CA-C-N	5.06	124.72	119.56
1	F	21	ASN	C-N-CA	5.06	124.72	119.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2688	0	2745	48	0
1	F	2688	0	2745	45	0
2	B	370	0	208	0	0
2	G	370	0	208	6	0
3	C	344	0	192	4	0
3	H	284	0	158	3	0
4	A	29	0	14	1	0
4	F	29	0	14	1	0
5	A	2	0	0	0	0
5	F	2	0	0	0	0
6	A	112	0	0	10	0
6	B	28	0	0	0	0
6	C	34	0	0	2	0
6	F	182	0	0	14	0
6	G	38	0	0	1	0
6	H	30	0	0	2	0
All	All	7230	0	6284	101	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 8.

All (101) 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)
3:H:866:DT:O2	6:H:927:HOH:O	1.81	0.97
1:F:317:ARG:NH2	6:F:634:HOH:O	2.08	0.83
1:F:18:MET:HE3	1:F:45:ASN:HD22	1.46	0.81
3:C:861:DG:OP1	6:C:931:HOH:O	2.01	0.78
1:A:250:ALA:O	6:A:590:HOH:O	2.02	0.77
1:F:246:GLU:OE2	6:F:504:HOH:O	2.04	0.73
3:C:859:DA:N3	6:C:918:HOH:O	2.22	0.73
3:H:866:DT:O4	6:H:923:HOH:O	2.07	0.71
1:A:132:ASN:O	1:A:134:LEU:N	2.25	0.69
1:F:113:VAL:O	6:F:641:HOH:O	2.11	0.69
1:A:37:ARG:NH1	6:A:570:HOH:O	2.05	0.69
1:A:96:ARG:NH2	1:A:233:ASP:OD1	2.25	0.69
1:A:217:LYS:NZ	6:A:605:HOH:O	2.27	0.68
1:F:195:MET:SD	1:F:214:ARG:NH1	2.67	0.67
1:F:127:ARG:NH1	1:F:159:ASN:OD1	2.28	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:293:ASP:O	6:F:594:HOH:O	2.14	0.65
1:A:235:ASN:ND2	1:A:237:GLU:OE2	2.31	0.64
1:F:297:GLN:OE1	6:F:631:HOH:O	2.15	0.63
1:A:54:ARG:NH1	6:A:588:HOH:O	2.34	0.61
1:A:85:HIS:ND1	1:A:134:LEU:HD21	2.17	0.59
1:A:174:GLN:NE2	6:A:584:HOH:O	2.14	0.59
1:F:262:ILE:HG22	1:F:266:LEU:HD22	1.87	0.57
1:F:129:THR:N	6:F:502:HOH:O	2.37	0.56
1:F:129:THR:HA	1:F:132:ASN:HB2	1.87	0.56
1:A:177:PRO:HB2	1:A:180:LYS:HG2	1.88	0.55
1:A:24:LEU:HB3	1:A:29:ILE:HG21	1.89	0.54
1:A:130:ILE:O	1:A:134:LEU:HB2	2.07	0.54
1:F:207:ASP:HB3	1:F:210:MET:HG2	1.90	0.54
1:F:240:ARG:NH1	2:G:843:RDG:OP1	2.40	0.54
1:A:291:LYS:HB3	1:A:331:LEU:HB3	1.89	0.54
1:F:127:ARG:HD2	1:F:138:ALA:O	2.07	0.54
1:F:127:ARG:NE	6:F:659:HOH:O	2.19	0.54
1:A:88:GLU:O	1:A:91:SER:OG	2.21	0.54
1:F:61:MET:HG3	2:G:837:DT:C6	2.43	0.53
1:A:291:LYS:HG3	1:A:297:GLN:HB3	1.91	0.52
1:A:285:ARG:HB2	1:A:337:THR:HB	1.91	0.52
1:F:61:MET:HE2	2:G:837:DT:N3	2.25	0.52
3:C:859:DA:H2''	3:C:860:DG:N7	2.25	0.52
1:F:323:ARG:NE	6:F:681:HOH:O	2.43	0.51
1:F:2:ARG:HD3	6:F:551:HOH:O	2.11	0.50
1:F:44:ALA:HB1	1:F:48:ALA:HB3	1.93	0.50
1:F:35:ARG:NH2	1:F:36:GLU:OE2	2.45	0.49
1:A:125:GLU:OE1	6:A:600:HOH:O	2.20	0.49
1:A:4:ILE:HD12	1:A:145:VAL:HA	1.95	0.49
1:A:208:LEU:HD13	1:A:223:TRP:CD1	2.48	0.49
1:A:340:ASP:HB2	1:A:341:PRO:HD3	1.95	0.49
1:F:31:ILE:O	1:F:42:SER:N	2.45	0.49
1:A:169:VAL:O	1:A:173:LEU:HB2	2.12	0.49
3:C:859:DA:H2''	3:C:860:DG:C8	2.49	0.48
1:F:40:VAL:HG13	2:G:840:DA:H5'	1.95	0.48
1:A:280:ASP:OD2	1:A:282:LEU:HB2	2.14	0.48
1:A:254:HIS:HB3	6:A:563:HOH:O	2.14	0.48
1:A:340:ASP:N	1:A:340:ASP:OD1	2.47	0.47
1:F:100:LEU:HD11	1:F:106:TYR:CE1	2.50	0.47
1:A:77:ASP:N	1:A:77:ASP:OD1	2.47	0.46
1:F:297:GLN:NE2	6:F:540:HOH:O	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:57:MET:HG3	1:F:61:MET:HE3	1.97	0.46
1:A:124:GLN:HG3	6:A:602:HOH:O	2.15	0.46
1:F:161:GLN:OE1	6:F:659:HOH:O	2.21	0.46
1:A:124:GLN:OE1	1:A:127:ARG:NH2	2.48	0.46
1:F:193:GLU:OE2	6:F:613:HOH:O	2.21	0.46
1:A:88:GLU:OE1	1:A:92:ARG:NH2	2.44	0.46
1:A:157:LYS:HE2	4:A:401:1FZ:O3G	2.16	0.46
1:A:3:LYS:NZ	1:A:117:GLY:O	2.45	0.46
1:A:272:ARG:O	1:A:276:LYS:HG2	2.16	0.46
1:A:3:LYS:NZ	1:A:119:ALA:H	2.14	0.45
1:F:103:ASP:OD2	1:F:104:GLU:HG3	2.16	0.45
1:A:82:ALA:O	1:A:86:ILE:HG23	2.15	0.45
1:F:291:LYS:HB3	1:F:331:LEU:HB3	1.97	0.45
2:G:854:DC:OP2	6:G:926:HOH:O	2.21	0.44
1:A:207:ASP:OD1	1:A:209:VAL:HG13	2.17	0.44
1:A:302:HIS:NE2	1:A:311:ASP:OD2	2.47	0.44
1:F:18:MET:HE2	1:F:25:ARG:O	2.17	0.44
1:F:210:MET:HG3	1:F:211:LEU:N	2.33	0.44
1:A:255:HIS:HE1	2:G:839:DT:O4	1.99	0.44
1:F:43:THR:HB	4:F:401:1FZ:H7	2.00	0.43
1:A:9:MET:HB2	1:A:103:ASP:HB2	2.00	0.43
1:F:321:ASP:OD2	6:F:626:HOH:O	2.21	0.43
1:A:173:LEU:O	1:A:200:CYS:HB2	2.18	0.43
1:A:240:ARG:HH21	1:A:277:VAL:HG11	1.82	0.43
1:F:323:ARG:O	1:F:327:ARG:NH2	2.49	0.43
1:F:18:MET:HE2	1:F:25:ARG:HA	2.01	0.43
1:A:37:ARG:NH2	6:A:570:HOH:O	2.52	0.43
1:F:93:TYR:OH	1:F:125:GLU:HG2	2.20	0.42
1:F:130:ILE:O	1:F:134:LEU:HB2	2.20	0.42
1:F:258:GLU:O	1:F:262:ILE:HG12	2.19	0.42
1:A:240:ARG:HD2	1:A:242:SER:O	2.19	0.42
1:A:272:ARG:NH1	6:A:595:HOH:O	2.51	0.42
1:F:121:LEU:HD23	1:F:121:LEU:HA	1.88	0.41
1:A:29:ILE:HG12	1:A:45:ASN:ND2	2.34	0.41
3:H:864:DC:H2'	3:H:865:DC:C6	2.54	0.41
1:F:176:LEU:HD12	1:F:177:PRO:HD2	2.01	0.41
1:F:88:GLU:O	1:F:91:SER:OG	2.28	0.41
1:A:3:LYS:HD3	1:A:119:ALA:HB2	2.02	0.41
1:A:237:GLU:H	1:A:237:GLU:CD	2.29	0.41
1:F:24:LEU:HA	1:F:27:ILE:HD11	2.02	0.41
1:A:12:PHE:CD2	1:A:103:ASP:HB3	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:146:LYS:NZ	6:F:597:HOH:O	2.30	0.41
1:A:181:ILE:HD11	1:A:200:CYS:SG	2.60	0.41
1:A:284:ALA:O	1:A:285:ARG:HG3	2.20	0.40
1:F:144:PRO:HD3	1:F:164:ILE:O	2.21	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%)	322 (95%)	12 (4%)	6 (2%)	6	4
1	F	340/342 (99%)	330 (97%)	9 (3%)	1 (0%)	36	39
All	All	680/684 (99%)	652 (96%)	21 (3%)	7 (1%)	12	10

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	129	THR
1	A	129	THR
1	A	114	HIS
1	A	133	GLU
1	A	235	ASN
1	A	236	SER
1	A	340	ASP

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	286/286 (100%)	265 (93%)	21 (7%)	13	13
1	F	286/286 (100%)	272 (95%)	14 (5%)	22	26
All	All	572/572 (100%)	537 (94%)	35 (6%)	17	18

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	40	VAL
1	F	112	SER
1	F	124	GLN
1	F	129	THR
1	F	136	LEU
1	F	175	THR
1	F	193	GLU
1	F	210	MET
1	F	249	MET
1	F	266	LEU
1	F	307	LEU
1	F	317	ARG
1	F	336	VAL
1	F	338	LEU
1	A	36	GLU
1	A	50	LYS
1	A	114	HIS
1	A	124	GLN
1	A	136	LEU
1	A	142	VAL
1	A	186	LYS
1	A	198	ARG
1	A	206	CYS
1	A	209	VAL
1	A	210	MET
1	A	214	ARG
1	A	237	GLU
1	A	239	LEU
1	A	240	ARG
1	A	243	VAL
1	A	307	LEU
1	A	332	VAL
1	A	336	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	338	LEU
1	A	340	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	128	GLN
1	F	132	ASN
1	F	255	HIS
1	F	297	GLN
1	A	132	ASN
1	A	156	ASN
1	A	255	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	G	843	2	28,31,32	1.95	9 (32%)	38,44,47	2.21	14 (36%)
2	RDG	B	843	2	28,31,32	1.99	9 (32%)	38,44,47	2.13	15 (39%)

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	G	843	2	-	2/12/26/27	0/4/4/4
2	RDG	B	843	2	-	4/12/26/27	0/4/4/4

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	843	RDG	O6-C6	4.76	1.32	1.23
2	B	843	RDG	C2-N2	4.66	1.44	1.34
2	G	843	RDG	O6-C6	4.56	1.32	1.23
2	G	843	RDG	C2-N2	4.36	1.43	1.34
2	B	843	RDG	C2'-C3'	-3.99	1.42	1.52
2	G	843	RDG	C2'-C3'	-3.94	1.42	1.52
2	B	843	RDG	C9-C10	2.58	1.41	1.34
2	G	843	RDG	C9-C10	2.57	1.41	1.34
2	G	843	RDG	C3'-C4'	-2.51	1.46	1.53
2	B	843	RDG	C4-N3	2.45	1.39	1.34
2	G	843	RDG	O5'-C5'	-2.32	1.37	1.44
2	B	843	RDG	C7-C12	2.27	1.41	1.32
2	G	843	RDG	C7-C12	2.27	1.40	1.32
2	B	843	RDG	C3'-C4'	-2.26	1.47	1.53
2	G	843	RDG	C4-N3	2.13	1.39	1.34
2	B	843	RDG	O5'-C5'	-2.12	1.38	1.44
2	B	843	RDG	O7-C10	-2.11	1.30	1.36
2	G	843	RDG	O7-C10	-2.08	1.30	1.36

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	843	RDG	C2-N3-C4	6.28	119.86	112.00
2	B	843	RDG	C2-N3-C4	6.17	119.72	112.00
2	G	843	RDG	C11-N2-C2	-5.19	116.75	123.03
2	G	843	RDG	C5-C4-N3	-4.91	120.57	128.39
2	B	843	RDG	C5-C4-N3	-4.78	120.78	128.39
2	B	843	RDG	C11-N2-C2	-4.64	117.42	123.03
2	G	843	RDG	C2-N1-C6	-3.39	120.45	124.55
2	G	843	RDG	N2-C2-N3	-3.05	116.00	120.19
2	G	843	RDG	C6-C5-N7	2.93	135.63	130.29
2	B	843	RDG	C6-C5-N7	2.84	135.45	130.29
2	B	843	RDG	N9-C4-N3	2.83	131.60	125.95
2	B	843	RDG	C2-N1-C6	-2.83	121.13	124.55
2	G	843	RDG	C4-C5-N7	-2.68	106.42	110.67
2	G	843	RDG	N9-C4-N3	2.57	131.09	125.95
2	B	843	RDG	C12-O7-C10	2.57	111.34	106.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	843	RDG	N2-C2-N3	-2.54	116.70	120.19
2	B	843	RDG	C4-C5-N7	-2.47	106.75	110.67
2	B	843	RDG	N9-C8-N7	-2.39	108.96	113.40
2	B	843	RDG	C8-N7-C5	2.39	108.51	104.26
2	G	843	RDG	C12-O7-C10	2.37	110.94	106.22
2	G	843	RDG	C8-N7-C5	2.35	108.44	104.26
2	G	843	RDG	C11-C10-C9	-2.33	125.10	133.07
2	G	843	RDG	N9-C8-N7	-2.32	109.09	113.40
2	G	843	RDG	C5-C6-N1	2.27	119.04	113.25
2	B	843	RDG	C10-C11-N2	2.26	117.68	112.69
2	B	843	RDG	C11-C10-C9	-2.19	125.60	133.07
2	B	843	RDG	C5-C6-N1	2.17	118.78	113.25
2	G	843	RDG	O7-C10-C11	2.16	124.90	117.50
2	B	843	RDG	O7-C10-C11	2.05	124.53	117.50

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	843	RDG	C9-C10-C11-N2
2	B	843	RDG	O7-C10-C11-N2
2	B	843	RDG	C3'-C4'-C5'-O5'
2	B	843	RDG	O4'-C4'-C5'-O5'
2	G	843	RDG	C9-C10-C11-N2
2	G	843	RDG	O7-C10-C11-N2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	843	RDG	1	0

5.5 Carbohydrates [\(i\)](#)

There are no oligosaccharides 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	$\# Z > 2$
4	1FZ	A	401	5	29,30,30	2.76	11 (37%)	41,47,47	2.11	10 (24%)
4	1FZ	F	401	5	29,30,30	2.63	12 (41%)	41,47,47	2.21	13 (31%)

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
4	1FZ	A	401	5	-	5/19/34/34	0/2/2/2
4	1FZ	F	401	5	-	5/19/34/34	0/2/2/2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	401	1FZ	O4-C4	9.10	1.40	1.23
4	F	401	1FZ	O4-C4	8.96	1.40	1.23
4	A	401	1FZ	PA-O1A	6.90	1.56	1.46
4	F	401	1FZ	PB-O2B	5.86	1.55	1.46
4	A	401	1FZ	C6-C5	3.56	1.40	1.34
4	F	401	1FZ	C3'-C4'	-3.45	1.43	1.53
4	F	401	1FZ	C6-C5	3.38	1.40	1.34
4	A	401	1FZ	C3'-C4'	-3.35	1.44	1.53
4	F	401	1FZ	C4-C5	-3.08	1.39	1.44
4	A	401	1FZ	PA-O2A	-2.97	1.48	1.56
4	A	401	1FZ	C4-C5	-2.92	1.40	1.44
4	F	401	1FZ	C2-N1	-2.83	1.34	1.38
4	A	401	1FZ	PB-O2B	2.78	1.50	1.46
4	A	401	1FZ	C2-N1	-2.75	1.34	1.38
4	A	401	1FZ	C2'-C3'	-2.61	1.46	1.52
4	A	401	1FZ	PA-N3A	2.56	1.70	1.63
4	F	401	1FZ	PB-O1B	-2.55	1.50	1.56
4	F	401	1FZ	C2'-C3'	-2.54	1.46	1.52
4	F	401	1FZ	PA-N3A	2.44	1.69	1.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	401	1FZ	C4-N3	-2.13	1.34	1.38
4	A	401	1FZ	C4-N3	-2.08	1.35	1.38
4	F	401	1FZ	PA-O1A	2.07	1.49	1.46
4	F	401	1FZ	C2-N3	-2.03	1.34	1.38

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	401	1FZ	C5-C4-N3	5.77	120.34	115.32
4	A	401	1FZ	N3-C2-N1	5.72	122.34	114.89
4	A	401	1FZ	C4-N3-C2	-5.63	119.96	127.34
4	A	401	1FZ	C5-C4-N3	5.48	120.09	115.32
4	F	401	1FZ	C4-N3-C2	-5.43	120.22	127.34
4	F	401	1FZ	N3-C2-N1	5.27	121.75	114.89
4	F	401	1FZ	O4-C4-C5	-4.44	119.84	124.92
4	A	401	1FZ	O4-C4-C5	-4.39	119.90	124.92
4	A	401	1FZ	O4'-C1'-N1	3.65	114.33	107.86
4	F	401	1FZ	C5-C6-N1	-3.24	119.80	123.31
4	F	401	1FZ	O4'-C1'-N1	3.20	113.54	107.86
4	F	401	1FZ	O5'-PA-O1A	-3.17	104.86	114.27
4	A	401	1FZ	C5-C6-N1	-3.16	119.88	123.31
4	F	401	1FZ	O5'-C5'-C4'	2.49	117.47	108.99
4	F	401	1FZ	C5M-C5-C4	2.31	121.25	118.78
4	F	401	1FZ	O2B-PB-N3A	-2.26	108.44	111.77
4	F	401	1FZ	O1A-PA-N3A	-2.26	108.45	111.77
4	F	401	1FZ	C1'-N1-C2	2.20	121.95	117.66
4	A	401	1FZ	C1'-N1-C2	2.15	121.86	117.66
4	A	401	1FZ	O5'-C5'-C4'	2.15	116.30	108.99
4	A	401	1FZ	O2-C2-N1	-2.13	120.02	122.80
4	A	401	1FZ	O2-C2-N3	-2.08	117.64	121.49
4	F	401	1FZ	O2-C2-N3	-2.04	117.73	121.49

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	401	1FZ	PB-N3A-PA-O5'
4	F	401	1FZ	PA-N3A-PB-O2B
4	F	401	1FZ	PB-O3B-PG-O1G
4	A	401	1FZ	PB-N3A-PA-O5'
4	A	401	1FZ	PB-O3B-PG-O1G
4	A	401	1FZ	PB-O3B-PG-O3G

Continued on next page...

Continued from previous page...

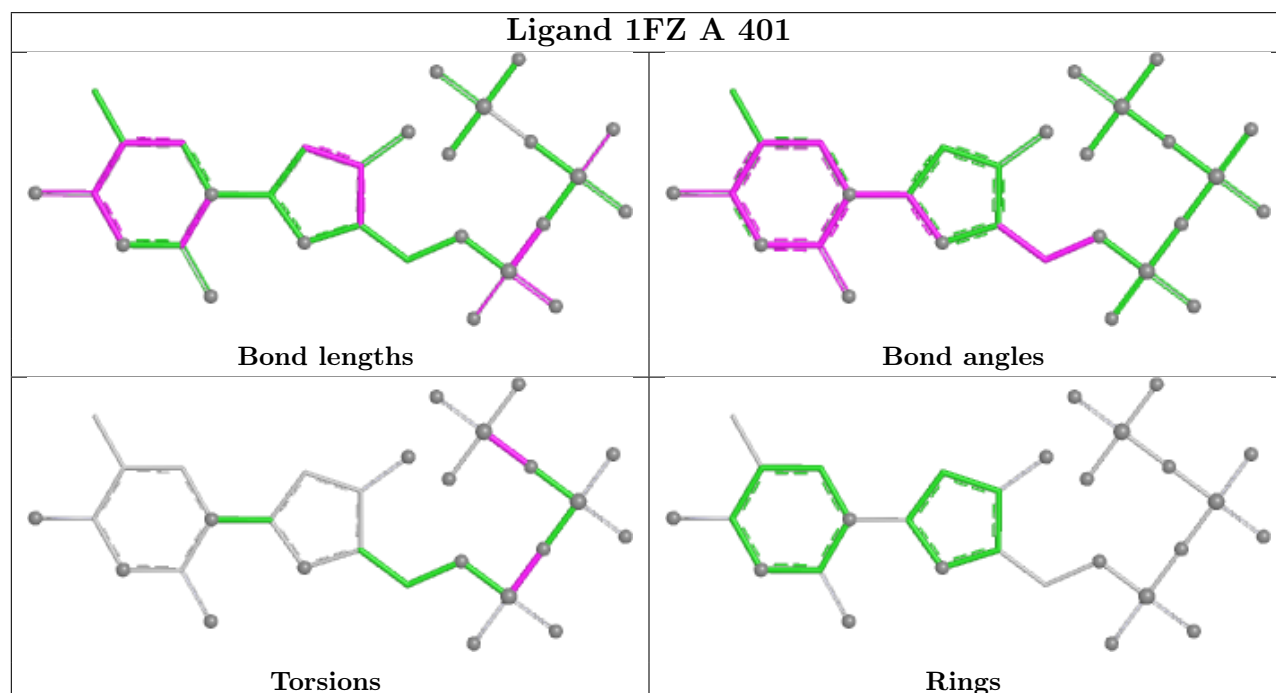
Mol	Chain	Res	Type	Atoms
4	F	401	1FZ	PB-O3B-PG-O3G
4	A	401	1FZ	PB-N3A-PA-O1A
4	F	401	1FZ	PB-O3B-PG-O2G
4	A	401	1FZ	PB-O3B-PG-O2G

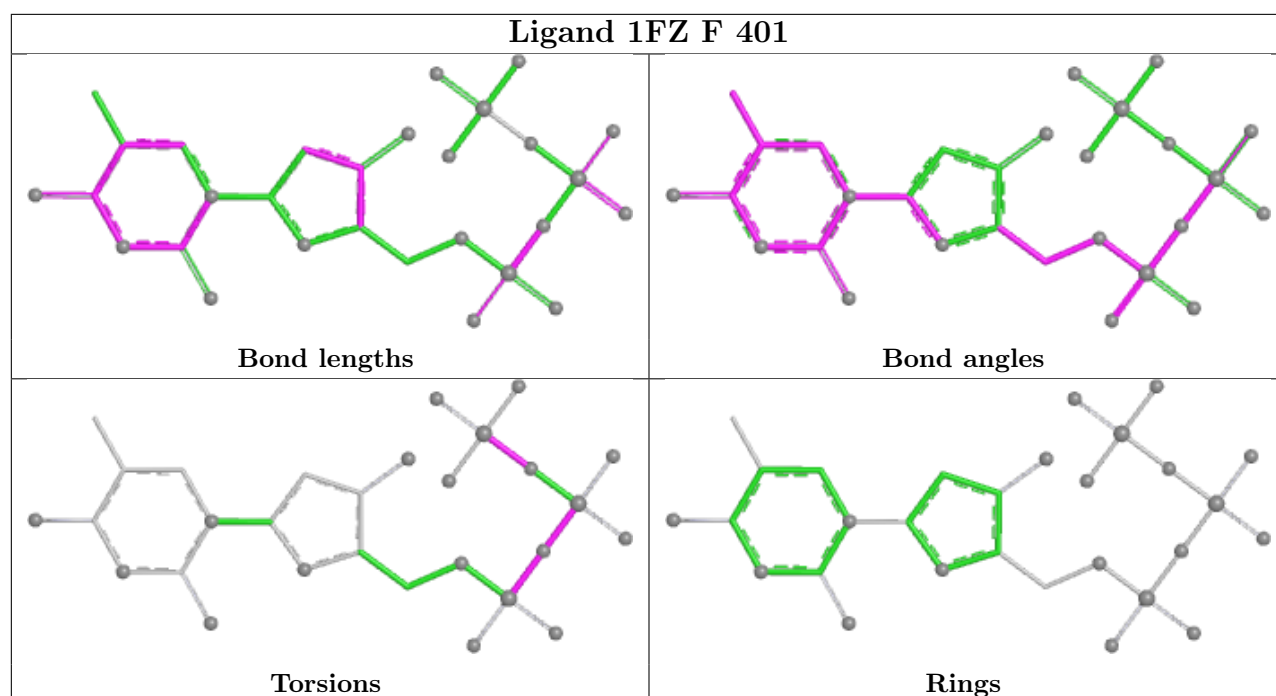
There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

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, 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%)	1.04	44 (12%) 7 6	19, 44, 62, 95	0
1	F	342/342 (100%)	0.58	26 (7%) 20 19	18, 33, 50, 70	0
2	B	17/18 (94%)	0.15	0 100 100	25, 43, 52, 58	0
2	G	17/18 (94%)	-0.12	1 (5%) 28 27	24, 33, 59, 68	0
3	C	17/18 (94%)	-0.04	1 (5%) 28 27	31, 36, 54, 54	0
3	H	14/18 (77%)	-0.27	0 100 100	24, 32, 43, 45	0
All	All	749/756 (99%)	0.74	72 (9%) 13 12	18, 38, 59, 95	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	0	GLY	7.3
1	A	341	PRO	6.0
1	A	0	GLY	4.7
1	A	76	PHE	4.4
1	F	129	THR	4.1
1	A	113	VAL	4.1
2	G	837	DT	3.8
1	A	339	LEU	3.8
1	F	194	ALA	3.6
1	F	341	PRO	3.4
1	F	206	CYS	3.3
1	A	37	ARG	3.3
1	A	279	PRO	3.3
1	A	116	HIS	3.2
1	A	210	MET	3.1
1	F	212	LEU	3.0
1	A	235	ASN	3.0
1	A	340	ASP	2.9
1	A	36	GLU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	205	ALA	2.9
1	A	282	LEU	2.9
1	A	303	VAL	2.9
1	A	275	ALA	2.9
1	F	112	SER	2.8
1	F	197	LEU	2.8
1	F	76	PHE	2.8
1	F	113	VAL	2.8
1	A	213	LYS	2.8
1	A	276	LYS	2.8
1	A	237	GLU	2.7
1	F	211	LEU	2.7
1	A	175	THR	2.7
1	F	186	LYS	2.7
1	F	61	MET	2.6
1	F	213	LYS	2.6
1	A	305	PRO	2.6
1	F	1	SER	2.6
1	A	215	PHE	2.5
1	A	239	LEU	2.5
1	A	119	ALA	2.4
1	F	191	LYS	2.4
1	A	241	LYS	2.4
1	A	307	LEU	2.4
1	A	186	LYS	2.4
3	C	857	DC	2.4
1	A	86	ILE	2.4
1	F	214	ARG	2.4
1	A	68	HIS	2.3
1	F	205	ALA	2.3
1	A	238	ARG	2.3
1	A	174	GLN	2.2
1	A	109	VAL	2.2
1	A	336	VAL	2.2
1	A	304	TRP	2.2
1	F	219	GLY	2.2
1	A	100	LEU	2.1
1	A	211	LEU	2.1
1	F	340	ASP	2.1
1	A	206	CYS	2.1
1	A	195	MET	2.1
1	A	120	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	195	MET	2.1
1	F	111	ASP	2.1
1	F	114	HIS	2.1
1	F	126	ILE	2.1
1	A	181	ILE	2.1
1	A	278	LYS	2.1
1	F	215	PHE	2.1
1	A	277	VAL	2.1
1	A	22	PRO	2.0
1	F	167	ALA	2.0
1	A	136	LEU	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. 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	B	843	28/29	0.94	0.09	27,36,47,52	0
2	RDG	G	843	28/29	0.96	0.07	18,27,41,53	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MG	A	403	1/1	0.86	0.15	45,45,45,45	0
5	MG	F	403	1/1	0.90	0.23	47,47,47,47	0
4	1FZ	A	401	29/29	0.96	0.07	20,30,37,39	0
5	MG	A	402	1/1	0.97	0.04	21,21,21,21	0
4	1FZ	F	401	29/29	0.98	0.05	15,23,31,33	0

Continued on next page...

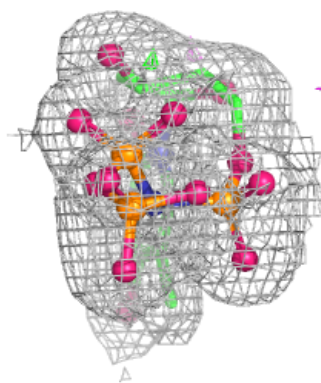
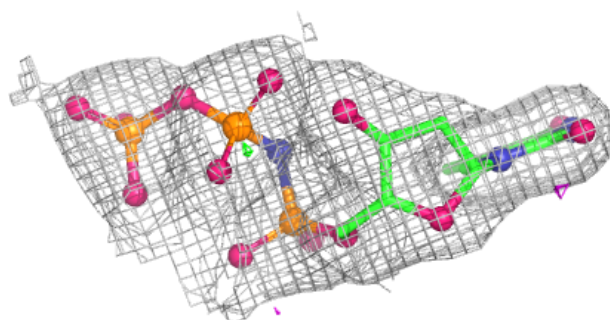
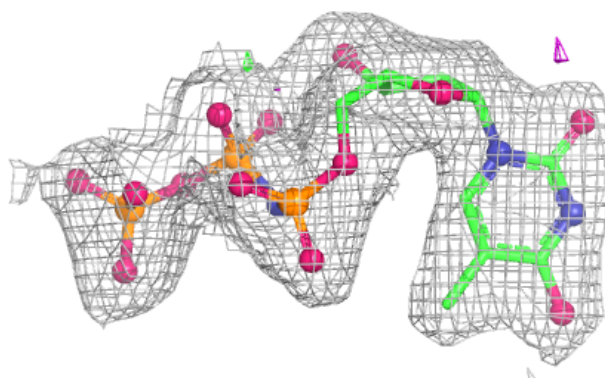
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MG	F	402	1/1	0.99	0.09	11,11,11,11	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.

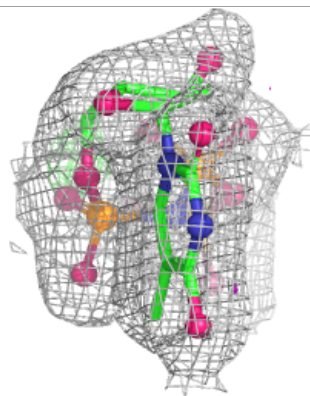
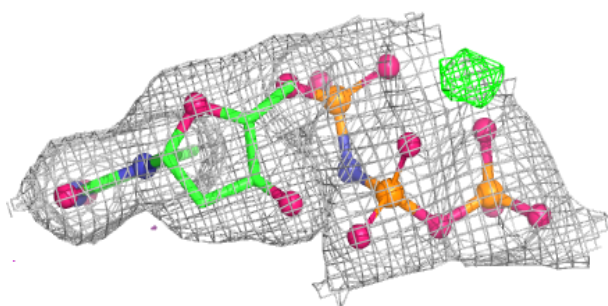
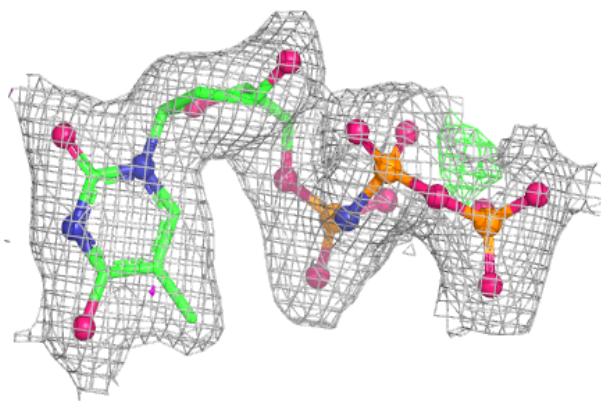
Electron density around 1FZ A 401:

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



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)



6.5 Other polymers [i](#)

There are no such residues in this entry.