



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 19, 2022 – 04:18 PM JST

PDB ID : 7Y7R
Title : QDE-1 in complex with DNA template, RNA primer and 3'-dGTP
Authors : Cui, R.X.; Gan, J.H.; Ma, J.B.
Deposited on : 2022-06-22
Resolution : 2.10 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 : 4.02b-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

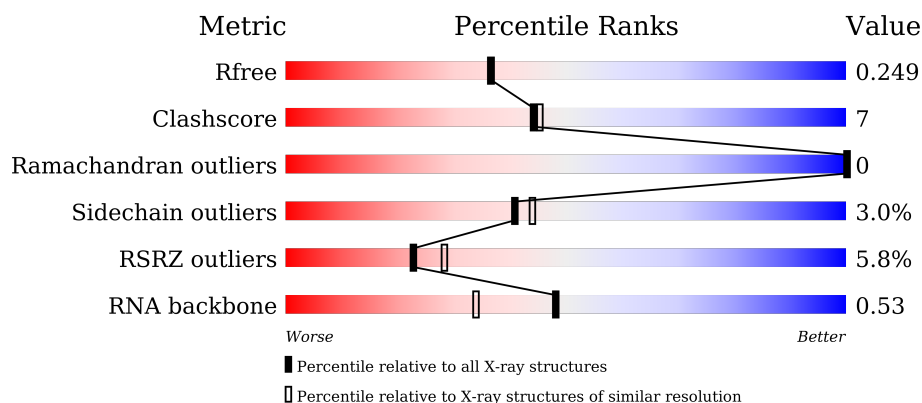
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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.



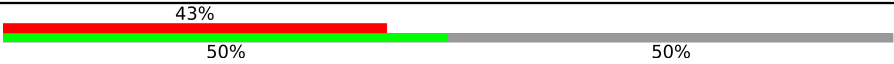

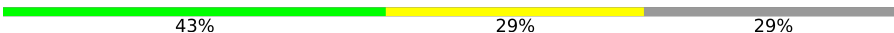
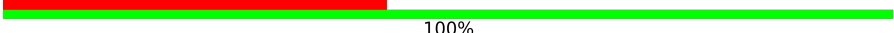
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)
RNA backbone	3102	1000 (2.54-1.66)

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	1026	<div> <div>4%</div> <div>76%</div> <div>15%</div> <div>8%</div> </div>
1	B	1026	<div> <div>6%</div> <div>71%</div> <div>15%</div> <div>13%</div> </div>
2	C	14	<div> <div>7%</div> <div>50%</div> <div>21%</div> <div>29%</div> </div>
2	E	14	<div> <div>14%</div> <div>64%</div> <div>21%</div> <div>14%</div> </div>

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Mol	Chain	Length	Quality of chain
2	H	14	 43% 50% 50%
3	D	7	 71% 29%
3	F	7	 43% 29% 29%
3	G	7	 43% 100%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 16197 atoms, of which 26 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	941	Total	C	N	O	S	0	6	0
			7567	4838	1315	1377	37			
1	B	897	Total	C	N	O	S	0	5	0
			7024	4458	1239	1294	33			

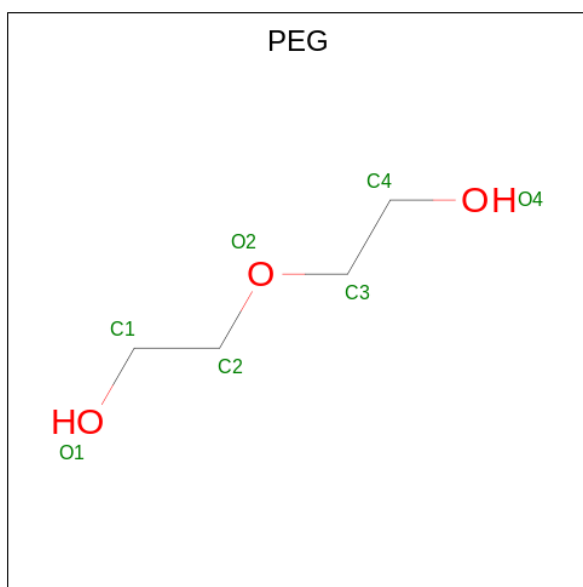
- Molecule 2 is a DNA chain called DNA (5'-D(*GP*AP*AP*CP*TP*AP*CP*CP*GP*TP*CP*GP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	10	Total	C	N	O	P	0	0	0
			205	97	38	60	10			
2	E	12	Total	C	N	O	P	0	0	0
			245	116	46	71	12			
2	H	7	Total	C	N	O	P	0	0	0
			142	68	28	40	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	7	Total	C	N	O	P	0	0	0
			144	66	26	46	6			
3	F	5	Total	C	N	O	P	0	0	0
			107	48	21	33	5			
3	G	7	Total	C	N	O	P	0	0	0
			144	66	26	46	6			

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



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

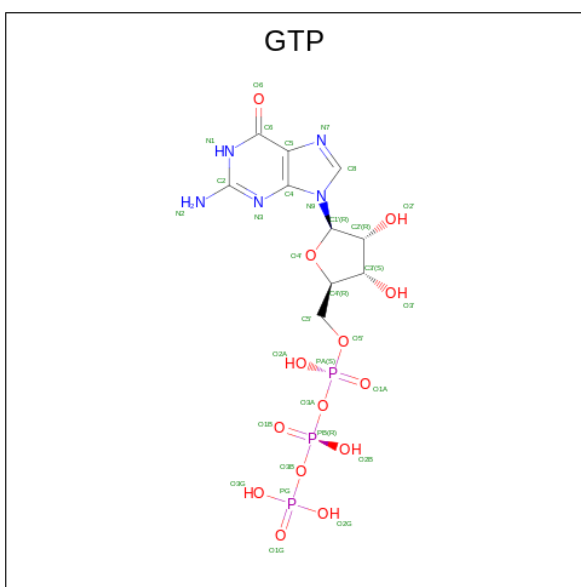
- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Ca	0	0
			2	2		
5	B	2	Total	Ca	0	0
			2	2		

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

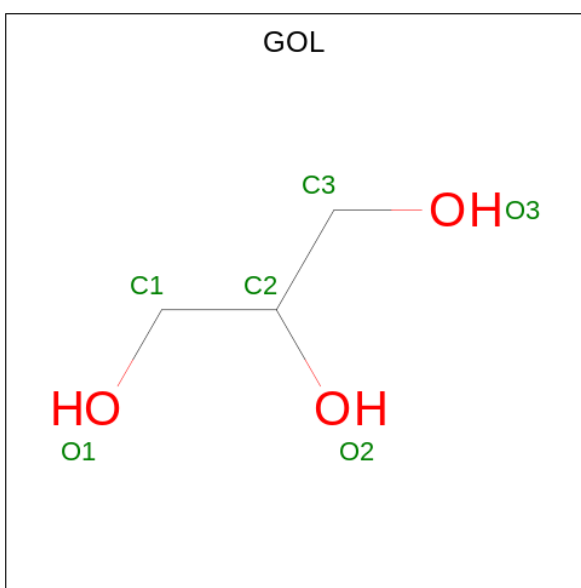
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	B	1	Total	Mg	0	0
			1	1		

- Molecule 7 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
7	B	1	Total 31	C 10	N 5	O 13	P 3	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



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

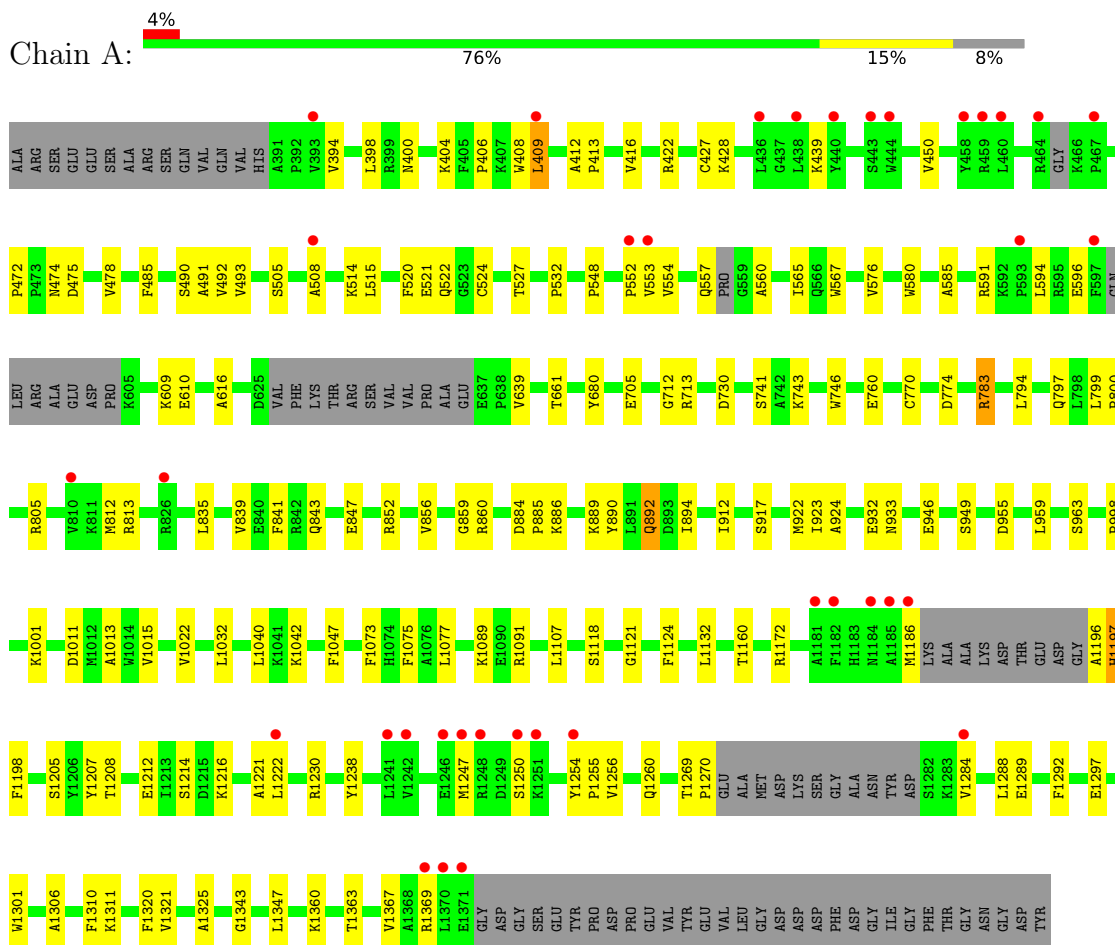
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	266	Total 266	O 266	0	0
9	B	209	Total 209	O 209	0	0
9	C	11	Total 11	O 11	0	0
9	D	7	Total 7	O 7	0	0
9	E	6	Total 6	O 6	0	0
9	F	7	Total 7	O 7	0	0

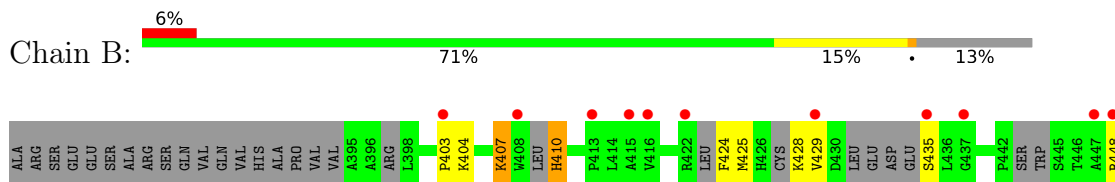
3 Residue-property plots [i](#)

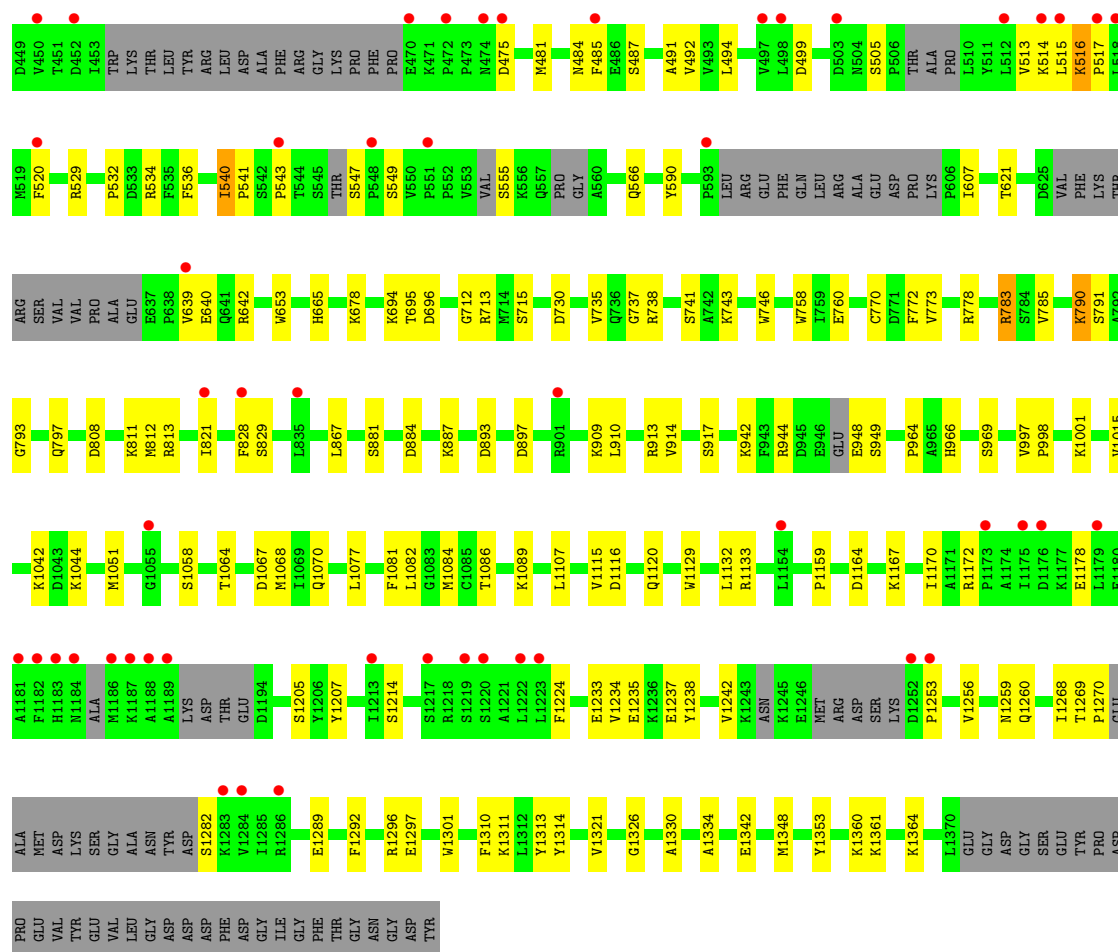
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: RNA-dependent RNA polymerase

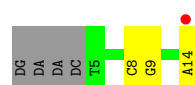


• Molecule 1: RNA-dependent RNA polymerase





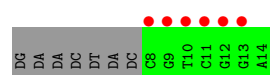
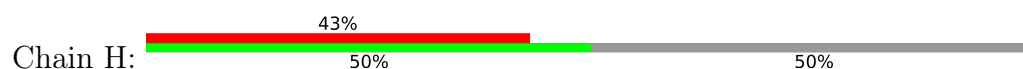
- Molecule 2: DNA (5'-D(*GP*AP*AP*CP*TP*AP*CP*CP*GP*TP*CP*GP*GP*A)-3')



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



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



- Molecule 3: RNA (5'-R(*UP*CP*CP*GP*AP*CP*G)-3')

Chain D:  71% 29%




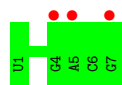
- Molecule 3: RNA (5'-R(*UP*CP*CP*GP*AP*CP*G)-3')

Chain F:  43% 29% 29%



- Molecule 3: RNA (5'-R(*UP*CP*CP*GP*AP*CP*G)-3')

Chain G:  43% 100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.37Å 122.17Å 114.92Å 90.00° 109.29° 90.00°	Depositor
Resolution (Å)	49.57 – 2.10 49.57 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.4 (49.57-2.10) 93.4 (49.57-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.10Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.207 , 0.249 0.207 , 0.249	Depositor DCC
R_{free} test set	7162 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	35.6	Xtrriage
Anisotropy	0.348	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16197	wwPDB-VP
Average B, all atoms (Å ²)	53.0	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 27.26 % 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 2.2690e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, GTP, MG, PEG, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.38	0/7756	0.58	3/10495 (0.0%)
1	B	0.39	0/7174	0.58	0/9673
2	C	0.76	0/229	0.85	0/351
2	E	0.69	0/274	0.84	0/420
2	H	0.70	0/159	0.84	0/244
3	D	0.40	0/160	0.93	0/247
3	F	0.34	0/119	0.89	0/183
3	G	0.27	0/160	0.73	0/247
All	All	0.40	0/16031	0.60	3/21860 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	548	PRO	CA-N-CD	-6.89	101.86	111.50
1	A	548	PRO	N-CD-CG	-5.87	94.39	103.20
1	A	548	PRO	CA-CB-CG	-5.30	93.93	104.00

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	7567	0	7457	103	0
1	B	7024	0	6780	102	0
2	C	205	0	113	4	0
2	E	245	0	135	2	0
2	H	142	0	80	0	0
3	D	144	0	76	3	0
3	F	107	0	54	2	0
3	G	144	0	76	0	0
4	A	7	10	10	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	31	0	10	0	0
7	B	31	0	10	1	0
8	B	12	16	16	2	0
9	A	266	0	0	4	0
9	B	209	0	0	2	0
9	C	11	0	0	0	0
9	D	7	0	0	1	0
9	E	6	0	0	0	0
9	F	7	0	0	0	0
All	All	16171	26	14817	202	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 7.

All (202) 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:922[A]:MET:HE1	1:A:1011:ASP:HB3	1.41	1.02
1:B:485:PHE:CD1	1:B:492:VAL:HB	2.05	0.92
1:B:485:PHE:HD1	1:B:492:VAL:HB	1.37	0.89
1:A:847:GLU:OE2	1:A:1360:LYS:HE2	1.74	0.86
1:A:552:PRO:HD2	1:A:553:VAL:H	1.45	0.81
1:A:1269:THR:HG23	1:A:1270:PRO:HD2	1.64	0.80
1:A:892:GLN:NE2	1:A:1186:MET:HB3	1.96	0.79
1:A:843:GLN:O	1:A:847:GLU:HG3	1.83	0.78
1:A:1256:VAL:O	1:A:1260:GLN:HG3	1.84	0.77
1:A:794:LEU:HD12	1:A:912:ILE:HB	1.68	0.75
1:A:1343:GLY:O	9:A:1601:HOH:O	2.06	0.73
1:B:942:LYS:HD2	1:B:944:ARG:HG2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:621:THR:OG1	1:B:640:GLU:O	2.08	0.72
1:A:949:SER:HB2	1:B:730:ASP:OD2	1.90	0.71
3:D:6:C:OP1	9:D:101:HOH:O	2.07	0.71
1:A:1270:PRO:HG2	1:A:1289:GLU:HG3	1.72	0.71
1:B:516:LYS:HE2	1:B:517:PRO:HD2	1.73	0.70
1:B:678:LYS:HD2	3:F:5:A:H4'	1.73	0.70
1:B:1089:LYS:HA	1:B:1107:LEU:HD13	1.74	0.68
1:B:1256:VAL:O	1:B:1260:GLN:HG3	1.91	0.68
1:A:835:LEU:HD13	1:A:841:PHE:CE1	2.28	0.68
1:B:1042:LYS:HE2	1:B:1044:LYS:HG2	1.77	0.67
1:B:665:HIS:HB2	1:B:1068:MET:HG3	1.75	0.67
1:A:783:ARG:HD2	3:D:6:C:H4'	1.76	0.66
1:B:964:PRO:HG3	7:B:1506:GTP:HN22	1.61	0.64
1:A:639:VAL:HG21	9:A:1623:HOH:O	1.98	0.62
1:A:505:SER:HB3	1:A:508:ALA:HB2	1.82	0.61
2:C:8:DC:H2'	2:C:9:DG:H8	1.66	0.61
1:A:1040:LEU:HD23	1:A:1124:PHE:CD1	2.36	0.61
1:A:963:SER:OG	9:A:1603:HOH:O	2.16	0.61
1:A:610:GLU:HG3	1:A:1077:LEU:CD2	2.32	0.60
1:A:860:ARG:NH1	1:B:1342:GLU:HA	2.17	0.59
1:B:1067:ASP:O	1:B:1070:GLN:HG3	2.02	0.59
1:A:565:ILE:HG12	1:A:1077:LEU:HD12	1.85	0.58
1:B:484:ASN:OD1	1:B:639:VAL:HG23	2.02	0.58
1:B:1116:ASP:HB3	1:B:1120:GLN:HG2	1.86	0.58
1:B:1269:THR:CG2	1:B:1270:PRO:HD2	2.34	0.58
1:B:1269:THR:HG23	1:B:1270:PRO:HD2	1.86	0.57
1:B:735:VAL:HG12	1:B:785:VAL:HG12	1.87	0.57
1:B:1159:PRO:HB3	1:B:1164:ASP:HB3	1.85	0.57
1:A:922[B]:MET:SD	1:A:1013:ALA:HB2	2.45	0.56
1:B:791:SER:H	8:B:1501:GOL:H31	1.69	0.56
2:C:8:DC:H2'	2:C:9:DG:C8	2.41	0.56
1:A:852:ARG:NH1	1:B:1361:LYS:HD2	2.21	0.56
1:B:808:ASP:CG	1:B:811:LYS:HD2	2.25	0.56
1:B:1270:PRO:HD3	1:B:1301:TRP:CE2	2.40	0.56
1:B:540:ILE:HG12	1:B:541:PRO:HD2	1.87	0.55
1:B:997:VAL:HG13	1:B:998:PRO:HD2	1.88	0.55
1:B:808:ASP:OD2	1:B:811:LYS:HD2	2.06	0.55
1:B:783:ARG:HD2	3:F:6:C:H4'	1.89	0.54
1:B:1270:PRO:CG	1:B:1289:GLU:HG3	2.37	0.54
1:B:1042:LYS:CE	1:B:1044:LYS:HG2	2.37	0.54
1:A:524:CYS:SG	1:A:527:THR:HG23	2.48	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:543:PRO:HD2	1:B:1077:LEU:HD22	1.90	0.53
1:A:557:GLN:HA	1:A:557:GLN:OE1	2.08	0.53
1:B:513:VAL:HG12	1:B:515:LEU:HD23	1.90	0.53
1:A:576:VAL:HG23	1:A:576:VAL:O	2.07	0.53
1:B:534:ARG:HD2	1:B:642:ARG:HD2	1.91	0.52
1:B:884:ASP:HB3	1:B:887:LYS:HB2	1.91	0.52
1:B:910:LEU:HD22	1:B:1167:LYS:HB2	1.92	0.52
1:A:493:VAL:HG21	1:A:521:GLU:HG3	1.91	0.52
1:A:1347:LEU:HD23	1:B:1334:ALA:HB3	1.91	0.52
1:B:773:VAL:O	1:B:778:ARG:NH1	2.40	0.52
1:A:412:ALA:HB1	1:A:416:VAL:HB	1.91	0.52
1:A:1214:SER:HB2	1:A:1221:ALA:HA	1.93	0.51
1:B:1253:PRO:HD2	1:B:1256:VAL:HG21	1.92	0.51
1:A:1310:PHE:HA	1:A:1321:VAL:HG11	1.91	0.51
1:B:1270:PRO:HG3	1:B:1289:GLU:HG3	1.92	0.51
1:A:813:ARG:NH2	1:A:1160:THR:O	2.39	0.51
1:B:797:GLN:HE22	1:B:964:PRO:CB	2.24	0.51
1:B:1235:GLU:HG3	1:B:1313:TYR:CD2	2.45	0.50
1:B:1270:PRO:HD3	1:B:1301:TRP:CD2	2.46	0.50
1:B:1234:VAL:HG21	1:B:1268:ILE:HD11	1.93	0.50
1:A:450:VAL:HG11	1:A:472:PRO:HD2	1.94	0.50
1:A:474:ASN:O	1:A:478:VAL:HG23	2.11	0.50
1:A:705:GLU:OE2	1:A:1001:LYS:NZ	2.25	0.50
1:A:839:VAL:HG22	1:A:1363:THR:HG23	1.94	0.50
1:B:491:ALA:HB1	1:B:532:PRO:HB3	1.94	0.49
1:A:884:ASP:OD1	1:A:885:PRO:HD2	2.11	0.49
1:B:791:SER:N	8:B:1501:GOL:H31	2.27	0.49
1:A:485:PHE:CD2	1:A:492:VAL:HB	2.47	0.49
1:A:554:VAL:HG12	1:A:560:ALA:HB1	1.94	0.49
1:A:1269:THR:HG23	1:A:1270:PRO:CD	2.40	0.49
1:B:893:ASP:O	1:B:897:ASP:OD1	2.31	0.49
1:A:514:LYS:HD3	1:A:594:LEU:HD13	1.93	0.49
1:A:552:PRO:CD	1:A:553:VAL:H	2.22	0.49
1:A:1091:ARG:NH1	9:A:1602:HOH:O	2.16	0.49
1:A:1297:GLU:HA	1:A:1297:GLU:OE1	2.12	0.49
1:A:1284:VAL:O	1:A:1288:LEU:HG	2.12	0.48
1:A:490:SER:HG	2:C:14:DA:H8	1.60	0.48
1:B:1081:PHE:HD1	1:B:1084:MET:HE2	1.78	0.48
1:A:797:GLN:NE2	2:C:8:DC:H4'	2.29	0.48
1:A:922[A]:MET:HE1	1:A:1011:ASP:CB	2.28	0.48
1:B:741:SER:HB3	1:B:770:CYS:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:PRO:HD2	1:A:416:VAL:HG21	1.95	0.48
1:A:1075:PHE:HE1	1:A:1118:SER:HA	1.78	0.47
1:A:1270:PRO:HG3	1:A:1301:TRP:CD2	2.49	0.47
1:B:403:PRO:HB3	1:B:425:MET:HE3	1.95	0.47
1:B:828:PHE:HB3	1:B:1178:GLU:HG3	1.97	0.47
1:B:1129:TRP:CE2	1:B:1133:ARG:HD2	2.50	0.47
1:A:552:PRO:HD2	1:A:553:VAL:N	2.23	0.47
1:A:852:ARG:O	1:A:856:VAL:HG23	2.15	0.47
1:B:1238:TYR:CD2	1:B:1242:VAL:HG21	2.49	0.47
1:B:590:TYR:HA	1:B:607:ILE:O	2.15	0.47
1:A:1306:ALA:CB	1:A:1325:ALA:HB1	2.45	0.46
1:A:890:TYR:CE2	1:A:894:ILE:HD11	2.51	0.46
3:D:5:A:C2'	3:D:6:C:H5'	2.45	0.46
1:B:966:HIS:ND1	1:B:1089:LYS:HE2	2.31	0.46
1:A:661:THR:HA	1:A:1047:PHE:HB3	1.96	0.46
1:B:793:GLY:HA2	1:B:914:VAL:H	1.80	0.46
1:B:1086:THR:HG21	2:E:7:DC:H1'	1.98	0.46
1:A:580:TRP:CZ3	1:A:616:ALA:HB2	2.51	0.46
1:A:713:ARG:HB2	1:A:760:GLU:OE2	2.15	0.46
1:B:790:LYS:HB2	1:B:790:LYS:HE2	1.71	0.45
1:B:1044:LYS:HB2	1:B:1044:LYS:HE3	1.81	0.45
1:B:529:ARG:HG2	1:B:653:TRP:CZ2	2.51	0.45
1:B:909:LYS:HA	1:B:909:LYS:HD2	1.72	0.45
1:A:799:LEU:HB2	1:A:800:PRO:HD3	1.99	0.45
1:A:812:MET:HG3	1:A:813:ARG:N	2.31	0.45
1:A:1363:THR:O	1:A:1367:VAL:HG12	2.16	0.45
1:A:1292:PHE:CD2	1:B:1205:SER:HB2	2.51	0.45
1:B:713:ARG:HB2	1:B:760:GLU:OE2	2.17	0.45
1:B:424:PHE:O	1:B:428:LYS:HA	2.16	0.45
1:B:737:GLY:C	1:B:738:ARG:HD2	2.37	0.45
1:B:1348:MET:HE2	1:B:1353:TYR:HA	1.99	0.45
1:B:867:LEU:HD21	1:B:1326:GLY:HA3	1.98	0.45
1:B:481:MET:HE2	1:B:481:MET:HB3	1.82	0.45
1:A:491:ALA:HB1	1:A:532:PRO:HB3	1.98	0.45
1:A:805:ARG:NE	1:A:805:ARG:HA	2.32	0.45
1:B:715:SER:HB3	1:B:758:TRP:CD1	2.52	0.45
1:A:705:GLU:HG2	1:A:998:PRO:HD2	1.99	0.44
1:A:1207:TYR:CE2	1:A:1311:LYS:HG2	2.52	0.44
1:A:394:VAL:HG22	1:A:553:VAL:HG22	1.98	0.44
1:B:969:SER:HA	9:B:1673:HOH:O	2.17	0.44
1:A:741:SER:HB3	1:A:770:CYS:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:923:ILE:HG22	1:A:924:ALA:N	2.32	0.44
1:A:1089:LYS:HA	1:A:1107:LEU:HD13	1.99	0.44
1:A:1089:LYS:HG3	1:A:1107:LEU:HB3	1.99	0.44
1:B:407:LYS:HA	1:B:410:HIS:HB2	2.00	0.44
1:B:881:SER:OG	1:B:1330:ALA:HB1	2.18	0.44
1:A:1132:LEU:C	1:A:1132:LEU:HD23	2.38	0.44
1:A:1238:TYR:CD2	1:A:1320:PHE:HB2	2.52	0.44
1:A:743:LYS:HB3	1:A:743:LYS:HE3	1.61	0.44
1:A:917:SER:HA	1:A:1015:VAL:O	2.18	0.43
1:A:522:GLN:OE1	1:A:680:TYR:CD2	2.71	0.43
1:A:610:GLU:HG3	1:A:1077:LEU:HD21	1.99	0.43
1:B:494:LEU:O	1:B:536:PHE:HD1	2.01	0.43
1:A:422:ARG:HG2	1:A:515:LEU:HB2	2.01	0.43
1:A:713:ARG:O	1:A:760:GLU:HG2	2.18	0.43
1:B:1310:PHE:O	1:B:1314:TYR:HB3	2.18	0.43
1:A:406:PRO:HB2	1:A:408:TRP:CD1	2.54	0.43
1:B:1082:LEU:HD21	1:B:1115:VAL:HG12	2.00	0.43
1:B:1051:MET:HA	1:B:1064:THR:OG1	2.19	0.43
1:A:1208:THR:O	1:A:1212:GLU:HG3	2.19	0.43
1:A:712:GLY:O	1:A:746:TRP:HA	2.18	0.42
1:A:585:ALA:HB2	1:A:1073:PHE:CZ	2.55	0.42
1:A:1270:PRO:HG3	1:A:1301:TRP:CE3	2.54	0.42
1:A:1254:TYR:HB3	1:A:1255:PRO:HD3	2.01	0.42
1:A:522:GLN:OE1	1:A:680:TYR:CE2	2.72	0.42
1:A:890:TYR:O	1:A:894:ILE:HG13	2.20	0.42
1:A:959:LEU:HG	1:A:1022:VAL:HG22	2.01	0.42
1:B:1296:ARG:HG3	1:B:1297:GLU:OE2	2.19	0.42
1:A:852:ARG:HD3	1:B:1361:LYS:HB2	2.01	0.42
1:A:1032:LEU:HD12	1:A:1032:LEU:HA	1.87	0.42
1:B:1084:MET:HE3	9:B:1704:HOH:O	2.19	0.42
1:B:694:LYS:HA	1:B:694:LYS:HD3	1.84	0.42
1:B:1310:PHE:HA	1:B:1321:VAL:HG11	2.01	0.42
1:A:1042:LYS:HA	1:A:1121:GLY:O	2.20	0.42
1:B:942:LYS:HD2	1:B:944:ARG:CG	2.47	0.42
1:B:797:GLN:HE22	1:B:964:PRO:CA	2.33	0.41
1:B:997:VAL:CG1	1:B:998:PRO:HD2	2.48	0.41
1:A:859:GLY:O	1:A:860:ARG:HB3	2.19	0.41
1:B:770:CYS:HB3	1:B:772:PHE:CE1	2.55	0.41
1:B:821:ILE:HG13	1:B:1170:ILE:HG23	2.01	0.41
1:B:1233:GLU:O	1:B:1237:GLU:HG2	2.21	0.41
1:A:932:GLU:O	1:A:933:ASN:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:695:THR:HG22	1:B:696:ASP:O	2.19	0.41
1:A:889:LYS:HB3	1:A:1198:PHE:CE1	2.55	0.41
1:B:1360:LYS:HE3	1:B:1364:LYS:HE3	2.01	0.41
1:A:1306:ALA:HB1	1:A:1325:ALA:HB1	2.01	0.41
1:B:516:LYS:HB3	1:B:517:PRO:HD2	2.03	0.41
1:B:797:GLN:HE22	1:B:964:PRO:HB3	1.84	0.41
1:B:1116:ASP:HB3	1:B:1120:GLN:CG	2.50	0.41
1:A:1205:SER:HB2	1:B:1292:PHE:CD2	2.56	0.41
1:B:712:GLY:O	1:B:746:TRP:HA	2.21	0.41
1:B:998:PRO:HG2	1:B:1001:LYS:HB2	2.01	0.41
2:E:4:DC:H3'	2:E:5:DT:H5''	2.03	0.41
1:A:398:LEU:HD22	1:A:567:TRP:CD2	2.56	0.41
1:A:730[B]:ASP:OD2	1:B:949:SER:HB2	2.21	0.41
1:B:812:MET:HG3	1:B:813:ARG:N	2.35	0.41
1:B:917:SER:HA	1:B:1015:VAL:O	2.21	0.41
1:B:1270:PRO:HG2	1:B:1289:GLU:HG3	2.02	0.40
1:A:475:ASP:OD1	1:A:475:ASP:N	2.52	0.40
1:A:591:ARG:HB2	1:A:609:LYS:HE3	2.04	0.40
1:B:514:LYS:O	1:B:514:LYS:HG2	2.21	0.40
1:B:1132:LEU:O	1:B:1132:LEU:HD23	2.20	0.40
1:A:1196:ALA:C	1:A:1197:HIS:ND1	2.75	0.40
1:A:400:ASN:HD21	1:A:404:LYS:HE3	1.85	0.40
1:A:409:LEU:HD23	1:A:409:LEU:HA	1.84	0.40
1:A:427:CYS:O	1:A:428:LYS:HB2	2.21	0.40
1:B:948:GLU:HG2	1:B:949:SER:N	2.37	0.40
1:B:1207:TYR:CE2	1:B:1311:LYS:HG2	2.57	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	933/1026 (91%)	914 (98%)	19 (2%)	0	100	100
1	B	862/1026 (84%)	841 (98%)	21 (2%)	0	100	100
All	All	1795/2052 (88%)	1755 (98%)	40 (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	814/894 (91%)	796 (98%)	18 (2%)	52	57
1	B	734/894 (82%)	705 (96%)	29 (4%)	31	32
All	All	1548/1788 (87%)	1501 (97%)	47 (3%)	41	44

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	409	LEU
1	A	439	LYS
1	A	520	PHE
1	A	596	GLU
1	A	774	ASP
1	A	783	ARG
1	A	886	LYS
1	A	892	GLN
1	A	946	GLU
1	A	955	ASP
1	A	1172	ARG
1	A	1197	HIS
1	A	1216	LYS
1	A	1222	LEU
1	A	1230	ARG
1	A	1247	MET
1	A	1250	SER
1	A	1369	ARG

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Mol	Chain	Res	Type
1	B	404	LYS
1	B	407	LYS
1	B	410	HIS
1	B	429	VAL
1	B	435	SER
1	B	448	ARG
1	B	475	ASP
1	B	487	SER
1	B	499	ASP
1	B	505	SER
1	B	516	LYS
1	B	520	PHE
1	B	540	ILE
1	B	547	SER
1	B	549	SER
1	B	555	SER
1	B	566	GLN
1	B	743[A]	LYS
1	B	743[B]	LYS
1	B	783	ARG
1	B	790	LYS
1	B	829	SER
1	B	913	ARG
1	B	1058	SER
1	B	1172	ARG
1	B	1214	SER
1	B	1224	PHE
1	B	1259	ASN
1	B	1282	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	400	ASN
1	A	522	GLN
1	A	892	GLN
1	B	797	GLN
1	B	1184	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	D	5/7 (71%)	0	0
3	F	3/7 (42%)	0	0
3	G	5/7 (71%)	0	0
All	All	13/21 (61%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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, 6 are monoatomic - leaving 5 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	GTP	B	1506	6,5	25,33,34	1.09	2 (8%)	29,52,54	1.48	6 (20%)
8	GOL	B	1502	-	5,5,5	1.05	0	5,5,5	0.94	0
8	GOL	B	1501	-	5,5,5	0.73	0	5,5,5	0.97	0
7	GTP	A	1505	5	25,33,34	1.14	2 (8%)	29,52,54	1.52	5 (17%)
4	PEG	A	1501	-	6,6,6	0.51	0	5,5,5	0.33	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	GTP	B	1506	6,5	-	1/18/34/38	0/3/3/3
8	GOL	B	1502	-	-	2/4/4/4	-
8	GOL	B	1501	-	-	0/4/4/4	-
7	GTP	A	1505	5	-	2/18/34/38	0/3/3/3
4	PEG	A	1501	-	-	1/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1505	GTP	C5-C6	-3.73	1.39	1.47
7	B	1506	GTP	C5-C6	-3.57	1.40	1.47
7	A	1505	GTP	C2-N3	2.07	1.38	1.33
7	B	1506	GTP	C2-N3	2.01	1.38	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1505	GTP	C5-C6-N1	3.28	119.75	113.95
7	B	1506	GTP	C5-C6-N1	3.23	119.65	113.95
7	A	1505	GTP	PA-O3A-PB	-3.06	122.34	132.83
7	A	1505	GTP	C8-N7-C5	2.99	108.68	102.99
7	B	1506	GTP	C8-N7-C5	2.93	108.58	102.99
7	B	1506	GTP	PB-O3B-PG	-2.76	123.37	132.83
7	A	1505	GTP	C2-N1-C6	-2.56	120.38	125.10
7	B	1506	GTP	C2-N1-C6	-2.50	120.50	125.10
7	B	1506	GTP	PA-O3A-PB	-2.38	124.65	132.83
7	A	1505	GTP	PB-O3B-PG	-2.33	124.83	132.83
7	B	1506	GTP	N1-C2-N3	-2.07	119.46	123.32

There are no chirality outliers.

All (6) torsion outliers are listed below:

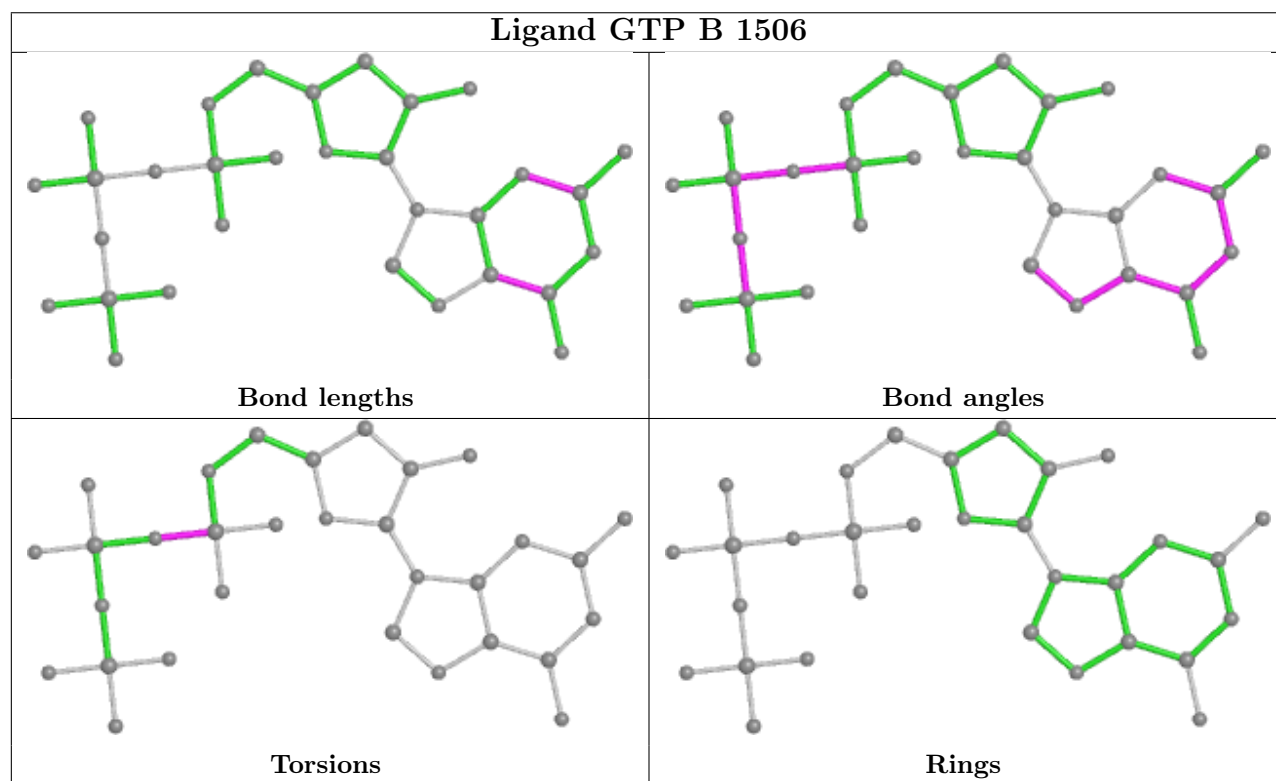
Mol	Chain	Res	Type	Atoms
7	A	1505	GTP	C5'-O5'-PA-O1A
8	B	1502	GOL	C1-C2-C3-O3
7	B	1506	GTP	PB-O3A-PA-O5'
7	A	1505	GTP	C5'-O5'-PA-O3A
8	B	1502	GOL	O2-C2-C3-O3
4	A	1501	PEG	C1-C2-O2-C3

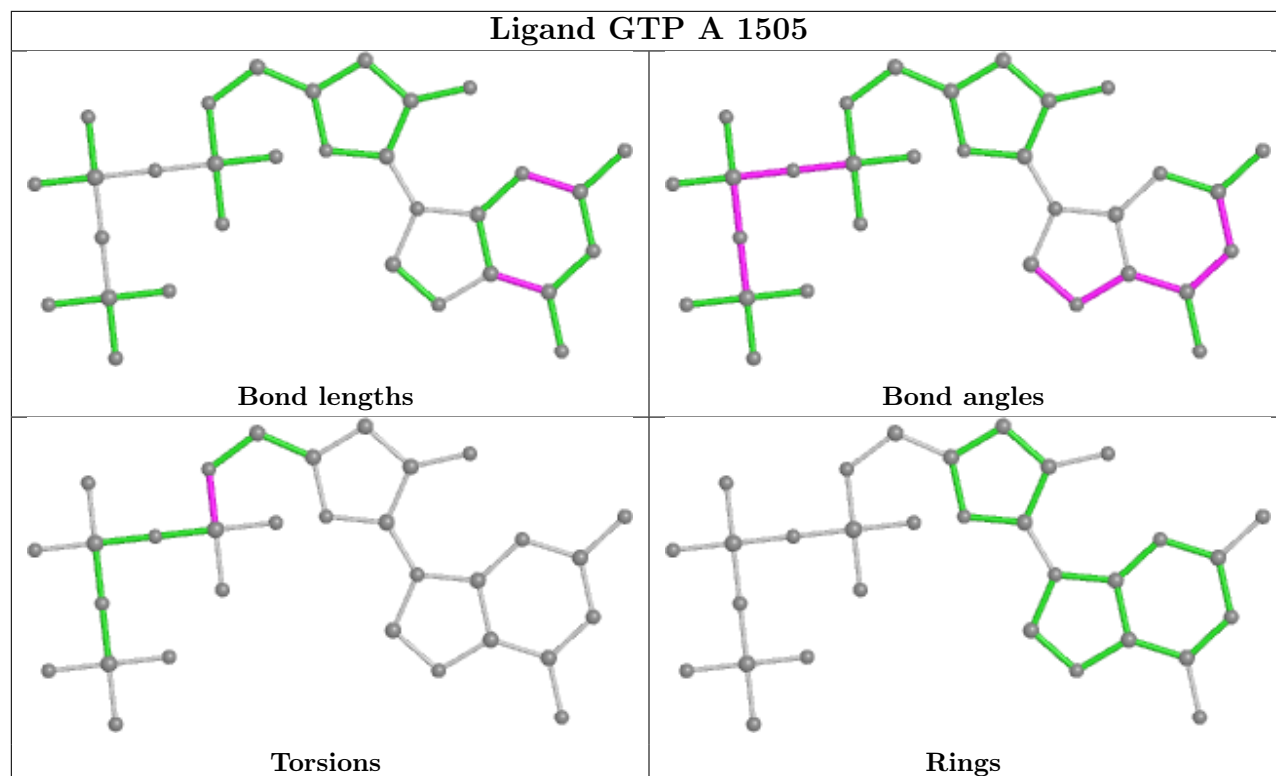
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1506	GTP	1	0
8	B	1501	GOL	2	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	941/1026 (91%)	0.24	37 (3%)	39	45	22, 47, 83, 114	0
1	B	897/1026 (87%)	0.43	61 (6%)	17	21	23, 50, 96, 117	0
2	C	10/14 (71%)	0.48	1 (10%)	7	9	41, 60, 111, 136	0
2	E	12/14 (85%)	0.84	2 (16%)	1	2	53, 78, 121, 143	2 (16%)
2	H	7/14 (50%)	3.43	6 (85%)	0	0	80, 108, 117, 117	6 (85%)
3	D	7/7 (100%)	-0.42	0	100	100	36, 64, 114, 125	0
3	F	5/7 (71%)	-0.45	0	100	100	46, 61, 102, 129	0
3	G	7/7 (100%)	1.89	3 (42%)	0	0	69, 87, 97, 98	7 (100%)
All	All	1886/2115 (89%)	0.35	110 (5%)	23	28	22, 49, 94, 143	15 (0%)

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1251	LYS	6.9
1	B	1188	ALA	6.4
1	B	416	VAL	5.8
1	B	1179	LEU	5.4
1	A	1185	ALA	5.3
1	B	520	PHE	5.0
1	B	1183	HIS	4.9
2	H	9	DG	4.9
1	B	821	ILE	4.7
1	B	1184	ASN	4.2
1	B	1213	ILE	4.1
1	B	828	PHE	4.0
2	H	10	DT	3.9
1	B	403	PRO	3.9
2	H	12	DG	3.9
3	G	7	G	3.8

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Mol	Chain	Res	Type	RSRZ
2	H	11	DC	3.8
1	B	1176	ASP	3.8
1	B	593	PRO	3.7
1	A	1370	LEU	3.7
1	A	458	TYR	3.6
1	B	497	VAL	3.6
1	A	1247	MET	3.6
2	H	8	DC	3.5
1	A	597	PHE	3.5
1	B	452	ASP	3.5
3	G	4	G	3.4
1	B	1154	LEU	3.4
1	B	1182	PHE	3.3
2	E	13	DG	3.3
1	A	459	ARG	3.3
1	B	518	LEU	3.2
1	A	1246	GLU	3.1
1	B	498	LEU	3.1
1	A	1242	VAL	3.1
1	B	835	LEU	3.1
1	A	440	TYR	3.1
1	B	475	ASP	3.0
1	A	508	ALA	3.0
1	A	436	LEU	3.0
1	B	503	ASP	3.0
1	A	826	ARG	3.0
1	B	1284	VAL	3.0
2	E	2	DA	3.0
1	B	1217	SER	2.9
1	A	1186	MET	2.9
1	B	543	PRO	2.9
1	A	444	TRP	2.9
1	B	639	VAL	2.9
1	B	1189	ALA	2.9
1	A	438	LEU	2.8
1	A	1284	VAL	2.8
1	B	517	PRO	2.7
2	C	14	DA	2.7
1	A	1369	ARG	2.7
1	B	548	PRO	2.7
1	A	1222	LEU	2.7
1	B	1186	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	515	LEU	2.7
1	A	467	PRO	2.6
1	B	447	ALA	2.6
1	A	464	ARG	2.6
1	B	472	PRO	2.6
2	H	13	DG	2.6
1	A	810	VAL	2.6
1	A	552	PRO	2.6
1	A	1181	ALA	2.6
1	B	435	SER	2.6
1	B	1283	LYS	2.5
1	B	415	ALA	2.5
1	B	485	PHE	2.5
1	A	593	PRO	2.5
1	B	901	ARG	2.5
1	A	1250	SER	2.5
1	B	437	GLY	2.5
1	B	1222	LEU	2.4
1	B	514	LYS	2.4
1	A	1182	PHE	2.4
1	B	1219	SER	2.4
1	A	1184	ASN	2.4
1	B	429	VAL	2.4
1	B	551	PRO	2.4
1	A	1248	ARG	2.4
1	B	408	TRP	2.4
1	B	1223	LEU	2.3
1	B	1175	ILE	2.3
1	A	409	LEU	2.3
1	A	460	LEU	2.3
1	A	1254	TYR	2.3
1	B	512	LEU	2.3
1	B	448	ARG	2.3
1	B	1252	ASP	2.3
3	G	5	A	2.2
1	B	1173	PRO	2.2
1	B	1055	GLY	2.2
1	B	1220	SER	2.2
1	A	553	VAL	2.1
1	B	450	VAL	2.1
1	A	1241	LEU	2.1
1	B	1286	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	470	GLU	2.1
1	B	1181	ALA	2.1
1	A	443	SER	2.0
1	B	474	ASN	2.0
1	B	413	PRO	2.0
1	A	1371	GLU	2.0
1	B	422	ARG	2.0
1	B	1187	LYS	2.0
1	B	1253	PRO	2.0
1	A	393	VAL	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.

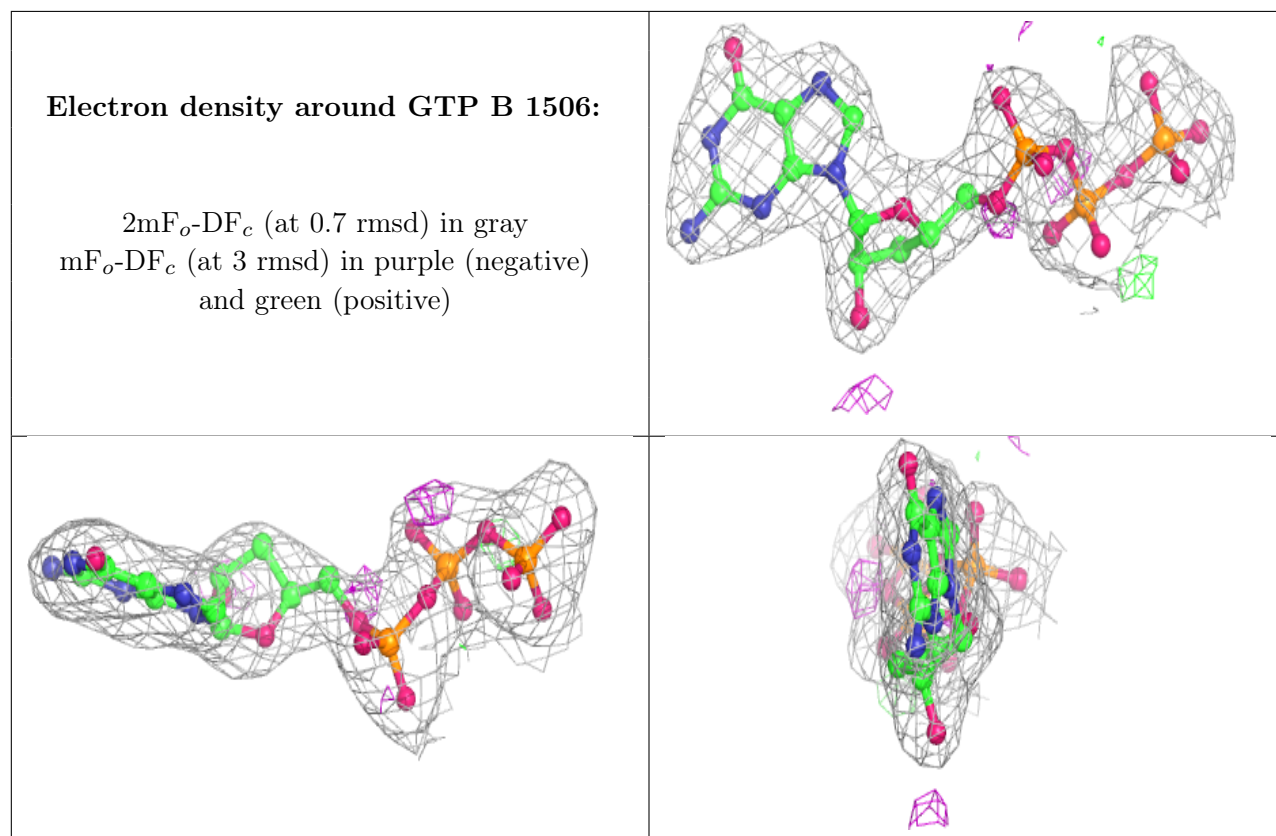
6.4 Ligands [i](#)

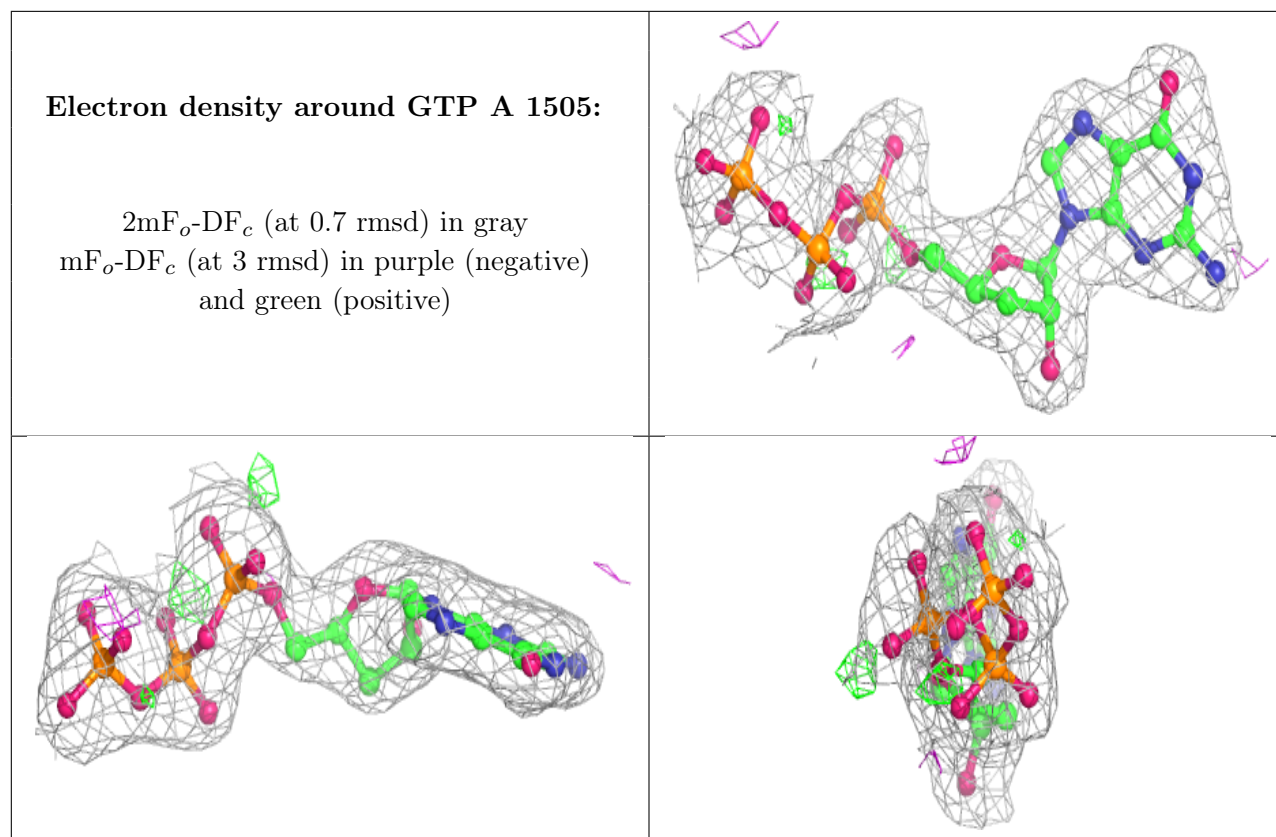
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	GOL	B	1502	6/6	0.86	0.13	54,78,93,101	0
8	GOL	B	1501	6/6	0.92	0.13	65,78,85,87	0
4	PEG	A	1501	7/7	0.96	0.15	53,64,74,74	0
5	CA	A	1502	1/1	0.98	0.13	38,38,38,38	0
7	GTP	B	1506	31/32	0.98	0.15	28,47,57,57	0
6	MG	B	1505	1/1	0.99	0.17	25,25,25,25	0
7	GTP	A	1505	31/32	0.99	0.17	25,37,49,54	0
5	CA	A	1503	1/1	0.99	0.12	35,35,35,35	0
5	CA	B	1503	1/1	0.99	0.14	31,31,31,31	0
5	CA	B	1504	1/1	0.99	0.13	33,33,33,33	0
6	MG	A	1504	1/1	1.00	0.16	33,33,33,33	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.