



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:54 PM UTC

PDB ID : 6UJY / pdb_00006ujy
Title : HIV-1 wild-type reverse transcriptase-DNA complex with (-)-3TC-TP
Authors : Lansdon, E.B.
Deposited on : 2019-10-03
Resolution : 2.59 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

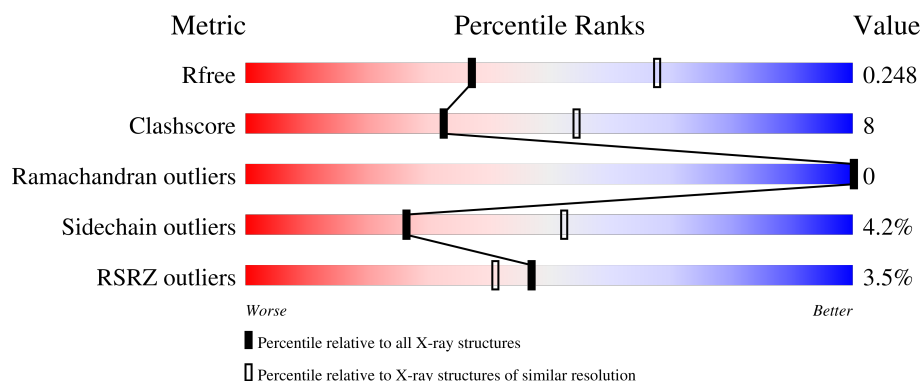
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	572	 3% 75% 20% . .
2	B	440	 4% 68% 18% . 11%
3	P	21	 67% 19% 14%
4	T	27	 4% 59% 22% 19%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8783 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 p66 Reverse transcriptase/RNaseH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	549	Total	C	N	O	S	0	0	0
			4471	2893	745	825	8			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP P04585
A	-10	GLY	-	expression tag	UNP P04585
A	-9	SER	-	expression tag	UNP P04585
A	-8	SER	-	expression tag	UNP P04585
A	-7	HIS	-	expression tag	UNP P04585
A	-6	HIS	-	expression tag	UNP P04585
A	-5	HIS	-	expression tag	UNP P04585
A	-4	HIS	-	expression tag	UNP P04585
A	-3	HIS	-	expression tag	UNP P04585
A	-2	HIS	-	expression tag	UNP P04585
A	-1	SER	-	expression tag	UNP P04585
A	0	SER	-	expression tag	UNP P04585
A	258	CYS	GLN	engineered mutation	UNP P04585
A	280	SER	CYS	engineered mutation	UNP P04585

- Molecule 2 is a protein called p51 Reverse transcriptase/RNaseH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	391	Total	C	N	O	S	0	0	0
			3238	2104	537	591	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P04585

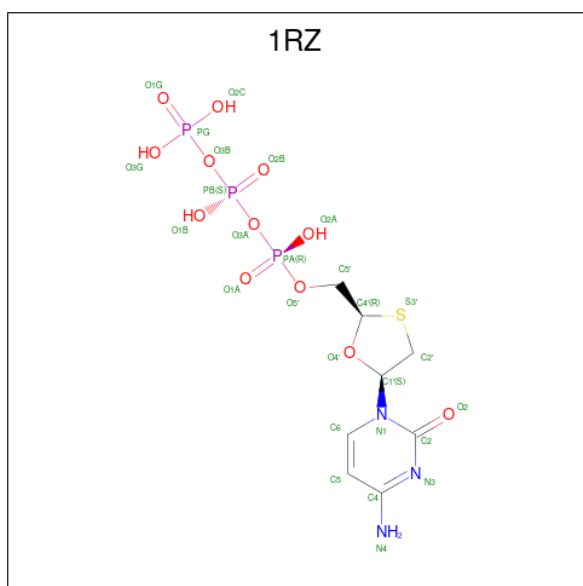
- Molecule 3 is a DNA chain called primer DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	18	Total	C	N	O	P	0	0	0
			360	172	62	109	17			

- Molecule 4 is a DNA chain called template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	T	22	Total	C	N	O	P	0	0	0
			460	214	95	129	22			

- Molecule 5 is Lamivudine Triphosphate (CCD ID: 1RZ) (formula: $C_8H_{14}N_3O_{12}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	1
			54	16	6	24	6	2	

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg	0	0
			1	1		

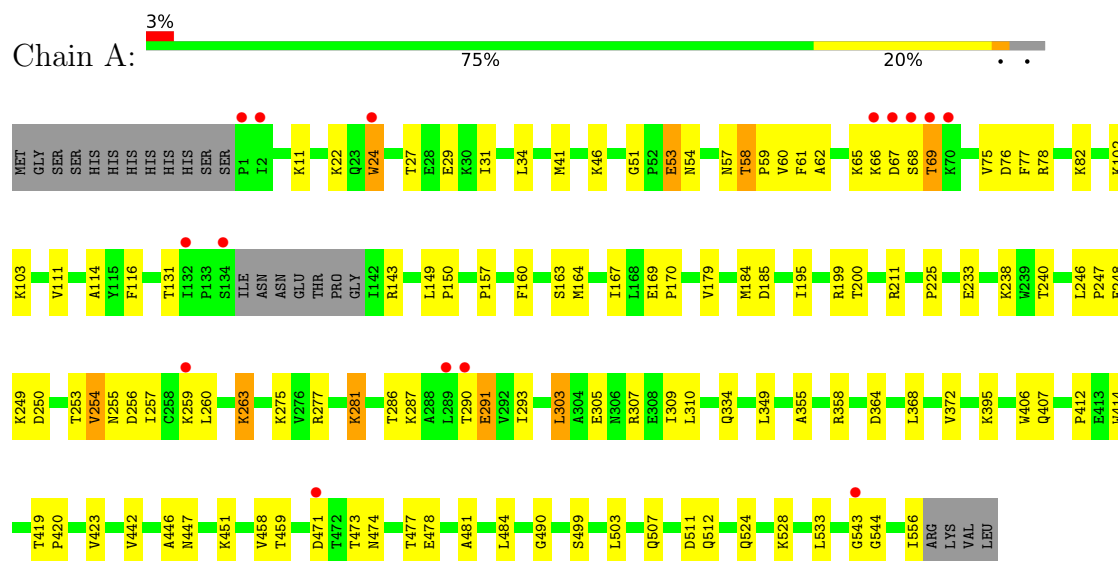
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	109	Total	O	0	0
			109	109		
8	B	54	Total	O	0	0
			54	54		
8	P	14	Total	O	0	0
			14	14		
8	T	12	Total	O	0	0
			12	12		

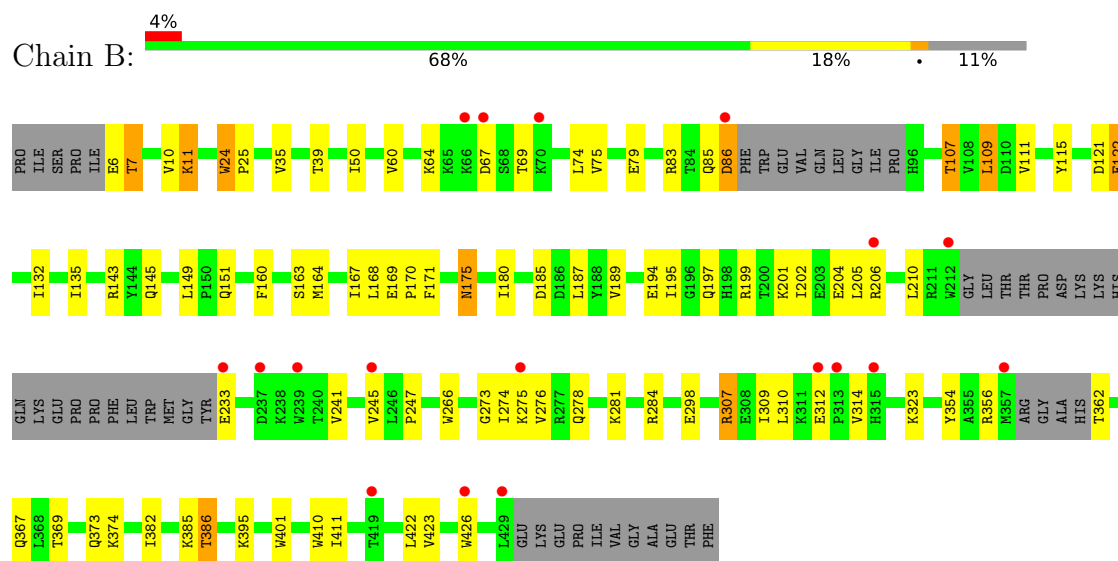
3 Residue-property plots [i](#)

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: p66 Reverse transcriptase/RNaseH



- Molecule 2: p51 Reverse transcriptase/RNaseH



- Molecule 3: primer DNA



● Molecule 4: template DNA



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	166.70Å 169.48Å 102.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.46 – 2.59 47.46 – 2.60	Depositor EDS
% Data completeness (in resolution range)	80.5 (47.46-2.59) 85.1 (47.46-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.9_1692, PHENIX 1.9_1692	Depositor
R, R_{free}	0.177 , 0.234 (Not available) , 0.248	Depositor DCC
R_{free} test set	2008 reflections (2.86%)	wwPDB-VP
Wilson B-factor (Å ²)	39.5	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8783	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, MG, 1RZ, DOC

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	0.57	1/4586 (0.0%)	0.89	8/6228 (0.1%)
2	B	0.57	0/3325	0.90	9/4513 (0.2%)
3	P	0.39	0/381	0.58	0/586
4	T	0.44	0/518	0.52	0/799
All	All	0.55	1/8810 (0.0%)	0.86	17/12126 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	65	LYS	C-O	5.13	1.29	1.23

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	312	GLU	CA-C-N	-6.45	113.30	120.14
2	B	312	GLU	C-N-CA	-6.45	113.30	120.14
1	A	58	THR	CA-C-N	6.28	126.04	119.76
1	A	58	THR	C-N-CA	6.28	126.04	119.76
1	A	225	PRO	O-C-N	5.94	123.94	121.15
1	A	51	GLY	CA-C-N	5.74	125.84	119.87
1	A	51	GLY	C-N-CA	5.74	125.84	119.87
1	A	250	ASP	N-CA-C	-5.63	107.06	114.04
2	B	24	TRP	CA-C-N	-5.48	114.28	119.76
2	B	24	TRP	C-N-CA	-5.48	114.28	119.76
1	A	291	GLU	N-CA-C	5.43	117.95	110.35
2	B	175	ASN	CA-C-N	5.35	125.17	119.28
2	B	175	ASN	C-N-CA	5.35	125.17	119.28
2	B	132	ILE	CA-C-N	5.31	125.29	120.03
2	B	132	ILE	C-N-CA	5.31	125.29	120.03
1	A	65	LYS	N-CA-C	5.29	118.04	109.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	382	ILE	N-CA-C	5.12	115.78	110.82

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	4471	0	4527	82	0
2	B	3238	0	3274	47	1
3	P	360	0	203	2	0
4	T	460	0	244	4	1
5	A	54	0	25	0	0
6	A	10	0	0	0	0
7	A	1	0	0	0	0
8	A	109	0	0	9	0
8	B	54	0	0	2	0
8	P	14	0	0	0	0
8	T	12	0	0	0	0
All	All	8783	0	8273	133	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (133) 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:A:247:PRO:O	1:A:307:ARG:NH2	2.14	0.80
1:A:478:GLU:HG2	1:A:499:SER:HB2	1.63	0.78
2:B:109:LEU:HD22	2:B:206:ARG:HD3	1.70	0.71
1:A:556:ILE:O	8:A:701:HOH:O	2.08	0.70
2:B:247:PRO:O	2:B:307:ARG:NH2	2.25	0.70
1:A:255:ASN:O	1:A:259:LYS:HG3	1.92	0.69
2:B:7:THR:HG21	2:B:121:ASP:HA	1.74	0.69
1:A:27:THR:HG22	1:A:29:GLU:H	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ARG:NH1	1:A:334:GLN:O	2.28	0.66
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.78	0.66
2:B:122:GLU:OE2	8:B:501:HOH:O	2.14	0.65
1:A:247:PRO:HB3	1:A:249:LYS:HE3	1.78	0.65
2:B:163:SER:O	2:B:167:ILE:HG13	1.97	0.65
1:A:53:GLU:H	1:A:53:GLU:CD	2.05	0.64
2:B:175:ASN:OD1	2:B:201:LYS:HE3	1.97	0.64
2:B:50:ILE:HD13	2:B:145:GLN:HB3	1.79	0.64
1:A:238:LYS:NZ	8:A:705:HOH:O	2.30	0.63
1:A:76:ASP:OD2	1:A:78:ARG:NH2	2.31	0.63
4:T:713:DC:H2'	4:T:714:DG:C8	2.33	0.63
1:A:54:ASN:O	1:A:143:ARG:NH2	2.28	0.62
1:A:447:ASN:HB2	1:A:556:ILE:HG23	1.81	0.61
2:B:79:GLU:HG3	2:B:83:ARG:HE	1.66	0.60
2:B:298:GLU:OE1	2:B:298:GLU:N	2.30	0.60
1:A:406:TRP:HZ3	1:A:507:GLN:HG2	1.65	0.60
1:A:511:ASP:OD1	1:A:512:GLN:HG3	2.01	0.60
1:A:277:ARG:NH2	1:A:355:ALA:O	2.35	0.60
1:A:233:GLU:OE1	8:A:703:HOH:O	2.17	0.59
1:A:131:THR:HG23	1:A:143:ARG:HG2	1.85	0.57
1:A:446:ALA:N	1:A:474:ASN:OD1	2.37	0.57
2:B:423:VAL:HA	2:B:426:TRP:CD1	2.39	0.57
1:A:60:VAL:HG12	1:A:75:VAL:HG22	1.87	0.57
2:B:160:PHE:CE2	2:B:164:MET:HG2	2.39	0.57
3:P:816:DG:H2'	3:P:817:DG:C8	2.40	0.56
4:T:712:DC:H2'	4:T:713:DC:C6	2.39	0.56
2:B:199:ARG:NE	2:B:233:GLU:OE2	2.36	0.56
1:A:157:PRO:HB3	1:A:184:MET:HE1	1.88	0.55
1:A:528:LYS:HE2	8:A:704:HOH:O	2.07	0.53
1:A:67:ASP:O	1:A:69:THR:OG1	2.26	0.53
1:A:246:LEU:HD11	1:A:310:LEU:HD12	1.90	0.53
2:B:323:LYS:O	2:B:385:LYS:NZ	2.38	0.53
1:A:407:GLN:NE2	8:A:707:HOH:O	2.42	0.52
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.91	0.52
1:A:111:VAL:HG21	1:A:164:MET:HE1	1.92	0.52
1:A:287:LYS:HD2	1:A:291:GLU:OE2	2.09	0.52
2:B:164:MET:HE1	2:B:168:LEU:HD11	1.91	0.52
2:B:386:THR:HG22	8:B:539:HOH:O	2.09	0.51
1:A:27:THR:HG22	1:A:29:GLU:N	2.24	0.51
1:A:103:LYS:HE3	1:A:179:VAL:HG11	1.93	0.51
2:B:356:ARG:HG3	2:B:367:GLN:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:LYS:HZ3	1:A:256:ASP:CG	2.19	0.50
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.92	0.50
2:B:180:ILE:HD13	2:B:205:LEU:HD11	1.93	0.50
1:A:478:GLU:CG	1:A:499:SER:HB2	2.37	0.49
1:A:246:LEU:HD22	1:A:260:LEU:HD12	1.94	0.49
1:A:255:ASN:O	1:A:259:LYS:CG	2.59	0.49
2:B:35:VAL:O	2:B:39:THR:HG23	2.12	0.49
2:B:278:GLN:O	2:B:281:LYS:HG2	2.13	0.49
2:B:266:TRP:CZ3	2:B:426:TRP:HB3	2.48	0.49
2:B:85:GLN:NE2	2:B:86:ASP:O	2.46	0.49
2:B:6:GLU:HG3	2:B:7:THR:N	2.28	0.49
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.95	0.48
2:B:281:LYS:HB2	2:B:284:ARG:NH1	2.28	0.48
1:A:451:LYS:HB3	1:A:471:ASP:HA	1.96	0.48
1:A:524:GLN:OE1	8:A:704:HOH:O	2.19	0.48
1:A:111:VAL:HB	1:A:185:ASP:HB2	1.95	0.48
1:A:195:ILE:O	1:A:199:ARG:HG3	2.14	0.48
1:A:478:GLU:HG3	8:A:714:HOH:O	2.14	0.47
1:A:24:TRP:HZ2	1:A:61:PHE:HD1	1.62	0.47
1:A:412:PRO:HD3	2:B:401:TRP:CH2	2.49	0.47
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.96	0.47
1:A:248:GLU:HG3	1:A:307:ARG:NH2	2.30	0.47
1:A:277:ARG:HH21	1:A:355:ALA:HB1	1.78	0.47
2:B:273:GLY:O	2:B:309:ILE:HD13	2.14	0.47
1:A:27:THR:O	1:A:31:ILE:HG13	2.15	0.47
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.50	0.47
1:A:281:LYS:HE3	1:A:281:LYS:HB3	1.70	0.47
2:B:107:THR:HG21	2:B:202:ILE:HG13	1.97	0.46
1:A:286:THR:HB	1:A:291:GLU:OE1	2.15	0.46
2:B:171:PHE:HE1	2:B:204:GLU:HG2	1.81	0.46
2:B:274:ILE:HD11	2:B:310:LEU:HD21	1.98	0.46
2:B:79:GLU:HG3	2:B:83:ARG:NE	2.30	0.46
2:B:369:THR:HG22	2:B:373:GLN:HE21	1.80	0.46
2:B:374:LYS:HD2	2:B:374:LYS:HA	1.75	0.46
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.97	0.45
1:A:478:GLU:HG2	1:A:499:SER:CB	2.39	0.45
2:B:143:ARG:HG2	2:B:143:ARG:HH11	1.81	0.45
1:A:358:ARG:HH11	1:A:358:ARG:HB3	1.82	0.45
1:A:406:TRP:CZ3	1:A:507:GLN:HG2	2.49	0.45
1:A:254:VAL:HG23	1:A:293:ILE:HD11	1.99	0.45
1:A:368:LEU:HD22	1:A:423:VAL:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ASN:HD21	1:A:259:LYS:HD3	1.83	0.44
1:A:46:LYS:HE2	1:A:116:PHE:O	2.17	0.44
1:A:58:THR:HG21	1:A:77:PHE:CD1	2.53	0.44
2:B:410:TRP:C	2:B:411:ILE:HG13	2.42	0.44
1:A:473:THR:O	1:A:477:THR:HG23	2.16	0.44
2:B:422:LEU:HD23	2:B:422:LEU:HA	1.76	0.44
1:A:395:LYS:HD2	1:A:414:TRP:CH2	2.53	0.44
1:A:349:LEU:HA	1:A:349:LEU:HD23	1.75	0.43
1:A:503:LEU:HD12	1:A:533:LEU:HD23	2.00	0.43
1:A:66:LYS:C	1:A:68:SER:N	2.74	0.43
1:A:211:ARG:NH1	8:A:711:HOH:O	2.50	0.43
2:B:395:LYS:HE3	3:P:813:DT:OP1	2.18	0.43
1:A:41:MET:HE2	1:A:46:LYS:HB3	2.00	0.43
1:A:169:GLU:HB3	1:A:170:PRO:HD3	2.00	0.42
2:B:160:PHE:HE2	2:B:164:MET:HG2	1.82	0.42
2:B:11:LYS:HA	2:B:11:LYS:HD2	1.60	0.42
1:A:11:LYS:HB2	1:A:11:LYS:HE2	1.76	0.42
1:A:419:THR:HA	1:A:420:PRO:HD2	1.85	0.42
1:A:253:THR:O	1:A:257:ILE:HG12	2.20	0.42
2:B:151:GLN:HB3	2:B:185:ASP:OD2	2.19	0.42
1:A:305:GLU:O	1:A:309:ILE:HG13	2.19	0.42
4:T:724:DT:H2'	4:T:725:DG:O4'	2.19	0.42
1:A:259:LYS:O	1:A:263:LYS:HG2	2.19	0.42
1:A:490:GLY:O	1:A:528:LYS:NZ	2.41	0.42
2:B:64:LYS:NZ	2:B:69:THR:HA	2.35	0.42
2:B:115:TYR:HB3	2:B:149:LEU:HB2	2.02	0.41
1:A:22:LYS:NZ	8:A:702:HOH:O	2.15	0.41
1:A:57:ASN:OD1	1:A:131:THR:OG1	2.31	0.41
1:A:484:LEU:HD12	1:A:484:LEU:HA	1.74	0.41
1:A:254:VAL:HG23	1:A:293:ILE:CD1	2.50	0.41
1:A:372:VAL:HG11	1:A:412:PRO:HD2	2.03	0.41
2:B:24:TRP:HB2	2:B:25:PRO:HD2	2.03	0.41
1:A:58:THR:HA	1:A:59:PRO:HD3	1.72	0.41
1:A:66:LYS:C	1:A:68:SER:H	2.29	0.41
1:A:163:SER:O	1:A:167:ILE:HG13	2.20	0.41
1:A:149:LEU:HA	1:A:150:PRO:HD3	1.92	0.41
2:B:180:ILE:HG23	2:B:189:VAL:HG22	2.02	0.40
1:A:543:GLY:HA2	1:A:544:GLY:HA2	1.64	0.40
2:B:354:TYR:OH	2:B:356:ARG:NE	2.54	0.40
1:A:24:TRP:HZ2	1:A:61:PHE:CD1	2.38	0.40
4:T:711:DC:H2'	4:T:712:DC:C6	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:201:LYS:O	2:B:204:GLU:HB3	2.21	0.40
1:A:303:LEU:HD21	1:A:307:ARG:NH1	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:314:VAL:O	4:T:725:DG:N2[3_554]	2.08	0.12

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	545/572 (95%)	518 (95%)	27 (5%)	0	100	100
2	B	383/440 (87%)	371 (97%)	12 (3%)	0	100	100
All	All	928/1012 (92%)	889 (96%)	39 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	490/511 (96%)	475 (97%)	15 (3%)	35	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	358/400 (90%)	337 (94%)	21 (6%)	18	38
All	All	848/911 (93%)	812 (96%)	36 (4%)	26	52

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	TRP
1	A	53	GLU
1	A	69	THR
1	A	82	LYS
1	A	102	LYS
1	A	200	THR
1	A	240	THR
1	A	254	VAL
1	A	263	LYS
1	A	275	LYS
1	A	281	LYS
1	A	290	THR
1	A	303	LEU
1	A	458	VAL
1	A	459	THR
2	B	7	THR
2	B	10	VAL
2	B	11	LYS
2	B	67	ASP
2	B	74	LEU
2	B	86	ASP
2	B	107	THR
2	B	109	LEU
2	B	122	GLU
2	B	135	ILE
2	B	194	GLU
2	B	195	ILE
2	B	197	GLN
2	B	210	LEU
2	B	241	VAL
2	B	245	VAL
2	B	275	LYS
2	B	276	VAL
2	B	307	ARG
2	B	362	THR
2	B	386	THR

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

Mol	Chain	Res	Type
1	A	265	ASN
1	A	278	GLN
1	A	520	GLN
2	B	137	ASN
2	B	147	ASN
2	B	258	GLN
2	B	269	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	DOC	P	822	4,3	16,19,20	2.26	7 (43%)	20,26,29	3.41	7 (35%)

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	DOC	P	822	4,3	-	0/7/18/19	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	822	DOC	C4-N3	4.47	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	822	DOC	C5-C4	-3.99	1.33	1.42
3	P	822	DOC	C4-N4	3.79	1.43	1.33
3	P	822	DOC	O4'-C1'	3.24	1.49	1.42
3	P	822	DOC	C6-C5	2.27	1.40	1.35
3	P	822	DOC	C3'-C2'	-2.27	1.47	1.54
3	P	822	DOC	O5'-C5'	-2.11	1.38	1.44

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	822	DOC	C2'-C1'-N1	11.79	134.75	112.40
3	P	822	DOC	O4'-C4'-C5'	5.52	119.28	109.34
3	P	822	DOC	O4'-C1'-N1	4.17	115.27	107.86
3	P	822	DOC	C4'-O4'-C1'	-3.99	106.04	109.81
3	P	822	DOC	O4'-C1'-C2'	-3.36	102.43	106.41
3	P	822	DOC	O2-C2-N3	-2.16	118.92	122.33
3	P	822	DOC	O4'-C4'-C3'	2.09	108.24	104.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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
5	1RZ	A	601[A]	7	27,28,28	2.19	3 (11%)	38,43,43	2.09	9 (23%)
6	SO4	A	602	-	4,4,4	0.31	0	6,6,6	0.23	0
6	SO4	A	603	-	4,4,4	0.25	0	6,6,6	0.17	0
5	1RZ	A	601[B]	7	27,28,28	1.99	3 (11%)	38,43,43	2.15	8 (21%)

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	1RZ	A	601[A]	7	-	7/22/31/31	0/2/2/2
5	1RZ	A	601[B]	7	-	4/22/31/31	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601[B]	1RZ	O2-C2	7.59	1.37	1.23
5	A	601[A]	1RZ	O2-C2	7.51	1.37	1.23
5	A	601[A]	1RZ	PA-O3A	6.82	1.66	1.59
5	A	601[B]	1RZ	PA-O3A	4.99	1.64	1.59
5	A	601[B]	1RZ	C6-C5	2.16	1.40	1.35
5	A	601[A]	1RZ	C6-C5	2.14	1.40	1.35

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601[B]	1RZ	O2-C2-N3	-6.18	112.58	122.33
5	A	601[A]	1RZ	O2-C2-N3	-6.13	112.66	122.33
5	A	601[A]	1RZ	O3A-PB-O2B	-5.77	93.36	110.70
5	A	601[B]	1RZ	O3A-PB-O2B	-5.72	93.51	110.70
5	A	601[B]	1RZ	O2A-PA-O3A	5.30	121.59	107.27
5	A	601[A]	1RZ	O2A-PA-O3A	4.72	120.02	107.27
5	A	601[A]	1RZ	O2-C2-N1	4.31	127.35	118.90
5	A	601[B]	1RZ	O2-C2-N1	4.31	127.34	118.90
5	A	601[B]	1RZ	O3A-PA-O1A	-3.14	101.24	110.70
5	A	601[B]	1RZ	O1B-PB-O2B	2.60	124.52	112.44
5	A	601[B]	1RZ	O4'-C4'-C5'	-2.48	103.62	109.61
5	A	601[A]	1RZ	O4'-C4'-C5'	-2.36	103.92	109.61
5	A	601[A]	1RZ	C5-C4-N4	2.27	124.60	120.63
5	A	601[B]	1RZ	C5-C4-N4	2.24	124.55	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601[A]	1RZ	O3A-PA-O1A	-2.21	104.06	110.70
5	A	601[A]	1RZ	O1B-PB-O3A	2.12	113.02	107.27
5	A	601[A]	1RZ	O1B-PB-O2B	2.08	122.14	112.44

There are no chirality outliers.

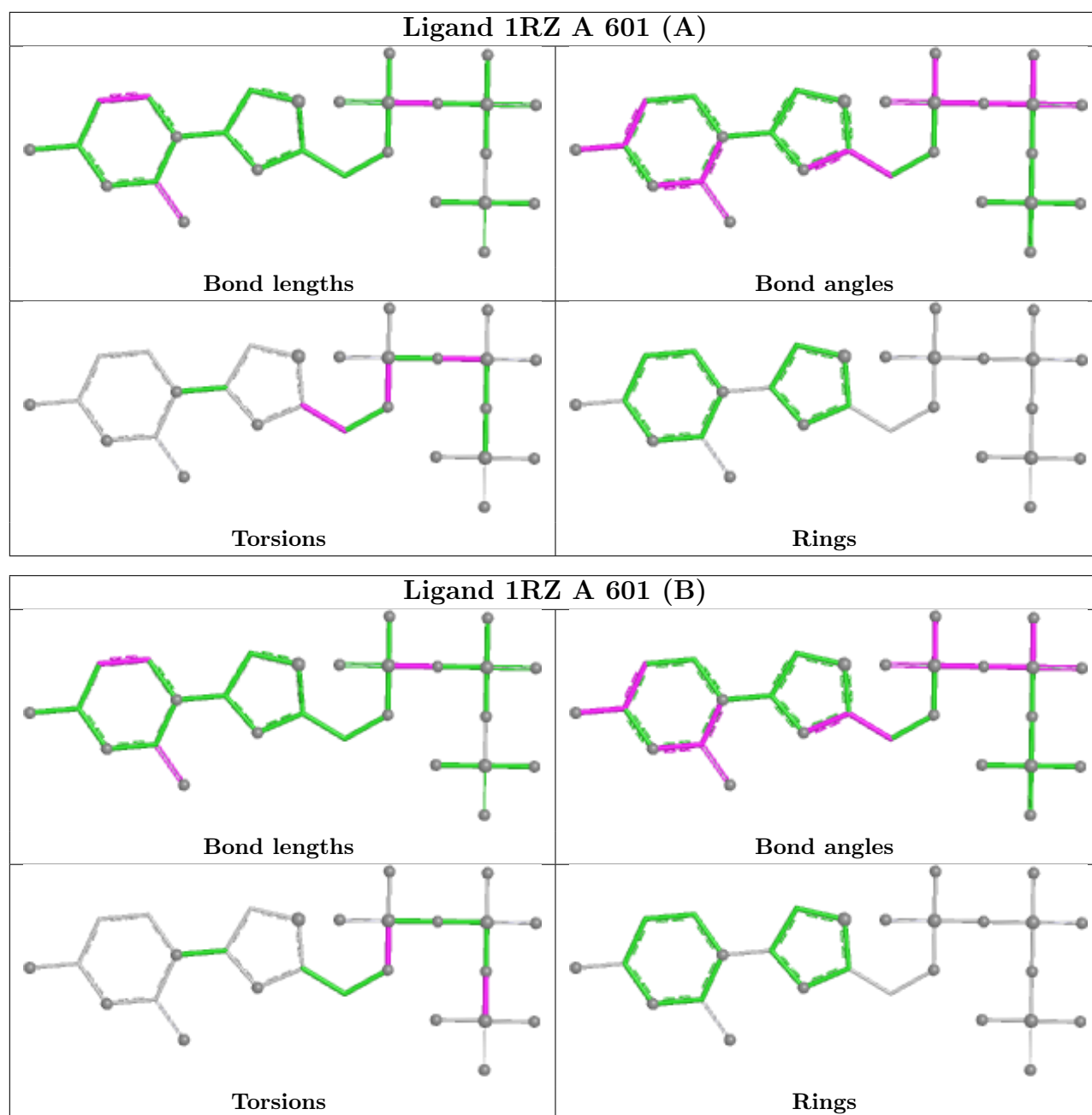
All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	601[A]	1RZ	C5'-O5'-PA-O1A
5	A	601[A]	1RZ	C5'-O5'-PA-O2A
5	A	601[B]	1RZ	PB-O3B-PG-O2C
5	A	601[B]	1RZ	C5'-O5'-PA-O1A
5	A	601[A]	1RZ	S3'-C4'-C5'-O5'
5	A	601[A]	1RZ	PA-O3A-PB-O2B
5	A	601[A]	1RZ	C5'-O5'-PA-O3A
5	A	601[B]	1RZ	C5'-O5'-PA-O3A
5	A	601[B]	1RZ	C5'-O5'-PA-O2A
5	A	601[A]	1RZ	PA-O3A-PB-O1B
5	A	601[A]	1RZ	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

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	549/572 (95%)	-0.02	15 (2%) 56 50	24, 42, 76, 108	0
2	B	391/440 (88%)	0.17	18 (4%) 37 32	24, 49, 78, 103	0
3	P	17/21 (80%)	-0.44	0 100 100	33, 51, 65, 67	0
4	T	22/27 (81%)	-0.21	1 (4%) 38 32	32, 61, 91, 104	0
All	All	979/1060 (92%)	0.04	34 (3%) 47 41	24, 45, 78, 108	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	24	TRP	4.8
2	B	212	TRP	4.7
1	A	67	ASP	4.1
2	B	429	LEU	3.9
1	A	69	THR	3.7
1	A	1	PRO	3.4
2	B	357	MET	3.3
1	A	68	SER	3.2
1	A	290	THR	3.1
2	B	275	LYS	2.8
1	A	70	LYS	2.7
2	B	313	PRO	2.7
1	A	66	LYS	2.7
2	B	245	VAL	2.6
2	B	206	ARG	2.5
1	A	132	ILE	2.5
1	A	134	SER	2.5
2	B	66	LYS	2.4
4	T	704	DG	2.4
2	B	315	HIS	2.3
1	A	543	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	471	ASP	2.3
2	B	233	GLU	2.3
2	B	237	ASP	2.3
2	B	239	TRP	2.2
1	A	2	ILE	2.2
2	B	419	THR	2.2
2	B	86	ASP	2.2
2	B	67	ASP	2.1
2	B	70	LYS	2.1
1	A	289	LEU	2.1
2	B	312	GLU	2.1
1	A	259	LYS	2.0
2	B	426	TRP	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
3	DOC	P	822	18/19	0.98	0.06	27,32,41,42	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	1RZ	A	601[A]	27/27	0.90	0.10	37,48,60,61	27
5	1RZ	A	601[B]	27/27	0.90	0.10	38,46,60,63	27
6	SO4	A	603	5/5	0.92	0.07	68,71,81,87	0
6	SO4	A	602	5/5	0.95	0.10	42,50,57,60	0

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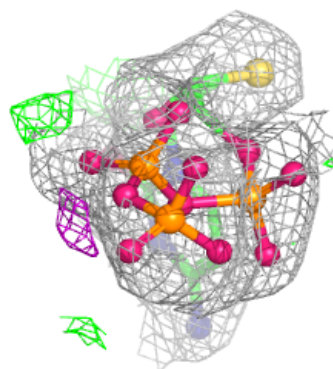
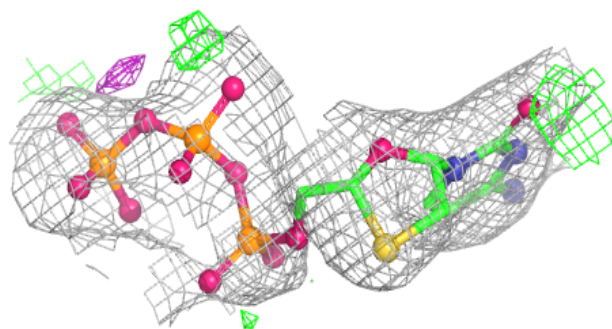
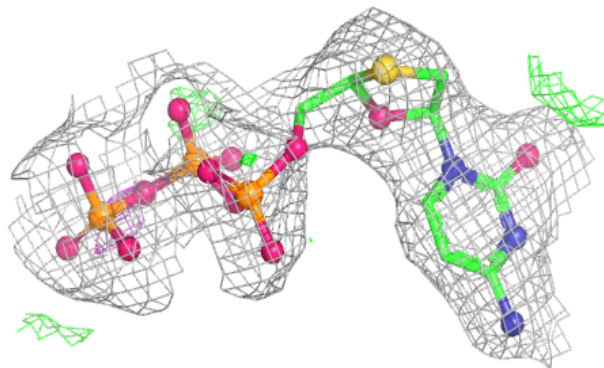
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	MG	A	604	1/1	0.98	0.04	45,45,45,45	0

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.

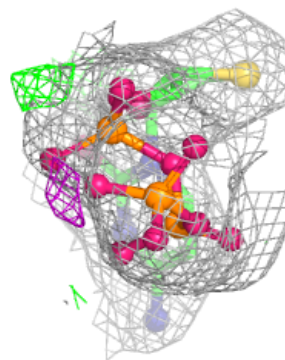
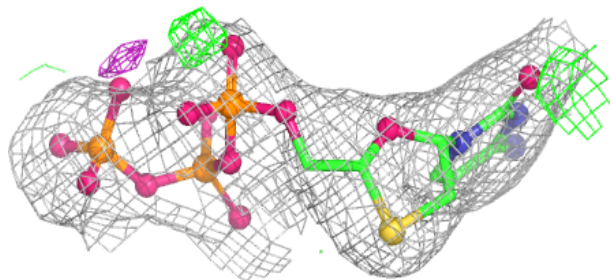
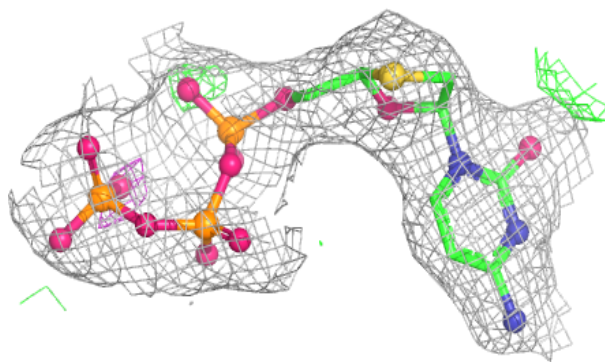
Electron density around 1RZ A 601 (A):

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 1RZ A 601 (B):

$2mF_o-DF_c$ (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.