



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 19, 2022 – 04:15 PM JST

PDB ID : 7Y7P  
Title : QDE-1 in complex with RNA template, RNA primer and AMPNPP  
Authors : Cui, R.X.; Gan, J.H.; Ma, J.B.  
Deposited on : 2022-06-22  
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](mailto: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>.

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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 : 2.30  
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) : 2.30

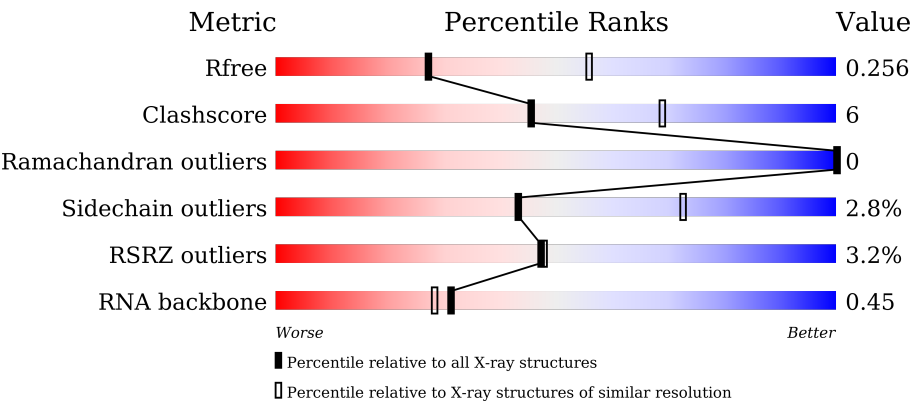
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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 <sub>free</sub>	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)
RNA backbone	3102	1159 (3.00-2.40)

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  $\geq 3$ , 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	1026	<div><div>2%</div><div><div></div><div>76%</div><div>15%</div><div>9%</div></div></div>
1	B	1026	<div><div>3%</div><div><div></div><div>75%</div><div>13%</div><div>12%</div></div></div>
2	C	14	<div><div>14%</div><div><div></div><div>21%</div><div>43%</div><div>14%</div><div>21%</div></div></div>
2	E	14	<div><div>14%</div><div><div></div><div>36%</div><div>43%</div><div>21%</div></div></div>

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Mol	Chain	Length	Quality of chain
3	D	7	<div><div></div><div>14%</div><div>86%</div><div>14%</div></div>
3	J	7	<div><div></div><div>29%</div><div>29%</div><div>43%</div><div>14%</div><div>14%</div></div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 15042 atoms, of which 18 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 RNA-dependent RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	934	Total	C	N	O	S	0	0	0
			7155	4577	1226	1320	32			
1	B	908	Total	C	N	O	S	0	0	0
			6905	4410	1187	1275	33			

- Molecule 2 is a RNA chain called RNA (5'-R(\*GP\*AP\*A\*CP\*UP\*AP\*UP\*GP\*GP\*UP\*C P\*GP\*GP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	11	Total	C	N	O	P	0	0	0
			231	104	42	75	10			
2	E	11	Total	C	N	O	P	0	0	0
			231	104	42	75	10			

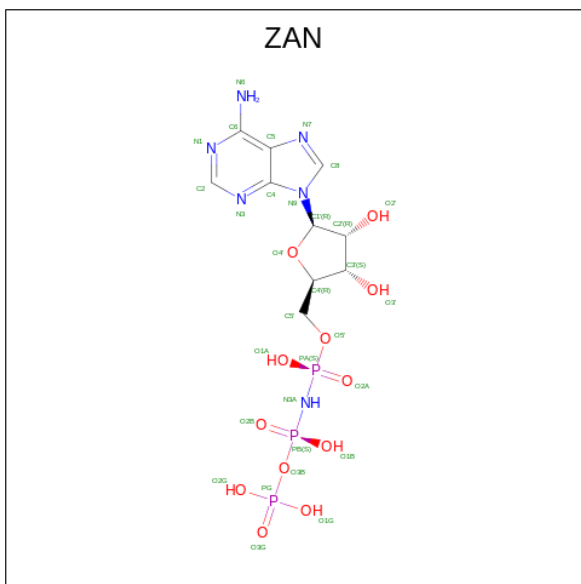
- Molecule 3 is a RNA chain called RNA (5'-R(\*UP\*CP\*CP\*GP\*AP\*CP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	7	Total	C	N	O	P	0	0	0
			142	65	24	47	6			
3	J	6	Total	C	N	O	P	0	0	0
			125	56	22	41	6			

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

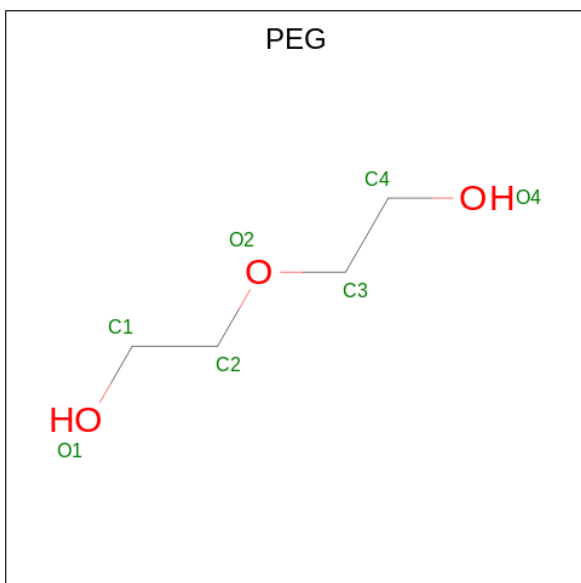
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Ca	0	0
			3	3		
4	B	3	Total	Ca	0	0
			3	3		
4	C	1	Total	Ca	0	0
			1	1		

- Molecule 5 is 5'-O-[(S)-hydroxy{[(S)-hydroxy(phosphonooxy)phosphoryl]amino}phosphoryl]adenosine (three-letter code: ZAN) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



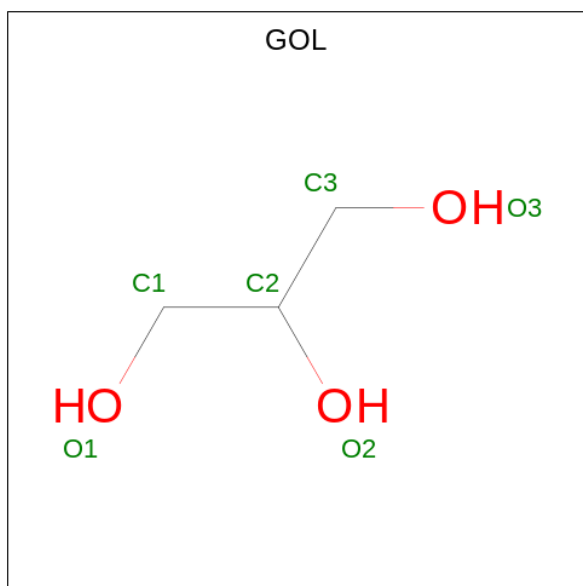
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	H	O	0	0
			14	3	8	3		

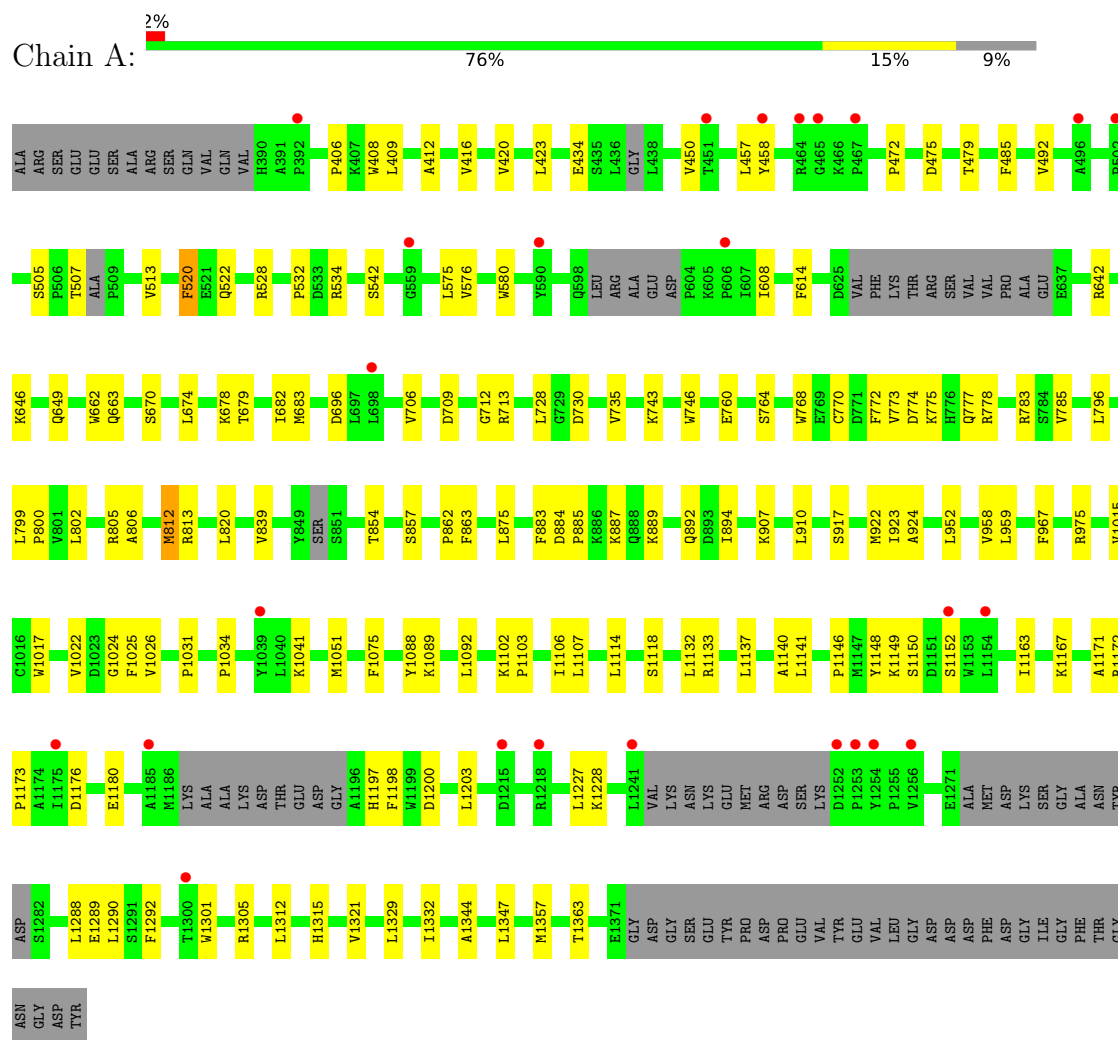
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	70	Total	O	0	0
			70	70		
8	B	67	Total	O	0	0
			67	67		
8	C	6	Total	O	0	0
			6	6		
8	D	2	Total	O	0	0
			2	2		
8	E	6	Total	O	0	0
			6	6		
8	J	2	Total	O	0	0
			2	2		

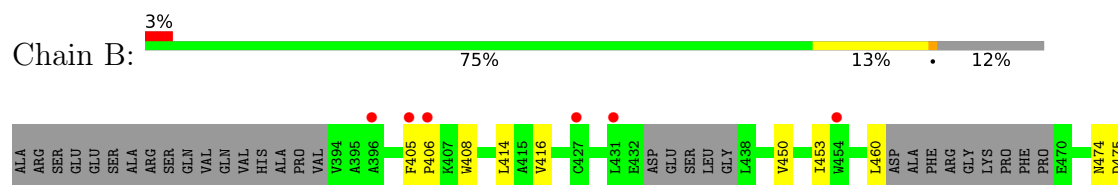
### 3 Residue-property plots

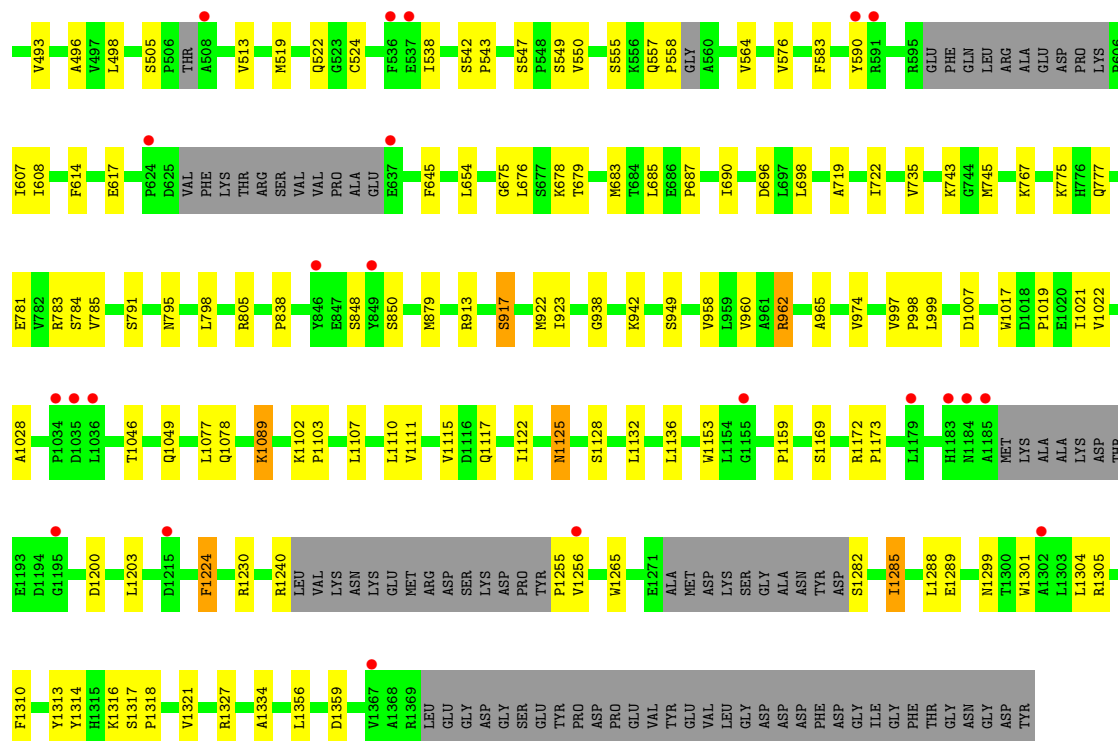
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

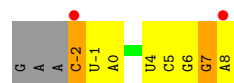
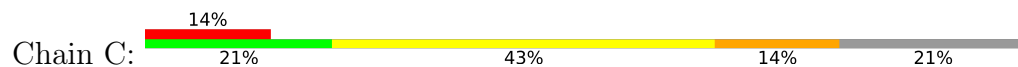


#### • Molecule 1: RNA-dependent RNA polymerase





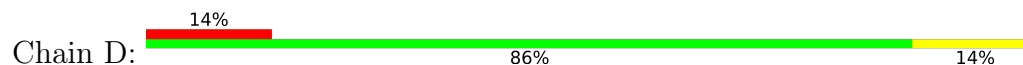
• Molecule 2: RNA (5'-R(\*GP\*AP\*A\*CP\*UP\*AP\*UP\*GP\*GP\*UP\*CP\*GP\*GP\*A)-3')



• Molecule 2: RNA (5'-R(\*GP\*AP\*A\*CP\*UP\*AP\*UP\*GP\*GP\*UP\*CP\*GP\*GP\*A)-3')



• Molecule 3: RNA (5'-R(\*UP\*CP\*CP\*GP\*AP\*CP\*C)-3')



• Molecule 3: RNA (5'-R(\*UP\*CP\*CP\*GP\*AP\*CP\*C)-3')







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.95Å 120.20Å 114.86Å 90.00° 109.62° 90.00°	Depositor
Resolution (Å)	29.62 – 2.70 29.62 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.0 (29.62-2.70) 98.0 (29.62-2.70)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.01 (at 2.72Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.223 , 0.254 0.226 , 0.256	Depositor DCC
$R_{free}$ test set	3462 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.3	Xtrriage
Anisotropy	0.384	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 55.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15042	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.28 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.6473e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: ZAN, CA, PEG, GOL

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	0.48	0/7338	0.63	0/9983
1	B	0.51	0/7080	0.64	0/9641
2	C	0.46	0/258	0.83	0/401
2	E	0.17	0/258	0.75	0/401
3	D	0.15	0/157	0.68	0/242
3	J	0.18	0/138	0.80	0/212
All	All	0.49	0/15229	0.65	0/20880

There are no bond length outliers.

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	7155	0	6706	93	0
1	B	6905	0	6419	86	0
2	C	231	0	116	3	0
2	E	231	0	116	1	0
3	D	142	0	77	1	0
3	J	125	0	66	2	0
4	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	3	0	0	1	0
4	C	1	0	0	0	0
5	A	31	0	17	1	0
5	B	31	0	16	0	0
6	B	7	10	10	0	0
7	B	6	8	8	0	0
8	A	70	0	0	3	0
8	B	67	0	0	1	0
8	C	6	0	0	0	0
8	D	2	0	0	0	0
8	E	6	0	0	0	0
8	J	2	0	0	0	0
All	All	15024	18	13551	181	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 6.

All (181) 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:1088:TYR:CD2	1:A:1088:TYR:CZ	2.37	1.06
1:A:1329:LEU:HA	1:A:1332:ILE:HD12	1.66	0.78
1:B:460:LEU:C	1:B:460:LEU:HD13	2.04	0.77
1:A:1227:LEU:HD11	1:A:1305:ARG:HG3	1.66	0.76
1:B:576:VAL:HG22	1:B:576:VAL:O	1.86	0.75
1:B:1288:LEU:HD23	1:B:1301:TRP:HE3	1.54	0.73
1:A:646:LYS:H	1:A:649:GLN:HE21	1.35	0.71
1:B:543:PRO:HB3	1:B:564:VAL:HG21	1.74	0.70
1:A:735:VAL:HG12	1:A:785:VAL:HG12	1.75	0.68
1:B:679:THR:HB	1:B:781:GLU:HB3	1.76	0.68
1:B:1007:ASP:OD2	4:B:1505:CA:CA	1.70	0.68
1:A:412:ALA:HB1	1:A:416:VAL:HG22	1.77	0.67
1:A:1132:LEU:O	1:A:1132:LEU:HD12	1.96	0.65
1:B:522:GLN:HB3	1:B:678:LYS:HB3	1.78	0.64
1:A:910:LEU:HD22	1:A:1163:ILE:HG23	1.78	0.64
1:A:1133:ARG:HA	1:A:1137:LEU:HD12	1.78	0.63
1:B:1288:LEU:HD23	1:B:1301:TRP:CE3	2.34	0.62
1:A:907:LYS:O	1:A:1167:LYS:HE3	2.01	0.60
1:A:959:LEU:HG	1:A:1022:VAL:HG22	1.84	0.59
1:B:498:LEU:CD2	1:B:513:VAL:HG22	2.31	0.59
1:B:1089:LYS:HA	1:B:1107:LEU:HD13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:549:SER:HB3	1:B:607:ILE:HD11	1.83	0.59
1:B:460:LEU:C	1:B:460:LEU:CD1	2.72	0.58
1:B:942:LYS:HD2	1:B:949:SER:HB3	1.87	0.57
1:A:409:LEU:HD21	1:A:420:VAL:HG11	1.86	0.57
1:A:1146:PRO:HD2	1:A:1149:LYS:HG3	1.86	0.57
1:B:1282:SER:HA	1:B:1285:ILE:HD13	1.85	0.57
1:B:496:ALA:HB3	1:B:538:ILE:HG22	1.87	0.56
1:A:674:LEU:HD21	1:A:743:LYS:HD3	1.88	0.56
1:B:958:VAL:HG23	1:B:974:VAL:HG23	1.87	0.56
1:B:547:SER:O	1:B:550:VAL:HG12	2.05	0.56
1:B:1200:ASP:HB3	1:B:1203:LEU:HG	1.86	0.56
1:B:538:ILE:HG12	1:B:614:PHE:HE2	1.71	0.56
1:B:791:SER:HA	1:B:917:SER:O	2.05	0.56
1:A:774:ASP:OD1	1:A:775:LYS:N	2.38	0.55
1:A:682:ILE:HG22	1:A:683:MET:HG2	1.88	0.55
1:B:735:VAL:HG12	1:B:785:VAL:HG12	1.89	0.55
1:A:1148:TYR:C	1:A:1150:SER:H	2.09	0.55
1:B:1117:GLN:HG3	1:B:1122:ILE:HB	1.89	0.55
1:A:773:VAL:O	1:A:778:ARG:NH1	2.39	0.54
1:A:679:THR:HG22	1:A:783:ARG:HB2	1.88	0.54
1:B:958:VAL:HG23	1:B:974:VAL:CG2	2.38	0.54
1:A:709:ASP:OD1	1:A:764:SER:HB2	2.07	0.53
1:B:543:PRO:HD2	1:B:1077:LEU:HD22	1.90	0.53
1:A:1228:LYS:HG2	1:A:1312:LEU:HD11	1.90	0.53
1:A:854:THR:HG21	1:A:862:PRO:HG3	1.91	0.53
1:B:942:LYS:HD2	1:B:949:SER:CB	2.38	0.53
1:A:875:LEU:HG	1:A:894:ILE:HG21	1.90	0.52
1:B:1282:SER:O	1:B:1285:ILE:HG12	2.09	0.52
1:B:576:VAL:O	1:B:576:VAL:CG2	2.57	0.52
1:B:683:MET:SD	1:B:685:LEU:HD11	2.50	0.51
1:B:1289:GLU:HA	1:B:1299:ASN:ND2	2.25	0.51
1:A:580:TRP:HB3	1:A:614:PHE:HB3	1.93	0.51
1:A:770:CYS:SG	1:A:777:GLN:NE2	2.83	0.51
1:A:662:TRP:CZ3	1:A:663:GLN:HG2	2.46	0.51
1:A:799:LEU:HB2	1:A:800:PRO:HD3	1.92	0.51
1:B:745:MET:HE2	1:B:923:ILE:HD11	1.93	0.51
1:A:952:LEU:C	1:A:952:LEU:HD12	2.31	0.51
1:B:1132:LEU:HD12	1:B:1136:LEU:HB2	1.93	0.50
1:B:1224:PHE:HE2	1:B:1304:LEU:HD11	1.77	0.50
1:B:1282:SER:HA	1:B:1285:ILE:CD1	2.42	0.50
1:B:1153:TRP:CD2	1:B:1159:PRO:HG3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:674:LEU:HD12	1:A:768:TRP:HZ3	1.77	0.50
1:A:713:ARG:HB2	1:A:760:GLU:OE2	2.11	0.50
1:A:1203:LEU:HD13	1:A:1329:LEU:HD22	1.92	0.50
1:B:805:ARG:NE	1:B:1028:ALA:HB2	2.26	0.50
1:A:805:ARG:O	1:A:1026:VAL:HG12	2.12	0.50
1:B:557:GLN:N	1:B:558:PRO:HD3	2.28	0.49
1:B:1125:ASN:H	1:B:1128:SER:HB2	1.77	0.49
1:A:922:MET:O	1:A:923:ILE:HD13	2.12	0.49
1:A:1347:LEU:HD23	1:B:1334:ALA:HB3	1.93	0.49
1:A:406:PRO:HG2	1:A:409:LEU:HB2	1.94	0.49
1:B:1289:GLU:HA	1:B:1299:ASN:HD22	1.77	0.49
1:A:802:LEU:HB3	1:A:812:MET:HE1	1.95	0.49
1:B:590:TYR:HA	1:B:608:ILE:HA	1.95	0.49
1:A:1172:ARG:N	1:A:1173:PRO:HD2	2.28	0.48
1:B:1313:TYR:HB3	1:B:1317:SER:HB2	1.95	0.48
1:B:783:ARG:HD2	3:J:6:C:H4'	1.96	0.48
1:B:1019:PRO:O	1:B:1022:VAL:N	2.46	0.48
1:A:883:PHE:CZ	1:A:1203:LEU:HD11	2.48	0.48
1:A:528:ARG:NH1	8:A:1607:HOH:O	2.38	0.48
1:A:485:PHE:HA	1:A:492:VAL:HG13	1.96	0.47
1:A:743:LYS:HB3	1:A:743:LYS:HE3	1.61	0.47
1:A:820:LEU:HD21	1:A:1171:ALA:HB2	1.95	0.47
1:A:770:CYS:HB3	1:A:772:PHE:CE1	2.49	0.47
1:A:883:PHE:HZ	1:A:1203:LEU:HD11	1.79	0.47
1:A:1344:ALA:HB1	1:B:1327:ARG:HD2	1.96	0.47
1:A:542:SER:HB3	1:A:608:ILE:HG23	1.97	0.47
1:A:839:VAL:HG22	1:A:1363:THR:HG23	1.96	0.47
1:B:416:VAL:HG22	1:B:453:ILE:CD1	2.44	0.47
1:B:958:VAL:HG12	1:B:1017:TRP:HB3	1.96	0.47
1:B:938:GLY:HA3	8:B:1625:HOH:O	2.14	0.46
1:A:576:VAL:HG23	1:A:576:VAL:O	2.15	0.46
1:B:783:ARG:NH1	1:B:784:SER:HB2	2.31	0.46
1:B:960:VAL:HG21	1:B:999:LEU:HD21	1.97	0.46
1:A:796:LEU:HD21	1:A:910:LEU:HB2	1.97	0.46
1:B:679:THR:CB	1:B:781:GLU:HB3	2.43	0.46
1:A:1092:LEU:HD21	1:A:1103:PRO:HB2	1.97	0.46
3:J:3:C:O2'	3:J:4:G:H5''	2.15	0.46
1:B:719:ALA:HA	1:B:722:ILE:HD12	1.97	0.46
1:B:1046:THR:HG23	1:B:1049:GLN:H	1.81	0.46
1:A:1344:ALA:CB	1:B:1327:ARG:HD2	2.46	0.46
1:A:1357:MET:HB3	1:B:1359:ASP:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:884:ASP:HB3	1:A:887:LYS:HB2	1.98	0.45
1:B:838:PRO:HA	1:B:879:MET:CE	2.47	0.45
1:A:1148:TYR:C	1:A:1150:SER:N	2.70	0.45
1:B:687:PRO:HA	1:B:690:ILE:HD12	1.99	0.45
1:B:493:VAL:HG12	1:B:519:MET:HG3	1.97	0.45
1:B:550:VAL:HG13	1:B:555:SER:OG	2.16	0.45
1:B:1102:LYS:N	1:B:1103:PRO:HD2	2.31	0.45
2:E:1:U:H2'	2:E:2:G:C8	2.52	0.45
1:A:967:PHE:CD1	1:A:1031:PRO:HG3	2.51	0.45
1:A:522:GLN:HB3	1:A:678:LYS:HB3	1.99	0.45
1:A:534:ARG:NH1	8:A:1601:HOH:O	2.31	0.45
1:A:696:ASP:HB3	1:A:706:VAL:HG13	1.98	0.45
1:A:806:ALA:HA	1:A:1024:GLY:O	2.17	0.45
1:A:1075:PHE:HE2	1:A:1118:SER:HA	1.82	0.45
1:A:884:ASP:OD1	1:A:885:PRO:HD2	2.17	0.44
1:B:997:VAL:HG13	1:B:998:PRO:HD2	1.98	0.44
1:A:1288:LEU:HD23	1:A:1301:TRP:HE3	1.82	0.44
1:B:922:MET:HE3	1:B:962:ARG:HD2	1.99	0.44
1:B:696:ASP:O	1:B:698:LEU:HD12	2.17	0.44
1:A:958:VAL:HG12	1:A:1017:TRP:HB3	1.99	0.44
1:B:838:PRO:HA	1:B:879:MET:HE3	1.99	0.44
1:B:913:ARG:HA	1:B:913:ARG:HD2	1.83	0.43
1:A:479:THR:HG21	1:A:520:PHE:HZ	1.83	0.43
1:B:654:LEU:HA	1:B:777:GLN:HE22	1.83	0.43
1:A:406:PRO:HB2	1:A:408:TRP:CD1	2.53	0.43
1:A:812:MET:HG3	1:A:813:ARG:N	2.32	0.43
1:A:923:ILE:HG22	1:A:924:ALA:N	2.33	0.43
1:A:1321:VAL:HG12	1:A:1329:LEU:HD11	2.00	0.43
1:A:1102:LYS:N	1:A:1103:PRO:HD2	2.33	0.43
1:A:889:LYS:HB3	1:A:1198:PHE:CE1	2.54	0.43
1:A:1140:ALA:C	1:A:1141:LEU:HD23	2.39	0.43
1:B:414:LEU:HD12	1:B:576:VAL:CG2	2.48	0.43
1:A:1089:LYS:HG3	1:A:1107:LEU:HB3	1.99	0.43
1:A:1290:LEU:HD22	1:A:1292:PHE:CE2	2.54	0.43
5:A:1504:ZAN:H7	5:A:1504:ZAN:H14	2.00	0.43
1:B:743:LYS:HE2	1:B:767:LYS:HE3	1.99	0.43
1:B:583:PHE:HE2	1:B:676:LEU:HD11	1.84	0.43
1:A:917:SER:HA	1:A:1015:VAL:O	2.18	0.43
1:A:1133:ARG:O	1:A:1137:LEU:HB2	2.19	0.43
1:B:962:ARG:O	1:B:965:ALA:HB2	2.19	0.43
1:A:1290:LEU:HD22	1:A:1292:PHE:HE2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:542:SER:HB3	1:B:608:ILE:HG23	2.00	0.42
1:B:406:PRO:HG2	1:B:408:TRP:HE1	1.84	0.42
1:A:450:VAL:HG11	1:A:472:PRO:HD2	2.02	0.42
1:A:805:ARG:HB2	1:A:1025:PHE:CE2	2.54	0.42
1:A:1200:ASP:HB3	1:A:1203:LEU:HB2	2.02	0.42
1:A:423:LEU:HD11	1:A:458:TYR:HE1	1.84	0.42
1:A:1197:HIS:CD2	1:A:1197:HIS:N	2.88	0.42
1:B:1021:ILE:N	1:B:1021:ILE:HD13	2.34	0.42
2:C:-2:C:H3'	2:C:-1:U:H5''	2.02	0.42
1:B:1316:LYS:C	1:B:1318:PRO:HD3	2.40	0.42
1:A:485:PHE:HB3	1:A:532:PRO:HB2	2.00	0.42
1:A:1289:GLU:O	1:A:1290:LEU:C	2.58	0.42
1:A:420:VAL:HG23	1:A:457:LEU:HD11	2.00	0.41
1:A:712:GLY:O	1:A:746:TRP:HA	2.21	0.41
1:B:1089:LYS:HB2	1:B:1107:LEU:HB3	2.02	0.41
1:B:1310:PHE:HA	1:B:1321:VAL:HG11	2.01	0.41
1:A:728:LEU:HD11	1:A:785:VAL:HG11	2.03	0.41
1:B:1172:ARG:N	1:B:1173:PRO:HD2	2.35	0.41
1:B:1265:TRP:CE2	1:B:1305:ARG:HD2	2.54	0.41
1:B:1314:TYR:O	1:B:1318:PRO:HG3	2.20	0.41
1:A:575:LEU:O	1:A:576:VAL:HG22	2.19	0.41
1:B:942:LYS:CG	1:B:949:SER:HB3	2.51	0.41
1:A:485:PHE:CD2	1:A:492:VAL:HG22	2.56	0.41
1:B:405:PHE:HA	1:B:406:PRO:HD3	1.92	0.41
1:A:805:ARG:HB3	1:A:1026:VAL:O	2.21	0.41
1:B:617:GLU:HA	1:B:645:PHE:O	2.21	0.41
1:A:642:ARG:HD2	8:A:1601:HOH:O	2.20	0.41
1:A:1133:ARG:HD2	1:A:1141:LEU:HA	2.04	0.40
1:B:1224:PHE:HD2	1:B:1224:PHE:HA	1.82	0.40
1:B:406:PRO:HG2	1:B:408:TRP:NE1	2.37	0.40
1:B:524:CYS:HB2	1:B:675:GLY:O	2.21	0.40
1:B:1111:VAL:O	1:B:1115:VAL:HG23	2.21	0.40
2:C:7:G:H1	3:D:2:C:H42	1.68	0.40
1:A:1114:LEU:HD23	1:A:1114:LEU:HA	1.89	0.40
2:C:4:U:H2'	2:C:5:C:O4'	2.21	0.40
1:A:1034:PRO:HG3	1:A:1106:ILE:HA	2.04	0.40
1:B:795:ASN:H	1:B:798:LEU:HD12	1.87	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	916/1026 (89%)	899 (98%)	17 (2%)	0	100	100
1	B	888/1026 (86%)	868 (98%)	20 (2%)	0	100	100
All	All	1804/2052 (88%)	1767 (98%)	37 (2%)	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	721/894 (81%)	702 (97%)	19 (3%)	46	75
1	B	689/894 (77%)	668 (97%)	21 (3%)	41	70
All	All	1410/1788 (79%)	1370 (97%)	40 (3%)	43	73

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

Mol	Chain	Res	Type
1	A	434	GLU
1	A	475	ASP
1	A	505	SER
1	A	507	THR
1	A	513	VAL
1	A	520	PHE
1	A	670	SER
1	A	730	ASP

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Mol	Chain	Res	Type
1	A	812	MET
1	A	857	SER
1	A	863	PHE
1	A	892	GLN
1	A	975	ARG
1	A	1041	LYS
1	A	1051	MET
1	A	1152	SER
1	A	1176	ASP
1	A	1180	GLU
1	A	1315	HIS
1	B	450	VAL
1	B	474	ASN
1	B	475	ASP
1	B	505	SER
1	B	775	LYS
1	B	848	SER
1	B	850	SER
1	B	917	SER
1	B	962	ARG
1	B	1078	GLN
1	B	1089	LYS
1	B	1110	LEU
1	B	1125	ASN
1	B	1169	SER
1	B	1224	PHE
1	B	1230	ARG
1	B	1240	ARG
1	B	1255	PRO
1	B	1256	VAL
1	B	1285	ILE
1	B	1356	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	649	GLN
1	A	777	GLN
1	A	827	GLN
1	A	899	GLN
1	A	1184	ASN
1	A	1197	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	10/14 (71%)	4 (40%)	2 (20%)
2	E	10/14 (71%)	3 (30%)	1 (10%)
3	D	6/7 (85%)	0	0
3	J	5/7 (71%)	2 (40%)	0
All	All	31/42 (73%)	9 (29%)	3 (9%)

All (9) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	0	A
2	C	6	G
2	C	7	G
2	C	8	A
2	E	0	A
2	E	5	C
2	E	7	G
3	J	3	C
3	J	5	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	C	-2	C
2	C	7	G
2	E	-2	C

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 7 are 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$
7	GOL	B	1502	-	5,5,5	0.08	0	5,5,5	0.25	0
5	ZAN	B	1506	4	29,33,33	1.12	4 (13%)	34,52,52	1.35	4 (11%)
6	PEG	B	1501	-	6,6,6	0.13	0	5,5,5	0.08	0
5	ZAN	A	1504	4	29,33,33	1.43	5 (17%)	34,52,52	1.62	5 (14%)

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	GOL	B	1502	-	-	2/4/4/4	-
5	ZAN	B	1506	4	-	5/15/38/38	0/3/3/3
6	PEG	B	1501	-	-	2/4/4/4	-
5	ZAN	A	1504	4	-	5/15/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1504	ZAN	PB-O2B	3.27	1.51	1.46
5	A	1504	ZAN	PA-O2A	3.23	1.51	1.46
5	B	1506	ZAN	PB-O2B	2.77	1.50	1.46
5	B	1506	ZAN	PA-O2A	2.59	1.50	1.46
5	A	1504	ZAN	C5-C4	2.49	1.47	1.40
5	A	1504	ZAN	PB-O3B	2.40	1.62	1.59
5	B	1506	ZAN	PA-O1A	-2.38	1.50	1.56
5	B	1506	ZAN	PB-O1B	-2.38	1.50	1.56
5	A	1504	ZAN	PA-O1A	-2.01	1.51	1.56

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1504	ZAN	O1A-PA-O2A	4.66	119.68	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1504	ZAN	O1B-PB-O2B	4.37	119.09	109.92
5	B	1506	ZAN	O1B-PB-O2B	4.28	118.90	109.92
5	B	1506	ZAN	O1A-PA-O2A	4.05	118.41	109.92
5	A	1504	ZAN	N3-C2-N1	-3.08	123.87	128.68
5	B	1506	ZAN	O5'-PA-O2A	-2.64	104.07	114.24
5	A	1504	ZAN	PB-O3B-PG	-2.56	123.60	132.62
5	A	1504	ZAN	C4-C5-N7	-2.54	106.75	109.40
5	B	1506	ZAN	C5-C6-N6	2.25	123.78	120.35

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1504	ZAN	PB-N3A-PA-O2A
5	A	1504	ZAN	C5'-O5'-PA-O1A
5	A	1504	ZAN	C5'-O5'-PA-O2A
5	A	1504	ZAN	C3'-C4'-C5'-O5'
5	B	1506	ZAN	PB-N3A-PA-O2A
5	B	1506	ZAN	C5'-O5'-PA-O1A
5	B	1506	ZAN	C5'-O5'-PA-O2A
5	B	1506	ZAN	C3'-C4'-C5'-O5'
7	B	1502	GOL	C1-C2-C3-O3
5	A	1504	ZAN	O4'-C4'-C5'-O5'
5	B	1506	ZAN	O4'-C4'-C5'-O5'
6	B	1501	PEG	O1-C1-C2-O2
7	B	1502	GOL	O2-C2-C3-O3
6	B	1501	PEG	O2-C3-C4-O4

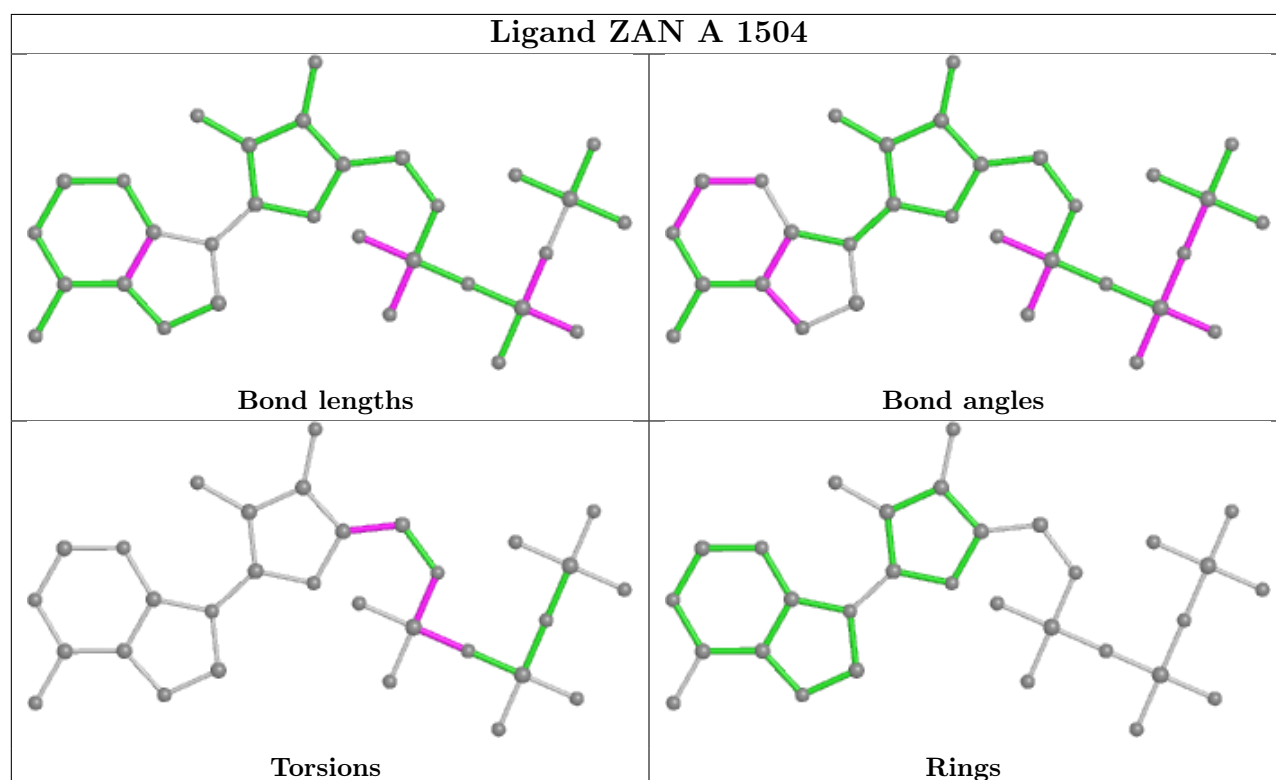
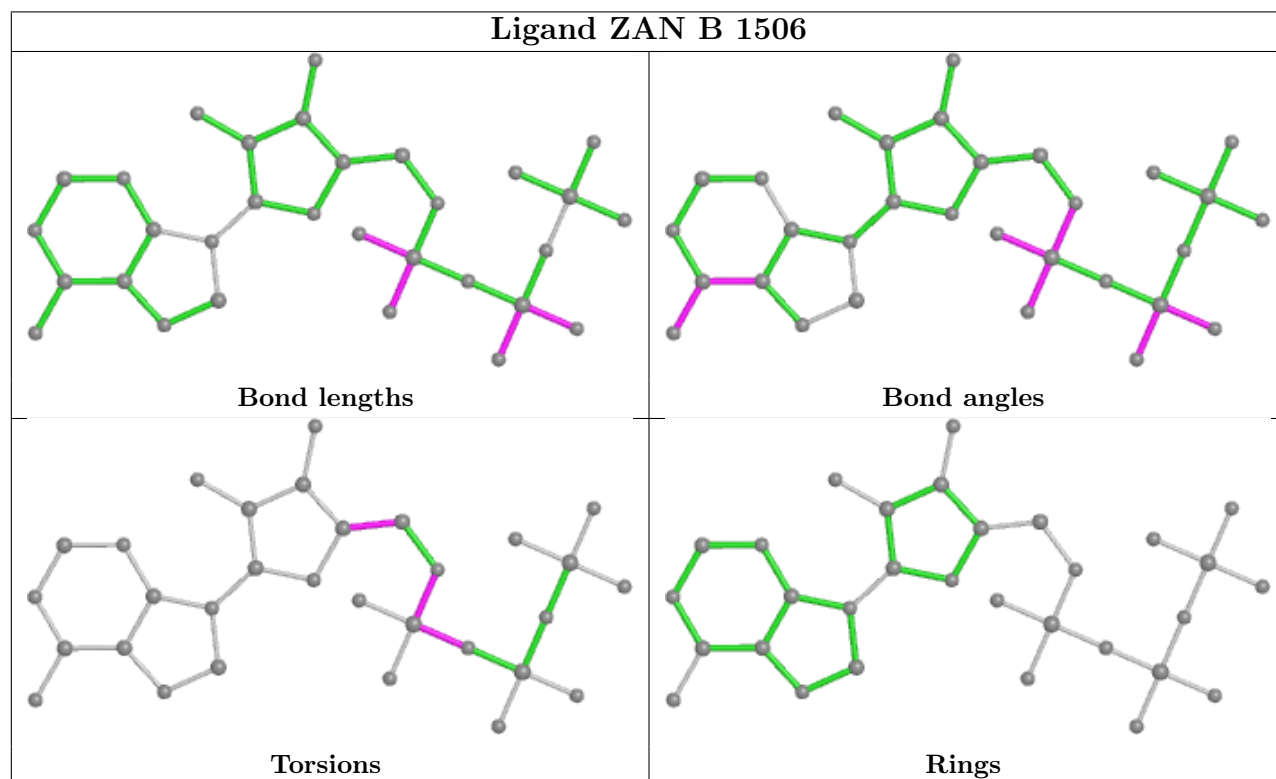
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1504	ZAN	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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	934/1026 (91%)	0.05	25 (2%) 54 55	37, 76, 114, 152	0
1	B	908/1026 (88%)	0.13	28 (3%) 49 49	39, 77, 122, 156	0
2	C	11/14 (78%)	0.34	2 (18%) 1 1	58, 71, 163, 164	0
2	E	11/14 (78%)	0.67	2 (18%) 1 1	64, 78, 169, 172	0
3	D	7/7 (100%)	0.60	1 (14%) 2 1	50, 72, 124, 138	0
3	J	6/7 (85%)	0.88	2 (33%) 0 0	54, 85, 132, 142	0
All	All	1877/2094 (89%)	0.10	60 (3%) 47 48	37, 76, 119, 172	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	8	A	4.4
1	B	1183	HIS	4.4
2	E	7	G	4.2
1	A	1241	LEU	4.1
3	D	1	U	4.1
1	A	1253	PRO	4.0
1	B	1184	ASN	3.8
2	C	8	A	3.7
1	B	1034	PRO	3.7
1	B	431	LEU	3.6
1	B	454	TRP	3.3
1	A	606	PRO	3.2
1	A	1254	TYR	3.1
2	C	-2	C	3.1
1	A	458	TYR	3.1
1	A	451	THR	3.0
1	A	467	PRO	3.0
3	J	2	C	2.9
1	B	405	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	1215	ASP	2.8
1	A	465	GLY	2.8
1	B	1036	LEU	2.7
1	A	1154	LEU	2.7
1	A	1256	VAL	2.7
1	B	1256	VAL	2.7
1	B	536	PHE	2.6
1	B	406	PRO	2.5
1	B	1302	ALA	2.5
1	A	502	PRO	2.5
1	B	624	PRO	2.5
1	A	464	ARG	2.5
1	B	1185	ALA	2.4
1	B	1179	LEU	2.4
1	B	590	TYR	2.4
1	B	846	TYR	2.4
1	B	396	ALA	2.3
1	B	537	GLU	2.3
1	B	1155	GLY	2.3
1	A	1215	ASP	2.3
1	A	590	TYR	2.2
1	A	559	GLY	2.2
1	A	1039	TYR	2.2
1	A	1152	SER	2.2
1	A	496	ALA	2.2
1	B	508	ALA	2.2
1	A	698	LEU	2.2
1	A	1185	ALA	2.2
1	B	427	CYS	2.2
1	A	392	PRO	2.1
1	B	849	TYR	2.1
1	A	1175	ILE	2.1
1	B	637	GLU	2.1
1	A	1300	THR	2.1
1	B	591	ARG	2.1
1	B	1035	ASP	2.1
1	B	1195	GLY	2.1
1	B	1367	VAL	2.0
1	A	1252	ASP	2.0
3	J	3	C	2.0
1	A	1218	ARG	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

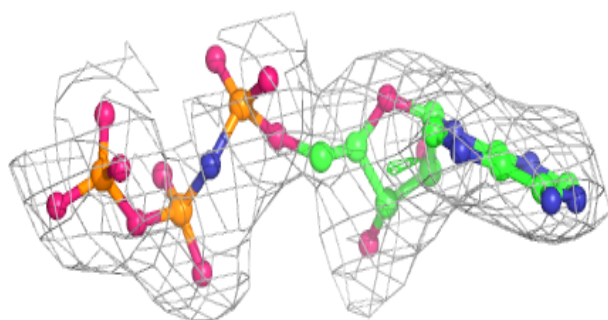
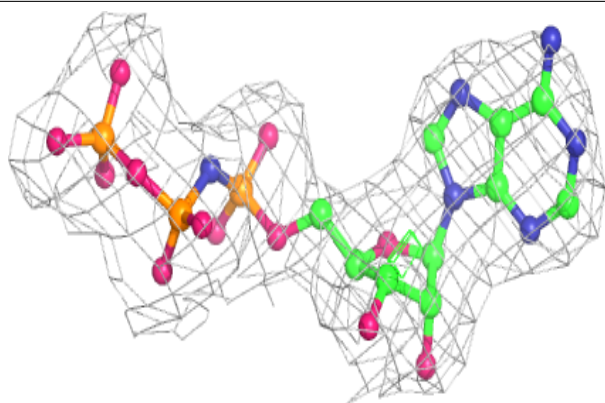
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	GOL	B	1502	6/6	0.88	0.26	63,80,110,110	0
4	CA	C	101	1/1	0.90	0.10	122,122,122,122	0
4	CA	A	1502	1/1	0.92	0.22	85,85,85,85	0
4	CA	B	1504	1/1	0.93	0.19	79,79,79,79	0
6	PEG	B	1501	7/7	0.94	0.33	63,76,88,88	0
5	ZAN	B	1506	31/31	0.96	0.17	41,55,66,81	0
5	ZAN	A	1504	31/31	0.97	0.18	41,52,64,76	0
4	CA	B	1505	1/1	0.98	0.15	51,51,51,51	0
4	CA	A	1503	1/1	0.98	0.09	46,46,46,46	0
4	CA	B	1503	1/1	0.99	0.16	44,44,44,44	0
4	CA	A	1501	1/1	0.99	0.13	42,42,42,42	0

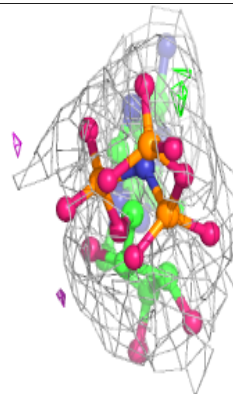
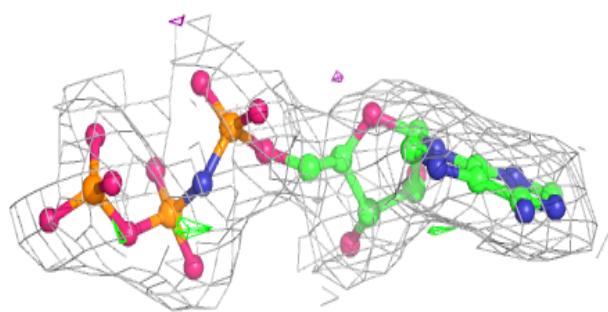
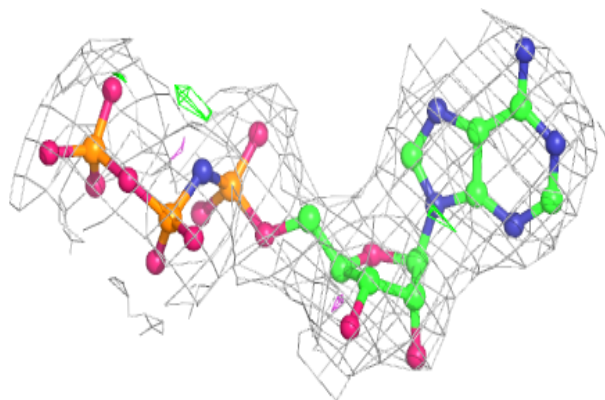
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ZAN B 1506:**

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

**Electron density around ZAN A 1504:**

$2mF_o - DF_c$  (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.