



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 12:20 PM BST

PDB ID : 6UJX
Title : HIV-1 wild-type reverse transcriptase-DNA complex with (-)-FTC-TP
Authors : Lansdon, E.B.
Deposited on : 2019-10-03
Resolution : 2.70 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 : 2.13.1
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) : 2.13.1

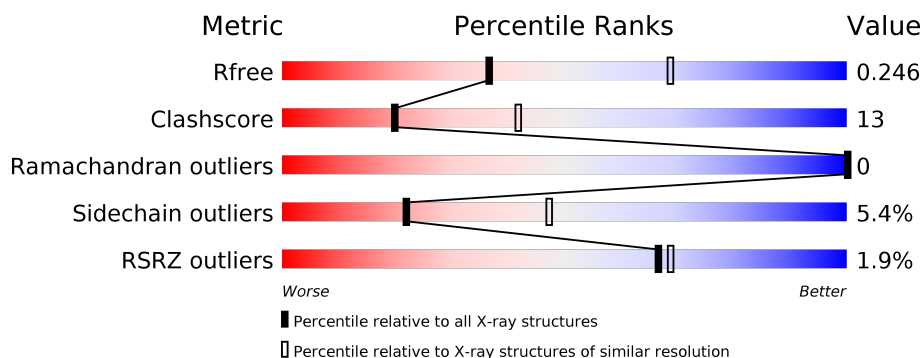
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	572	<div> <div>2%</div> <div> <div></div> <div>70%</div> <div>24%</div> <div>• •</div> </div> </div>
2	B	440	<div> <div>2%</div> <div> <div></div> <div>62%</div> <div>26%</div> <div>• 10%</div> </div> </div>
3	P	21	<div> <div></div> <div> <div>52%</div> <div>33%</div> <div>14%</div> </div> </div>
4	T	27	<div> <div></div> <div> <div>41%</div> <div>41%</div> <div>19%</div> </div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8759 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	548	Total	C	N	O	S	0	0	0
			4463	2887	744	824	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	398	Total	C	N	O	S	0	0	0
			3287	2134	549	598	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 DNA primer.

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 DNA template.

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 SULFATE ION (three-letter code: SO4) (formula: O₄S).

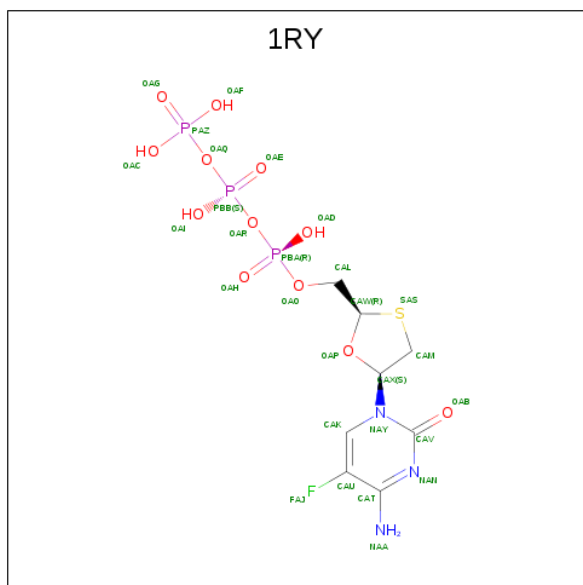


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	P	1	Total	O	S	0	0
			5	4	1		
5	T	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 7 is [(2R,5S)-5-(4-azanyl-5-fluoranyl-2-oxidanylidene-pyrimidin-1-yl)-1,3-oxathiolan-2-yl]methoxy-oxidanyl-phosphoryl phosphono hydrogen phosphate (three-letter code: 1RY) (formula: C₈H₁₃FN₃O₁₂P₃S) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	A	1	Total	C	F	N	O	P	S	
			56	16	2	6	24	6	2	

- Molecule 8 is water.

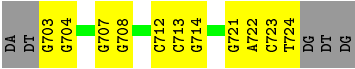
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	67	Total O 67 67	0	0
8	B	34	Total O 34 34	0	0
8	P	5	Total O 5 5	0	0
8	T	6	Total O 6 6	0	0



- Molecule 3: DNA primer



- Molecule 4: DNA template



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	169.80Å 167.69Å 103.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.60 – 2.70 47.60 – 2.70	Depositor EDS
% Data completeness (in resolution range)	89.1 (47.60-2.70) 88.5 (47.60-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.73 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.9_1692, PHENIX 1.9_1692	Depositor
R, R_{free}	0.197 , 0.244 0.199 , 0.246	Depositor DCC
R_{free} test set	1995 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	44.5	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8759	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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: 1RY, MG, SO4, 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	0.50	0/4578	0.59	0/6217
2	B	0.45	0/3377	0.58	0/4584
3	P	0.91	1/381 (0.3%)	1.01	0/586
4	T	0.91	0/518	0.87	0/799
All	All	0.54	1/8854 (0.0%)	0.64	0/12186

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	821	DC	C3'-O3'	-5.51	1.36	1.44

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4463	0	4516	110	0
2	B	3287	0	3325	92	0
3	P	360	0	203	7	0
4	T	460	0	244	14	0
5	A	10	0	0	1	0
5	P	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	T	5	0	0	0	0
6	A	1	0	0	0	0
7	A	56	0	26	3	0
8	A	67	0	0	3	0
8	B	34	0	0	0	0
8	P	5	0	0	0	0
8	T	6	0	0	0	0
All	All	8759	0	8314	214	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 13.

All (214) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:425:LEU:HA	2:B:428:GLN:HG3	1.48	0.94
1:A:417:VAL:HG12	1:A:419:THR:HG23	1.48	0.93
1:A:390:LYS:HB3	1:A:417:VAL:HG21	1.53	0.91
4:T:703:DG:H2''	4:T:704:DG:H5''	1.55	0.86
2:B:28:GLU:HG3	2:B:135:ILE:HD11	1.56	0.85
4:T:703:DG:C2'	4:T:704:DG:H5''	2.06	0.84
4:T:703:DG:H2'	4:T:704:DG:C2	2.13	0.84
2:B:35:VAL:O	2:B:39:THR:HG23	1.79	0.83
2:B:79:GLU:HG3	2:B:83:ARG:NH1	1.94	0.82
1:A:24:TRP:HB2	1:A:25:PRO:HD2	1.63	0.80
2:B:120:LEU:HD12	2:B:125:ARG:HG2	1.63	0.80
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.22	0.79
2:B:365:VAL:O	2:B:369:THR:HG23	1.82	0.79
1:A:27:THR:HG22	1:A:29:GLU:H	1.46	0.79
1:A:390:LYS:HB3	1:A:417:VAL:CG2	2.13	0.78
1:A:404:GLU:OE1	1:A:428:GLN:NE2	2.13	0.77
1:A:372:VAL:HG11	1:A:411:ILE:HG23	1.64	0.77
2:B:247:PRO:O	2:B:307:ARG:NH2	2.19	0.76
2:B:423:VAL:HA	2:B:426:TRP:CD1	2.21	0.75
4:T:712:DC:H2'	4:T:713:DC:C6	2.22	0.75
1:A:253:THR:HG22	1:A:292:VAL:HG22	1.69	0.74
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.71	0.72
1:A:131:THR:CG2	1:A:143:ARG:HD2	2.21	0.71
1:A:131:THR:HG22	1:A:143:ARG:HG2	1.72	0.71
1:A:197:GLN:NE2	8:A:702:HOH:O	2.24	0.70
2:B:302:GLU:O	2:B:306:ASN:ND2	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.73	0.69
2:B:79:GLU:HG3	2:B:83:ARG:HH11	1.58	0.69
1:A:473:THR:O	1:A:477:THR:HG23	1.94	0.68
1:A:111:VAL:HB	1:A:185:ASP:HB2	1.79	0.65
3:P:816:DG:H2'	3:P:817:DG:C8	2.32	0.65
1:A:27:THR:HG22	1:A:29:GLU:N	2.11	0.65
1:A:103:LYS:HE3	1:A:179:VAL:HG11	1.79	0.64
2:B:369:THR:HG22	2:B:398:TRP:CZ3	2.33	0.64
1:A:70:LYS:HE3	1:A:70:LYS:HA	1.79	0.64
4:T:713:DC:H2'	4:T:714:DG:C8	2.33	0.63
1:A:286:THR:HG21	1:A:293:ILE:HD11	1.80	0.63
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.80	0.63
4:T:703:DG:H2'	4:T:704:DG:N3	2.14	0.62
2:B:154:LYS:O	2:B:157:PRO:HD2	2.00	0.62
1:A:246:LEU:HD22	1:A:260:LEU:HD12	1.82	0.62
1:A:357:MET:HA	1:A:357:MET:CE	2.30	0.61
2:B:86:ASP:OD1	2:B:86:ASP:N	2.23	0.61
1:A:31:ILE:O	1:A:35:VAL:HG13	2.00	0.61
1:A:454:LYS:NZ	1:A:554:ALA:HB3	2.16	0.61
2:B:50:ILE:HD13	2:B:145:GLN:HB2	1.82	0.60
2:B:332:GLN:OE1	2:B:428:GLN:NE2	2.24	0.60
2:B:425:LEU:HA	2:B:428:GLN:CG	2.27	0.60
2:B:53:GLU:OE1	2:B:53:GLU:N	2.28	0.59
1:A:131:THR:HG22	1:A:143:ARG:CG	2.32	0.59
1:A:131:THR:HG22	1:A:143:ARG:HD2	1.85	0.58
1:A:265:ASN:OD1	1:A:353:LYS:NZ	2.29	0.58
1:A:500:GLN:HG2	2:B:422:LEU:CD2	2.33	0.58
1:A:473:THR:HG23	1:A:476:LYS:HD2	1.86	0.58
1:A:28:GLU:OE2	1:A:32:LYS:HE3	2.04	0.57
2:B:164:MET:HG2	2:B:182:GLN:OE1	2.03	0.57
2:B:66:LYS:CG	2:B:67:ASP:H	2.15	0.57
2:B:266:TRP:CZ3	2:B:426:TRP:HB3	2.38	0.57
2:B:82:LYS:HE2	2:B:413:GLU:OE2	2.04	0.57
1:A:286:THR:CG2	1:A:293:ILE:HD11	2.35	0.57
1:A:436:GLY:HA2	5:A:601:SO4:O4	2.05	0.56
1:A:60:VAL:HG12	1:A:75:VAL:HG22	1.88	0.56
1:A:131:THR:HG22	1:A:143:ARG:CD	2.36	0.55
1:A:417:VAL:HG12	1:A:419:THR:CG2	2.30	0.55
1:A:46:LYS:HE2	1:A:116:PHE:O	2.07	0.55
7:A:604[B]:1RY:H6	7:A:604[B]:1RY:PBB	2.47	0.55
2:B:28:GLU:CG	2:B:135:ILE:HD11	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:LYS:HZ1	1:A:554:ALA:HB3	1.72	0.54
1:A:511:ASP:OD1	1:A:512:GLN:HG3	2.07	0.54
1:A:35:VAL:O	1:A:39:THR:HG23	2.08	0.54
1:A:41:MET:HB3	1:A:47:ILE:HG12	1.90	0.54
2:B:24:TRP:HB2	2:B:25:PRO:HD2	1.89	0.54
2:B:344:GLU:O	2:B:347:LYS:HB2	2.08	0.54
1:A:115:TYR:CE2	1:A:156:SER:HB3	2.42	0.53
2:B:107:THR:HG21	2:B:202:ILE:HG13	1.89	0.53
2:B:298:GLU:O	2:B:301:LEU:HB2	2.08	0.53
1:A:27:THR:O	1:A:31:ILE:HG13	2.08	0.53
3:P:816:DG:H2'	3:P:817:DG:H8	1.72	0.53
1:A:73:LYS:HE3	1:A:146:TYR:OH	2.08	0.53
1:A:494:ASN:HB3	2:B:289:LEU:HD22	1.90	0.52
2:B:103:LYS:HD2	2:B:191:SER:CA	2.40	0.52
1:A:89:GLU:HG3	4:T:708:DG:OP1	2.09	0.52
4:T:723:DC:H2''	4:T:724:DT:H71	1.92	0.52
1:A:367:GLN:NE2	1:A:512:GLN:OE1	2.43	0.51
2:B:425:LEU:HD23	2:B:425:LEU:O	2.10	0.51
2:B:47:ILE:HD12	2:B:144:TYR:CD1	2.46	0.51
2:B:297:GLU:O	2:B:301:LEU:HG	2.11	0.51
2:B:417:VAL:HG12	2:B:417:VAL:O	2.10	0.51
1:A:54:ASN:O	1:A:143:ARG:NH2	2.43	0.50
1:A:448:ARG:NH2	3:P:806:DT:H1'	2.27	0.50
2:B:102:LYS:O	2:B:103:LYS:HG2	2.10	0.50
1:A:371:ALA:O	1:A:375:ILE:HG13	2.12	0.50
2:B:7:THR:HG22	2:B:119:PRO:HB2	1.94	0.50
2:B:263:LYS:HA	2:B:426:TRP:CZ3	2.46	0.50
1:A:483:TYR:CE1	1:A:520:GLN:HB3	2.46	0.50
2:B:115:TYR:CD2	2:B:156:SER:HB3	2.47	0.49
1:A:246:LEU:CD1	1:A:310:LEU:HD12	2.42	0.49
2:B:195:ILE:HG22	2:B:199:ARG:CZ	2.42	0.49
4:T:721:DG:H2''	4:T:722:DA:C8	2.46	0.49
1:A:281:LYS:O	1:A:284:ARG:HG3	2.13	0.49
1:A:362:THR:OG1	1:A:363:ASN:N	2.46	0.49
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.94	0.49
2:B:410:TRP:C	2:B:411:ILE:HG13	2.32	0.49
1:A:246:LEU:HD11	1:A:310:LEU:CD1	2.43	0.49
3:P:815:DG:H2''	3:P:816:DG:C8	2.48	0.49
1:A:50:ILE:HD12	1:A:54:ASN:HB3	1.95	0.48
2:B:366:LYS:HD2	2:B:405:TYR:CD1	2.48	0.48
2:B:191:SER:OG	2:B:198:HIS:ND1	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.47	0.48
4:T:703:DG:H2'	4:T:704:DG:N2	2.28	0.48
2:B:330:GLN:NE2	2:B:338:THR:OG1	2.44	0.48
3:P:815:DG:H2''	3:P:816:DG:H8	1.79	0.48
2:B:380:ILE:O	2:B:384:GLY:HA2	2.14	0.47
2:B:424:LYS:O	2:B:428:GLN:HG2	2.15	0.47
1:A:500:GLN:HG2	2:B:422:LEU:HD22	1.94	0.47
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.50	0.47
2:B:112:GLY:HA3	2:B:151:GLN:OE1	2.15	0.47
1:A:420:PRO:CB	1:A:421:PRO:HA	2.45	0.47
2:B:266:TRP:CH2	2:B:426:TRP:HB3	2.50	0.47
2:B:65:LYS:O	2:B:68:SER:HB3	2.15	0.47
1:A:412:PRO:HD3	2:B:401:TRP:CH2	2.50	0.47
1:A:112:GLY:HA2	7:A:604[A]:1RY:OAF	2.15	0.47
2:B:157:PRO:HG3	2:B:184:MET:HA	1.98	0.46
1:A:247:PRO:O	1:A:307:ARG:NH2	2.42	0.46
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.97	0.46
1:A:24:TRP:HB2	1:A:25:PRO:CD	2.42	0.46
2:B:253:THR:HA	2:B:292:VAL:HA	1.96	0.46
2:B:66:LYS:HG2	2:B:67:ASP:H	1.80	0.46
2:B:193:LEU:HD11	2:B:201:LYS:HG3	1.97	0.46
2:B:425:LEU:CA	2:B:428:GLN:HG3	2.34	0.46
1:A:242:GLN:HB3	1:A:243:PRO:HD2	1.98	0.45
2:B:242:GLN:OE1	2:B:429:LEU:HD12	2.15	0.45
1:A:30:LYS:NZ	4:T:704:DG:H1	2.14	0.45
1:A:67:ASP:O	1:A:69:THR:N	2.49	0.45
1:A:542:ILE:O	1:A:545:ASN:HB3	2.16	0.45
2:B:309:ILE:HG22	2:B:309:ILE:O	2.16	0.45
4:T:712:DC:H2'	4:T:713:DC:H6	1.74	0.45
1:A:57:ASN:OD1	1:A:131:THR:HG23	2.17	0.45
1:A:328:GLU:HG3	1:A:390:LYS:HB2	1.98	0.45
1:A:335:GLY:HA2	1:A:367:GLN:OE1	2.16	0.45
1:A:380:ILE:O	1:A:384:GLY:HA2	2.16	0.45
1:A:503:LEU:HD11	1:A:507:GLN:HE21	1.81	0.45
2:B:350:LYS:HG2	2:B:351:THR:N	2.31	0.45
1:A:131:THR:CG2	1:A:143:ARG:CD	2.91	0.45
2:B:46:LYS:HE3	2:B:116:PHE:CD2	2.52	0.45
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.99	0.44
1:A:275:LYS:HD2	1:A:332:GLN:OE1	2.17	0.44
1:A:450:THR:O	1:A:451:LYS:HB2	2.17	0.44
1:A:103:LYS:HE3	1:A:179:VAL:CG1	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:173:LYS:HD3	2:B:174:GLN:N	2.33	0.44
2:B:257:ILE:HG22	2:B:283:LEU:HD11	2.00	0.44
2:B:303:LEU:O	2:B:307:ARG:HG3	2.18	0.44
2:B:106:VAL:HG21	2:B:236:PRO:HG2	2.00	0.44
2:B:355:ALA:O	2:B:356:ARG:HG2	2.18	0.44
1:A:276:VAL:O	1:A:280:SER:HB2	2.17	0.43
2:B:74:LEU:HD11	2:B:409:THR:HA	2.00	0.43
1:A:395:LYS:HD2	1:A:414:TRP:CH2	2.54	0.43
1:A:58:THR:HG21	1:A:77:PHE:CD1	2.53	0.43
1:A:157:PRO:HG2	4:T:707:DG:O4'	2.19	0.43
1:A:245:VAL:HG23	1:A:245:VAL:O	2.19	0.43
1:A:419:THR:O	1:A:419:THR:OG1	2.32	0.43
1:A:121:ASP:O	1:A:125:ARG:HG3	2.19	0.43
1:A:122:GLU:HG3	8:A:747:HOH:O	2.18	0.43
1:A:451:LYS:HB3	1:A:471:ASP:HA	2.00	0.43
2:B:353:LYS:HB3	2:B:353:LYS:HE2	1.85	0.43
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.58	0.43
2:B:388:LYS:HG2	2:B:413:GLU:HB2	2.00	0.43
2:B:422:LEU:HD12	2:B:422:LEU:HA	1.84	0.43
1:A:34:LEU:HD23	1:A:34:LEU:HA	1.74	0.42
1:A:508:ALA:HB3	8:A:745:HOH:O	2.18	0.42
1:A:169:GLU:HB3	1:A:170:PRO:CD	2.43	0.42
2:B:103:LYS:HD2	2:B:191:SER:N	2.33	0.42
2:B:332:GLN:OE1	2:B:332:GLN:HA	2.18	0.42
2:B:242:GLN:OE1	2:B:353:LYS:HD3	2.19	0.42
1:A:8:VAL:HA	1:A:9:PRO:HD3	1.91	0.42
1:A:156:SER:HB2	1:A:157:PRO:HD3	2.02	0.42
1:A:303:LEU:HD12	1:A:303:LEU:O	2.19	0.42
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.53	0.42
2:B:201:LYS:HD3	2:B:201:LYS:HA	1.73	0.42
2:B:382:ILE:HG22	2:B:383:TRP:CE2	2.55	0.42
2:B:66:LYS:HG2	2:B:67:ASP:N	2.34	0.42
1:A:289:LEU:HD11	3:P:817:DG:H4'	2.02	0.42
1:A:389:PHE:HB3	1:A:391:LEU:HD21	2.00	0.42
1:A:43:LYS:HE3	1:A:43:LYS:HB2	1.71	0.42
1:A:246:LEU:HD11	1:A:310:LEU:HD11	2.02	0.41
2:B:303:LEU:HD23	2:B:303:LEU:HA	1.78	0.41
1:A:121:ASP:OD1	1:A:122:GLU:N	2.53	0.41
1:A:262:GLY:HA3	3:P:819:DG:O4'	2.20	0.41
1:A:24:TRP:CZ2	4:T:704:DG:C8	3.08	0.41
1:A:281:LYS:O	1:A:284:ARG:CG	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:276:VAL:HG13	2:B:276:VAL:O	2.20	0.41
2:B:28:GLU:HG3	2:B:135:ILE:CD1	2.38	0.41
1:A:266:TRP:O	1:A:269:GLN:HG2	2.21	0.41
2:B:50:ILE:HG21	2:B:145:GLN:HB2	2.02	0.41
2:B:126:LYS:HA	2:B:145:GLN:OE1	2.20	0.41
2:B:193:LEU:CD1	2:B:201:LYS:HG3	2.50	0.41
2:B:79:GLU:CG	2:B:83:ARG:NH1	2.74	0.41
1:A:324:ASP:O	1:A:343:GLN:HG2	2.21	0.41
1:A:67:ASP:C	1:A:69:THR:H	2.24	0.41
1:A:498:ASP:CG	1:A:538:ALA:HB2	2.40	0.41
2:B:148:VAL:O	2:B:150:PRO:HD3	2.21	0.41
7:A:604[B]:1RY:CAL	7:A:604[B]:1RY:PBB	3.08	0.41
2:B:320:ASP:OD2	2:B:323:LYS:HG3	2.21	0.41
1:A:411:ILE:CG2	1:A:412:PRO:HD2	2.51	0.40
2:B:103:LYS:HE2	2:B:179:VAL:HG12	2.03	0.40
1:A:3:SER:OG	1:A:5:ILE:HG22	2.21	0.40
2:B:195:ILE:H	2:B:195:ILE:HG13	1.45	0.40
2:B:258:GLN:HG2	2:B:283:LEU:HD13	2.03	0.40
2:B:393:ILE:HG21	2:B:398:TRP:HB2	2.04	0.40
1:A:28:GLU:HA	1:A:31:ILE:HD12	2.02	0.40
1:A:38:CYS:SG	1:A:132:ILE:CD1	3.04	0.40
1:A:93:GLY:C	1:A:94:ILE:HD13	2.42	0.40
2:B:183:TYR:CE1	2:B:184:MET:HG2	2.56	0.40
1:A:420:PRO:HB2	1:A:421:PRO:HA	2.03	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	544/572 (95%)	513 (94%)	31 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	392/440 (89%)	364 (93%)	28 (7%)	0	100	100
All	All	936/1012 (92%)	877 (94%)	59 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	489/511 (96%)	466 (95%)	23 (5%)	26	54
2	B	362/400 (90%)	339 (94%)	23 (6%)	17	39
All	All	851/911 (93%)	805 (95%)	46 (5%)	22	47

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	TRP
1	A	35	VAL
1	A	40	GLU
1	A	41	MET
1	A	70	LYS
1	A	110	ASP
1	A	173	LYS
1	A	179	VAL
1	A	194	GLU
1	A	200	THR
1	A	209	LEU
1	A	211	ARG
1	A	220	LYS
1	A	240	THR
1	A	258	CYS
1	A	280	SER
1	A	324	ASP
1	A	334	GLN

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Mol	Chain	Res	Type
1	A	340	GLN
1	A	357	MET
1	A	418	ASN
1	A	503	LEU
1	A	523	GLU
2	B	67	ASP
2	B	69	THR
2	B	72	ARG
2	B	86	ASP
2	B	107	THR
2	B	154	LYS
2	B	163	SER
2	B	179	VAL
2	B	194	GLU
2	B	195	ILE
2	B	276	VAL
2	B	286	THR
2	B	292	VAL
2	B	330	GLN
2	B	340	GLN
2	B	357	MET
2	B	362	THR
2	B	386	THR
2	B	388	LYS
2	B	396	GLU
2	B	418	ASN
2	B	422	LEU
2	B	429	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	3,4	14,19,20	2.33	7 (50%)	13,26,29	4.20	5 (38%)

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	3,4	-	1/4/18/19	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	4.53	1.42	1.35
3	P	822	DOC	O4'-C1'	3.29	1.49	1.42
3	P	822	DOC	C5-C4	-3.12	1.33	1.41
3	P	822	DOC	O5'-C5'	-2.76	1.38	1.44
3	P	822	DOC	C4-N4	2.51	1.42	1.35
3	P	822	DOC	O4'-C4'	2.31	1.49	1.44
3	P	822	DOC	C3'-C2'	-2.11	1.48	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	822	DOC	C2'-C1'-N1	11.62	134.37	112.48
3	P	822	DOC	O4'-C4'-C5'	5.87	119.17	109.52
3	P	822	DOC	C2-N3-C4	4.16	120.56	116.34
3	P	822	DOC	O4'-C1'-C2'	-3.86	102.49	106.67
3	P	822	DOC	C4'-O4'-C1'	-3.85	106.18	109.81

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	P	822	DOC	O4'-C1'-N1-C6

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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	$\# Z > 2$
7	1RY	A	604[B]	6	22,29,29	1.41	4 (18%)	28,45,45	1.73	8 (28%)
7	1RY	A	604[A]	6	22,29,29	1.37	4 (18%)	28,45,45	1.56	6 (21%)
5	SO4	A	602	-	4,4,4	0.19	0	6,6,6	0.21	0
5	SO4	P	901	-	4,4,4	0.17	0	6,6,6	0.29	0
5	SO4	A	601	-	4,4,4	0.24	0	6,6,6	0.21	0
5	SO4	T	801	-	4,4,4	0.20	0	6,6,6	0.17	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	1RY	A	604[B]	6	-	7/19/31/31	0/2/2/2
7	1RY	A	604[A]	6	-	4/19/31/31	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	604[B]	1RY	CAV-NAN	-3.80	1.30	1.38
7	A	604[A]	1RY	CAV-NAN	-3.59	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	604[B]	1RY	CAX-NAY	-2.53	1.41	1.49
7	A	604[B]	1RY	OAP-CAX	-2.48	1.36	1.42
7	A	604[B]	1RY	CAM-SAS	-2.48	1.73	1.81
7	A	604[A]	1RY	CAM-SAS	-2.43	1.74	1.81
7	A	604[A]	1RY	CAX-NAY	-2.11	1.43	1.49
7	A	604[A]	1RY	OAP-CAX	-2.10	1.37	1.42

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	604[B]	1RY	CAU-CAT-NAA	-4.38	117.87	121.47
7	A	604[A]	1RY	CAU-CAT-NAA	-3.54	118.56	121.47
7	A	604[A]	1RY	NAA-CAT-NAN	3.35	121.76	117.03
7	A	604[B]	1RY	NAA-CAT-NAN	3.23	121.60	117.03
7	A	604[B]	1RY	PBB-OAQ-PAZ	-3.13	122.10	132.83
7	A	604[A]	1RY	PBB-OAQ-PAZ	-2.99	122.57	132.83
7	A	604[B]	1RY	OAF-PAZ-OAC	2.47	117.09	107.64
7	A	604[A]	1RY	CAX-CAM-SAS	2.40	109.72	104.03
7	A	604[B]	1RY	OAO-PBA-OAH	2.31	118.09	109.07
7	A	604[B]	1RY	CAX-CAM-SAS	2.26	109.40	104.03
7	A	604[B]	1RY	FAJ-CAU-CAK	2.23	121.89	117.51
7	A	604[A]	1RY	OAF-PAZ-OAC	2.15	115.84	107.64
7	A	604[B]	1RY	OAP-CAW-CAL	-2.06	104.18	109.56
7	A	604[A]	1RY	FAJ-CAU-CAK	2.05	121.54	117.51

There are no chirality outliers.

All (11) torsion outliers are listed below:

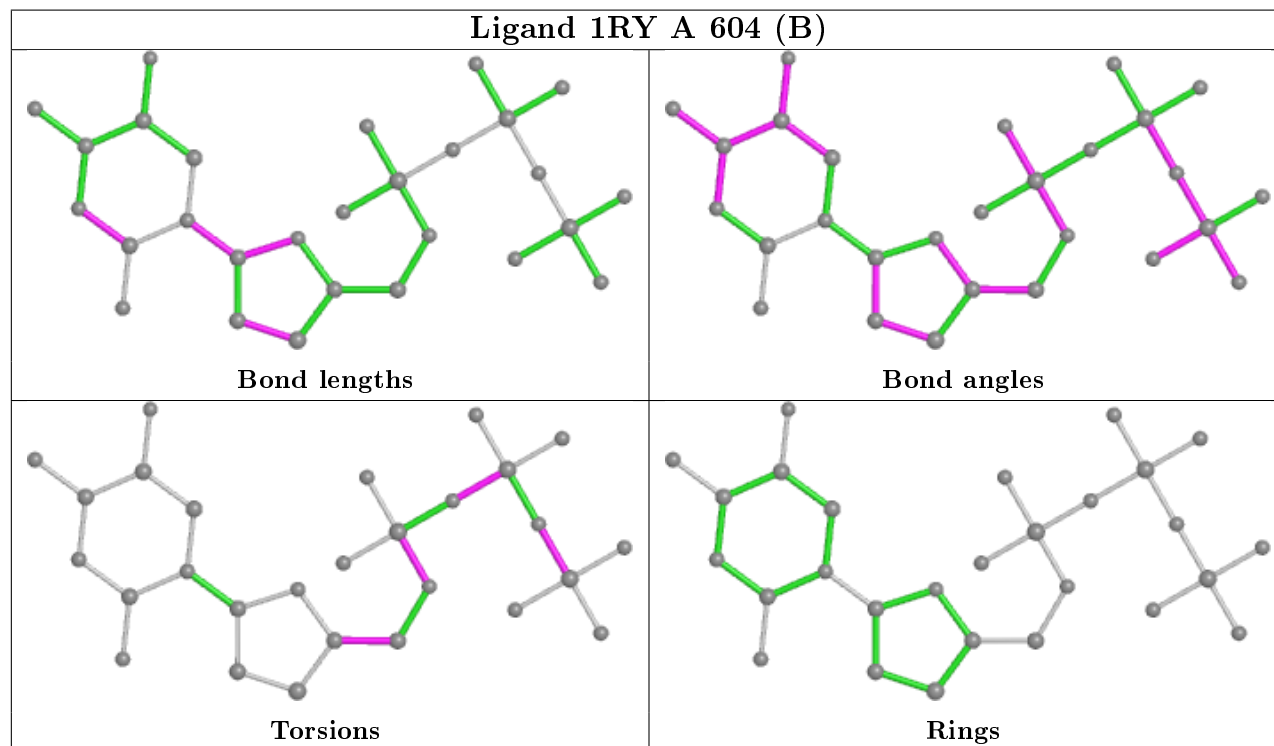
Mol	Chain	Res	Type	Atoms
7	A	604[B]	1RY	PBB-OAQ-PAZ-OAC
7	A	604[B]	1RY	CAL-OAO-PBA-OAH
7	A	604[A]	1RY	PBB-OAQ-PAZ-OAF
7	A	604[B]	1RY	CAL-OAO-PBA-OAD
7	A	604[A]	1RY	PBA-OAR-PBB-OAE
7	A	604[B]	1RY	PBA-OAR-PBB-OAE
7	A	604[B]	1RY	OAO-CAL-CAW-SAS
7	A	604[A]	1RY	PBA-OAR-PBB-OAQ
7	A	604[B]	1RY	CAL-OAO-PBA-OAR
7	A	604[B]	1RY	PBA-OAR-PBB-OAI
7	A	604[A]	1RY	PBB-OAR-PBA-OAH

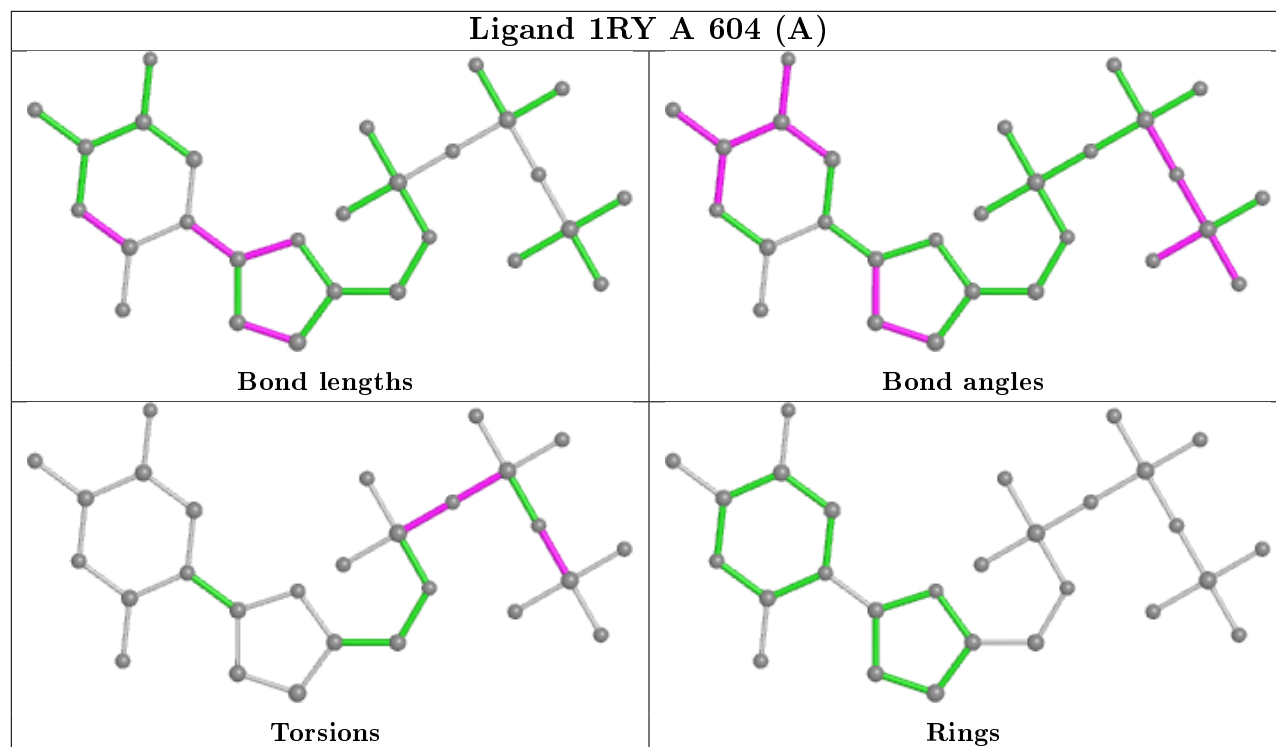
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	604[B]	1RY	2	0
7	A	604[A]	1RY	1	0
5	A	601	SO4	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	548/572 (95%)	-0.19	10 (1%) 68 70	19, 35, 68, 101	0
2	B	398/440 (90%)	0.02	9 (2%) 60 62	20, 46, 78, 99	0
3	P	17/21 (80%)	-0.73	0 100 100	27, 49, 61, 63	0
4	T	22/27 (81%)	-0.25	0 100 100	26, 56, 86, 98	0
All	All	985/1060 (92%)	-0.12	19 (1%) 66 69	19, 39, 74, 101	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	95	PRO	3.7
1	A	62	ALA	3.3
1	A	289	LEU	3.2
1	A	67	ASP	3.2
1	A	133	PRO	3.0
2	B	358	ARG	2.8
2	B	233	GLU	2.7
2	B	237	ASP	2.7
2	B	212	TRP	2.5
2	B	311	LYS	2.5
1	A	26	LEU	2.3
1	A	32	LYS	2.2
2	B	5	ILE	2.2
1	A	449	GLU	2.2
2	B	178	ILE	2.2
1	A	68	SER	2.2
2	B	360	ALA	2.1
1	A	70	LYS	2.1
1	A	22	LYS	2.0

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

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	0.17	27,32,41,42	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

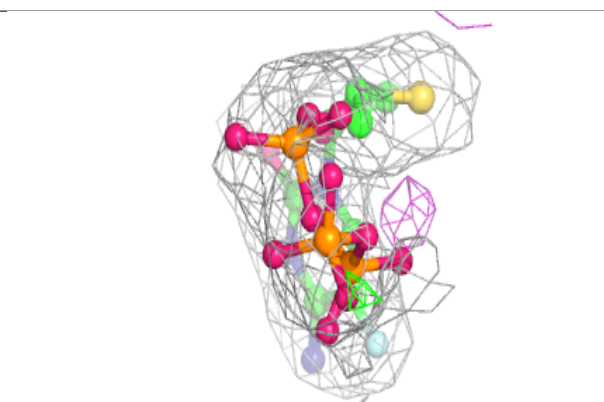
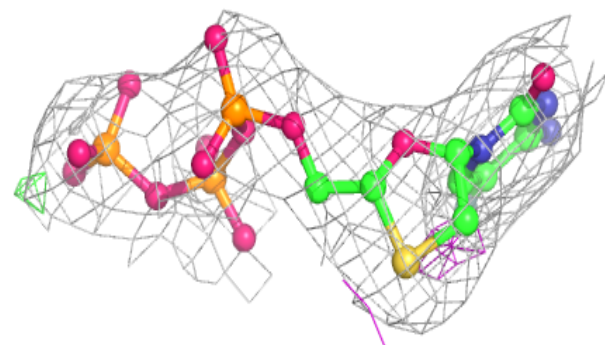
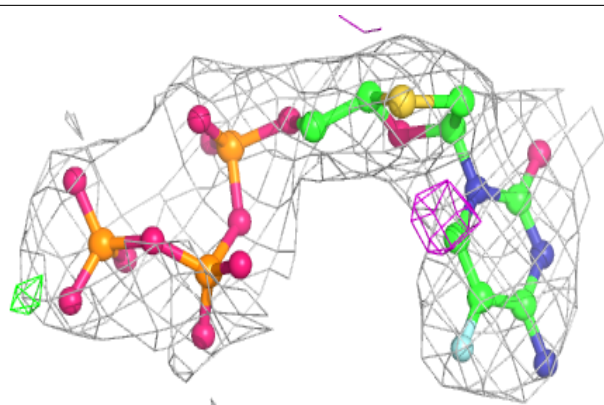
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	SO4	P	901	5/5	0.86	0.32	67,73,85,100	0
5	SO4	T	801	5/5	0.86	0.34	66,71,92,101	0
5	SO4	A	602	5/5	0.94	0.11	55,64,81,82	0
7	1RY	A	604[A]	28/28	0.95	0.15	30,34,48,49	28
7	1RY	A	604[B]	28/28	0.95	0.15	31,34,48,49	28
6	MG	A	603	1/1	0.96	0.08	41,41,41,41	0
5	SO4	A	601	5/5	0.97	0.11	35,38,46,49	0

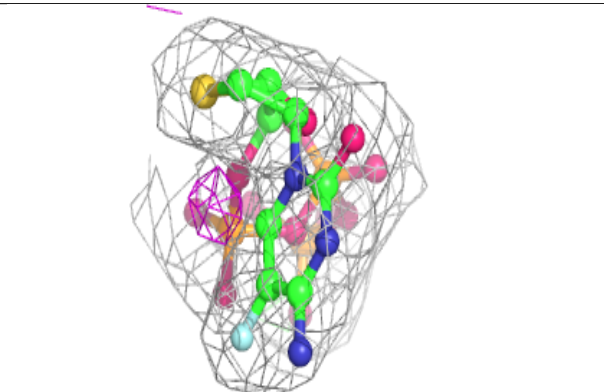
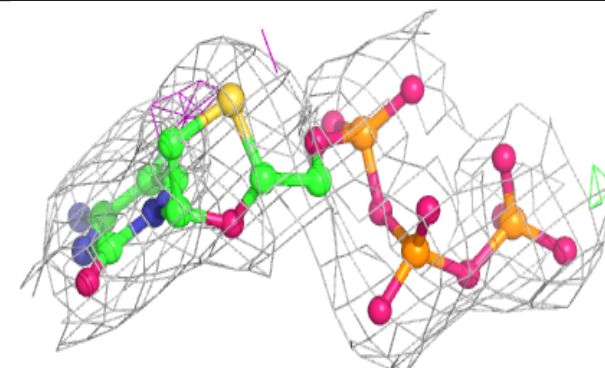
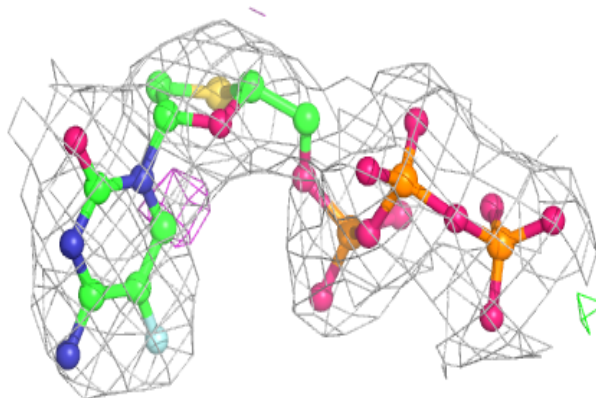
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 1RY A 604 (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 1RY A 604 (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

There are no such residues in this entry.