



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 10:21 am BST

PDB ID : 3AVW
Title : Structure of viral RNA polymerase complex 4
Authors : Takeshita, D.; Tomita, K.
Deposited on : 2011-03-08
Resolution : 2.60 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 : 2.11
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) : 2.11

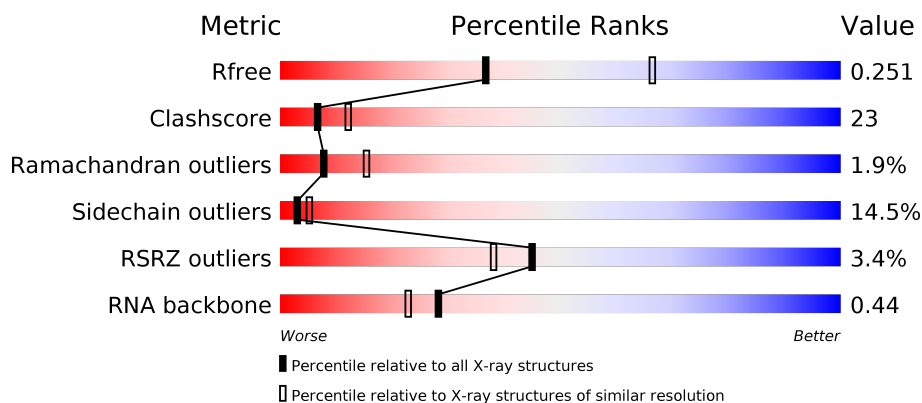
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION




The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)
RNA backbone	3102	1040 (2.90-2.30)

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	1289	
2	G	8	
3	T	12	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9843 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 Elongation factor Ts, Elongation factor Tu, LINKER, Q beta replicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1203	Total	C	N	O	S	0	0	0
			9287	5865	1605	1772	45			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	284	HIS	-	LINKER	UNP P0A6P3
A	1284	HIS	-	EXPRESSION TAG	UNP Q8LTE0
A	1285	HIS	-	EXPRESSION TAG	UNP Q8LTE0
A	1286	HIS	-	EXPRESSION TAG	UNP Q8LTE0
A	1287	HIS	-	EXPRESSION TAG	UNP Q8LTE0
A	1288	HIS	-	EXPRESSION TAG	UNP Q8LTE0
A	1289	HIS	-	EXPRESSION TAG	UNP Q8LTE0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	8	Total	C	N	O	P	0	0	0
			167	76	31	53	7			

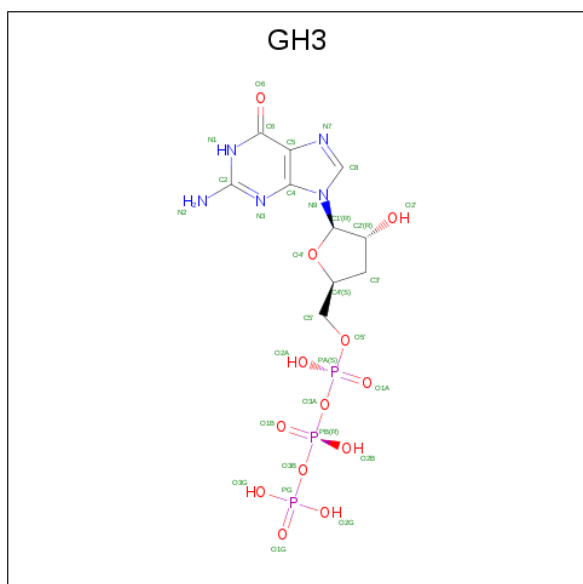
- Molecule 3 is a RNA chain called RNA (5'-R(*AP*UP*CP*GP*UP*GP*GP*AP*CP*CP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	12	Total	C	N	O	P	0	0	0
			252	114	46	81	11			

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Ca 2 2	0	0

- Molecule 5 is 3'-DEOXY-GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GH3) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$).



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

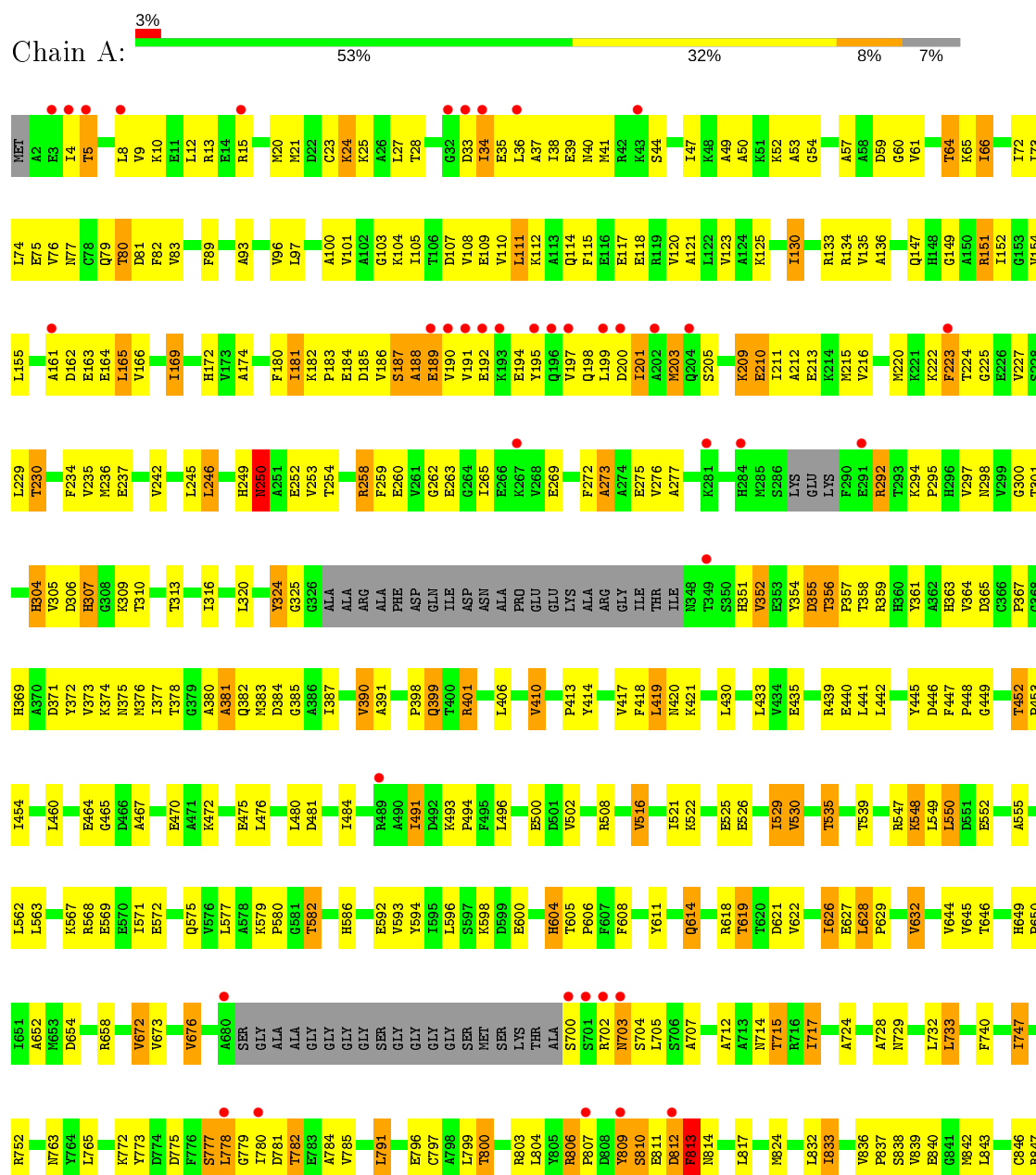
- Molecule 6 is water.

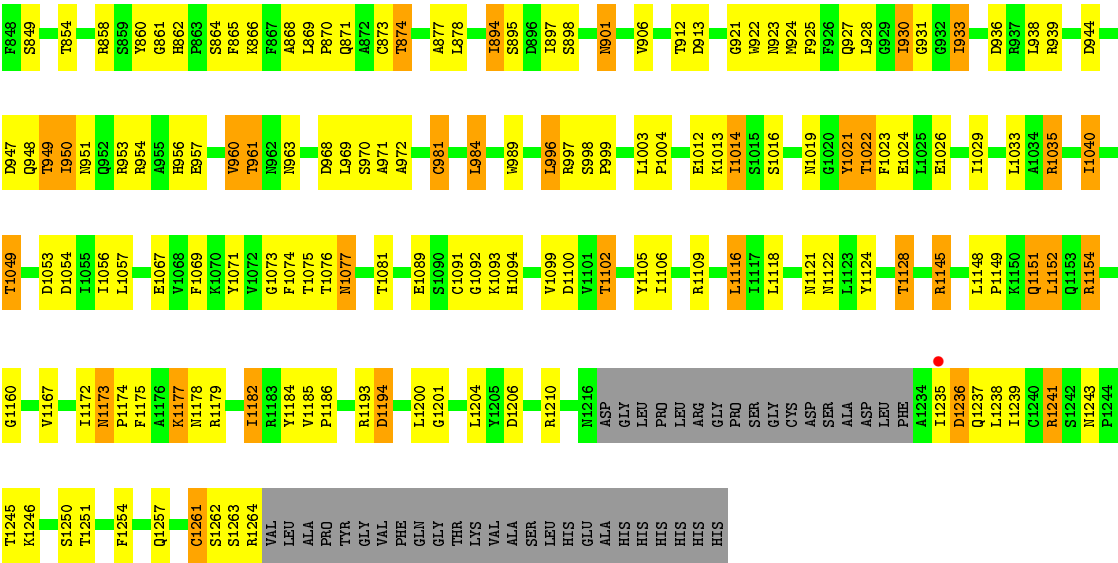
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	92	Total O 92 92	0	0
6	G	3	Total O 3 3	0	0
6	T	9	Total O 9 9	0	0

3 Residue-property plots

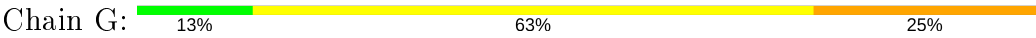
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Elongation factor Ts, Elongation factor Tu, LINKER, Q beta replicase

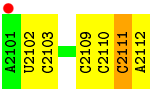




● Molecule 2: RNA (5'-R(*GP*GP*GP*UP*CP*CP*AP*C)-3')



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	140.02Å 256.83Å 101.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.60 41.84 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.1 (19.99-2.60) 98.8 (41.84-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.201 , 0.253 0.201 , 0.251	Depositor DCC
R_{free} test set	2831 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	52.4	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.017 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.024 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9843	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA, GH3

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	0.49	1/9456 (0.0%)	0.62	0/12787
2	G	0.59	0/186	1.03	1/288 (0.3%)
3	T	0.73	0/281	1.09	1/436 (0.2%)
All	All	0.50	1/9923 (0.0%)	0.65	2/13511 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	981	CYS	CB-SG	-5.05	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2008	C	O4'-C1'-N1	5.67	112.74	108.20
3	T	2103	C	C6-N1-C2	-5.11	118.26	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	849	SER	Peptide

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	9287	0	9273	445	0
2	G	167	0	87	6	0
3	T	252	0	132	4	0
4	A	2	0	0	0	0
5	T	31	0	12	1	0
6	A	92	0	0	2	0
6	G	3	0	0	0	0
6	T	9	0	0	0	0
All	All	9843	0	9504	452	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 23.

All (452) 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:1019:ASN:HB3	1:A:1022:THR:HG22	1.25	1.15
1:A:491:ILE:HD12	1:A:491:ILE:H	1.17	1.06
1:A:968:ASP:H	1:A:1081:THR:HG22	1.26	0.98
1:A:949:THR:HG23	1:A:953:ARG:HH12	1.27	0.97
1:A:961:THR:HG22	1:A:963:ASN:H	1.26	0.97
1:A:292:ARG:HE	1:A:292:ARG:H	1.04	0.96
1:A:1154:ARG:HH11	1:A:1154:ARG:HG3	1.28	0.95
1:A:806:ARG:HG2	1:A:806:ARG:O	1.69	0.93
1:A:714:ASN:HD21	1:A:1254:PHE:H	1.04	0.92
1:A:399:GLN:HE21	1:A:399:GLN:H	1.18	0.91
1:A:949:THR:HG23	1:A:953:ARG:NH1	1.86	0.90
1:A:862:HIS:HD2	1:A:864:SER:H	1.18	0.90
1:A:1019:ASN:HB3	1:A:1022:THR:CG2	2.02	0.89
1:A:1173:ASN:ND2	1:A:1175:PHE:H	1.72	0.87
1:A:273:ALA:O	1:A:276:VAL:HG12	1.74	0.87
1:A:949:THR:CG2	1:A:953:ARG:HH12	1.87	0.87
1:A:1100:ASP:OD1	1:A:1102:THR:HG23	1.77	0.84
1:A:59:ASP:O	1:A:77:ASN:HB2	1.77	0.84
1:A:448:PRO:O	1:A:452:THR:HG22	1.79	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1124:TYR:O	1:A:1128:THR:HB	1.79	0.82
1:A:954:ARG:NH1	1:A:1049:THR:HB	1.95	0.82
1:A:49:ALA:HB2	1:A:123:VAL:HG11	1.59	0.82
1:A:491:ILE:CD1	1:A:491:ILE:H	1.93	0.81
1:A:356:THR:HG22	1:A:359:ARG:H	1.45	0.81
1:A:65:LYS:HG2	1:A:101:VAL:HG21	1.62	0.81
1:A:838:SER:HB2	1:A:840:GLU:OE1	1.81	0.80
1:A:611:TYR:HB3	1:A:626:ILE:HD11	1.64	0.79
1:A:378:THR:HG23	1:A:380:ALA:H	1.48	0.79
1:A:324:TYR:CD1	1:A:357:PRO:HD3	2.18	0.78
1:A:301:THR:HB	1:A:363:HIS:NE2	1.98	0.78
1:A:120:VAL:HA	1:A:123:VAL:HG12	1.63	0.77
1:A:375:ASN:HA	1:A:378:THR:HG22	1.65	0.77
1:A:579:LYS:O	1:A:582:THR:HB	1.85	0.77
1:A:491:ILE:HD12	1:A:491:ILE:N	1.98	0.77
1:A:516:VAL:HG22	1:A:555:ALA:HA	1.67	0.77
1:A:372:TYR:CE1	1:A:410:VAL:HG21	2.19	0.76
1:A:307:HIS:CD2	1:A:391:ALA:H	2.04	0.76
1:A:292:ARG:H	1:A:292:ARG:NE	1.83	0.76
1:A:947:ASP:OD1	1:A:949:THR:HB	1.85	0.76
1:A:198:GLN:HA	1:A:201:ILE:HD12	1.67	0.75
1:A:961:THR:CG2	1:A:963:ASN:H	1.98	0.75
1:A:862:HIS:CD2	1:A:864:SER:H	2.05	0.74
1:A:413:PRO:HB2	1:A:414:TYR:CD1	2.22	0.74
1:A:714:ASN:ND2	1:A:1254:PHE:H	1.83	0.73
1:A:399:GLN:H	1:A:399:GLN:NE2	1.85	0.73
1:A:250:ASN:HD22	1:A:250:ASN:N	1.87	0.73
1:A:954:ARG:HH11	1:A:1049:THR:HB	1.53	0.72
1:A:212:ALA:O	1:A:216:VAL:HG23	1.89	0.71
1:A:1173:ASN:HD22	1:A:1173:ASN:C	1.94	0.71
1:A:374:LYS:HE3	1:A:594:TYR:CZ	2.26	0.71
1:A:627:GLU:HG2	1:A:644:VAL:HB	1.73	0.70
1:A:25:LYS:O	1:A:28:THR:HG22	1.91	0.70
1:A:1173:ASN:HD22	1:A:1175:PHE:H	1.39	0.70
1:A:420:ASN:ND2	1:A:421:LYS:HG3	2.07	0.70
1:A:211:ILE:O	1:A:215:MET:HG3	1.92	0.69
1:A:398:PRO:O	1:A:401:ARG:HG2	1.92	0.69
1:A:300:GLY:HA3	1:A:383:MET:SD	2.31	0.69
1:A:399:GLN:HE21	1:A:399:GLN:N	1.89	0.69
1:A:700:SER:O	1:A:1179:ARG:HD3	1.93	0.68
1:A:103:GLY:O	1:A:105:ILE:HG13	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:SER:O	1:A:47:ILE:HG22	1.93	0.68
1:A:796:GLU:O	1:A:800:THR:HG23	1.92	0.68
1:A:80:THR:HG22	1:A:83:VAL:H	1.58	0.68
1:A:806:ARG:H	1:A:807:PRO:HD3	1.59	0.67
1:A:372:TYR:HE1	1:A:410:VAL:HG21	1.59	0.67
1:A:310:THR:O	1:A:313:THR:HG22	1.95	0.67
1:A:120:VAL:HA	1:A:123:VAL:CG1	2.24	0.67
1:A:417:VAL:HB	1:A:454:ILE:HG13	1.76	0.67
1:A:1077:ASN:O	1:A:1081:THR:HG23	1.95	0.66
1:A:874:THR:HG22	1:A:877:ALA:H	1.60	0.66
1:A:220:MET:HA	1:A:223:PHE:HB3	1.77	0.66
1:A:1154:ARG:HG3	1:A:1154:ARG:NH1	1.98	0.66
1:A:442:LEU:HD13	1:A:452:THR:HG21	1.78	0.66
1:A:529:ILE:HD13	1:A:529:ILE:O	1.95	0.66
1:A:249:HIS:C	1:A:250:ASN:HD22	1.99	0.65
1:A:80:THR:HG23	1:A:82:PHE:H	1.62	0.65
1:A:618:ARG:NH1	1:A:652:ALA:O	2.29	0.65
1:A:1173:ASN:ND2	1:A:1175:PHE:N	2.44	0.65
1:A:871:GLN:HE21	1:A:921:GLY:HA3	1.61	0.65
1:A:187:SER:HB3	1:A:190:VAL:HG12	1.78	0.65
1:A:811:GLU:HG3	1:A:813:PHE:HB2	1.78	0.65
1:A:151:ARG:HB2	1:A:151:ARG:HH21	1.63	0.64
1:A:375:ASN:HA	1:A:378:THR:CG2	2.27	0.64
1:A:8:LEU:HG	1:A:27:LEU:HD21	1.78	0.64
1:A:526:GLU:HG2	1:A:539:THR:HG22	1.79	0.64
1:A:598:LYS:HD3	1:A:604:HIS:HB2	1.80	0.64
1:A:1182:ILE:HD11	1:A:1184:TYR:CZ	2.33	0.64
1:A:292:ARG:HE	1:A:292:ARG:N	1.87	0.64
1:A:1236:ASP:O	1:A:1239:ILE:HG12	1.98	0.63
1:A:356:THR:HG22	1:A:359:ARG:N	2.13	0.63
1:A:187:SER:C	1:A:189:GLU:H	2.02	0.63
1:A:969:LEU:HD21	1:A:1069:PHE:CD2	2.33	0.63
1:A:717:ILE:C	1:A:717:ILE:HD13	2.19	0.63
1:A:530:VAL:HG22	1:A:652:ALA:HB2	1.81	0.63
1:A:803:ARG:NH1	1:A:1071:TYR:O	2.32	0.62
1:A:775:ASP:OD2	1:A:1109:ARG:HD3	1.99	0.62
1:A:210:GLU:CD	1:A:210:GLU:H	2.00	0.62
1:A:365:ASP:O	1:A:367:PRO:HD3	2.00	0.62
1:A:309:LYS:HD2	1:A:365:ASP:OD2	1.99	0.62
1:A:181:ILE:HG12	1:A:182:LYS:HG3	1.80	0.61
1:A:75:GLU:O	1:A:75:GLU:HG3	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ASP:HB3	1:A:36:LEU:HB3	1.81	0.61
1:A:298:ASN:HB2	1:A:382:GLN:HE22	1.65	0.61
1:A:356:THR:HG21	1:A:481:ASP:OD1	2.01	0.61
1:A:870:PRO:HB2	1:A:895:SER:HB3	1.83	0.61
1:A:163:GLU:HG2	1:A:164:GLU:N	2.15	0.61
1:A:529:ILE:HD11	1:A:575:GLN:OE1	1.99	0.61
1:A:901:ASN:HD22	1:A:901:ASN:C	2.04	0.60
1:A:183:PRO:HD3	1:A:230:THR:HB	1.84	0.60
1:A:930:ILE:HD11	1:A:1021:TYR:CG	2.36	0.60
1:A:702:ARG:CB	1:A:705:LEU:HB3	2.31	0.60
1:A:24:LYS:NZ	1:A:24:LYS:HA	2.17	0.60
1:A:729:ASN:HD21	1:A:740:PHE:H	1.49	0.60
1:A:1094:HIS:H	1:A:1102:THR:HG22	1.67	0.60
1:A:1173:ASN:HD22	1:A:1174:PRO:N	2.00	0.60
1:A:1121:ASN:HD21	1:A:1167:VAL:H	1.49	0.59
1:A:997:ARG:HD2	1:A:1014:ILE:O	2.02	0.59
1:A:649:HIS:HB2	1:A:650:PRO:CD	2.32	0.59
1:A:181:ILE:HG23	1:A:185:ASP:OD1	2.02	0.59
1:A:572:GLU:O	1:A:575:GLN:HG3	2.02	0.59
1:A:316:ILE:O	1:A:320:LEU:HB2	2.03	0.59
1:A:704:SER:HA	1:A:707:ALA:HB3	1.84	0.58
1:A:24:LYS:HZ2	1:A:24:LYS:HA	1.69	0.58
1:A:72:ILE:HG13	1:A:136:ALA:O	2.04	0.58
1:A:96:VAL:HA	1:A:115:PHE:CZ	2.39	0.58
1:A:1245:THR:O	1:A:1246:LYS:HD3	2.03	0.58
1:A:951:ASN:OD1	1:A:1049:THR:HG23	2.04	0.58
1:A:227:VAL:HG22	1:A:227:VAL:O	2.03	0.58
1:A:924:MET:HE1	1:A:928:LEU:HD11	1.86	0.58
1:A:806:ARG:N	1:A:807:PRO:HD3	2.19	0.58
1:A:356:THR:CG2	1:A:359:ARG:H	2.16	0.57
1:A:894:ILE:HD11	1:A:897:ILE:HB	1.86	0.57
1:A:111:LEU:HA	1:A:114:GLN:HB3	1.85	0.57
1:A:174:ALA:O	1:A:258:ARG:NH1	2.37	0.57
1:A:209:LYS:HE3	1:A:213:GLU:OE2	2.04	0.57
1:A:262:GLY:HA2	1:A:265:ILE:HD12	1.86	0.57
1:A:951:ASN:OD1	1:A:1049:THR:CG2	2.52	0.57
1:A:809:TYR:O	1:A:810:SER:HB2	2.04	0.57
1:A:21:MET:HE3	1:A:430:LEU:HD23	1.87	0.56
1:A:229:LEU:O	1:A:242:VAL:HB	2.05	0.56
1:A:968:ASP:N	1:A:1081:THR:HG22	2.10	0.56
1:A:120:VAL:CA	1:A:123:VAL:HG12	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:GLU:CD	1:A:1210:ARG:HH12	2.09	0.56
1:A:21:MET:HA	1:A:21:MET:CE	2.35	0.56
1:A:72:ILE:HD11	1:A:135:VAL:CG2	2.35	0.56
1:A:80:THR:HG23	1:A:82:PHE:N	2.20	0.56
1:A:931:GLY:O	1:A:1024:GLU:HG2	2.06	0.56
1:A:1182:ILE:HG12	1:A:1184:TYR:CE2	2.40	0.56
1:A:385:GLY:HA3	1:A:484:ILE:HD12	1.88	0.56
1:A:1177:LYS:HA	1:A:1177:LYS:HE3	1.88	0.55
1:A:276:VAL:HG13	1:A:277:ALA:N	2.21	0.55
1:A:380:ALA:O	1:A:381:ALA:HB2	2.06	0.55
1:A:1014:ILE:O	1:A:1014:ILE:HD13	2.07	0.55
1:A:800:THR:HG21	1:A:1073:GLY:HA2	1.89	0.55
1:A:73:ILE:HG23	1:A:259:PHE:CE1	2.41	0.55
3:T:2111:C:H5'	3:T:2112:A:OP2	2.07	0.55
1:A:20:MET:HA	1:A:20:MET:HE3	1.87	0.55
1:A:4:ILE:HD11	1:A:28:THR:HA	1.88	0.55
1:A:629:PRO:HD2	1:A:632:VAL:CG1	2.37	0.55
1:A:1160:GLY:O	3:T:2109:C:H4'	2.07	0.55
1:A:1185:VAL:HG23	1:A:1186:PRO:HD2	1.88	0.55
1:A:34:ILE:H	1:A:34:ILE:HD12	1.72	0.54
1:A:108:VAL:O	1:A:111:LEU:HD23	2.08	0.54
1:A:182:LYS:HB2	1:A:185:ASP:OD2	2.06	0.54
1:A:933:ILE:HG12	1:A:989:TRP:HH2	1.72	0.54
1:A:1077:ASN:HD22	1:A:1077:ASN:C	2.09	0.54
1:A:301:THR:HG22	1:A:365:ASP:HA	1.89	0.54
1:A:439:ARG:NH1	1:A:449:GLY:O	2.40	0.54
1:A:1182:ILE:HD11	1:A:1184:TYR:OH	2.06	0.54
1:A:1206:ASP:O	1:A:1210:ARG:HG3	2.06	0.54
1:A:373:VAL:O	1:A:377:ILE:HG12	2.07	0.54
1:A:111:LEU:HD23	1:A:112:LYS:H	1.73	0.53
1:A:356:THR:HG23	1:A:358:THR:H	1.73	0.53
1:A:1121:ASN:ND2	1:A:1167:VAL:H	2.06	0.53
1:A:163:GLU:HG2	1:A:164:GLU:H	1.70	0.53
1:A:930:ILE:HD11	1:A:1021:TYR:CB	2.39	0.53
1:A:981:CYS:SG	1:A:1014:ILE:HG13	2.49	0.53
1:A:351:HIS:CG	1:A:351:HIS:O	2.62	0.53
1:A:874:THR:HG22	1:A:877:ALA:N	2.23	0.53
1:A:182:LYS:HB3	1:A:184:GLU:OE2	2.09	0.53
1:A:161:ALA:HB1	1:A:165:LEU:HB3	1.91	0.52
1:A:199:LEU:O	1:A:203:MET:HG3	2.09	0.52
1:A:1151:GLN:H	1:A:1151:GLN:HE21	1.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:833:ILE:HG23	1:A:989:TRP:CE2	2.44	0.52
1:A:861:GLY:O	1:A:866:LYS:HE3	2.09	0.52
1:A:37:ALA:O	1:A:41:MET:HG3	2.09	0.52
1:A:220:MET:HA	1:A:223:PHE:CB	2.40	0.52
1:A:586:HIS:CD2	1:A:676:VAL:HG21	2.45	0.52
1:A:93:ALA:HA	1:A:96:VAL:HG12	1.92	0.52
1:A:52:LYS:C	1:A:54:GLY:H	2.13	0.52
1:A:654:ASP:O	1:A:673:VAL:HG21	2.10	0.52
1:A:833:ILE:HG23	1:A:989:TRP:NE1	2.25	0.52
1:A:1177:LYS:HE3	1:A:1178:ASN:N	2.25	0.52
1:A:187:SER:C	1:A:189:GLU:N	2.63	0.52
1:A:548:LYS:HG3	1:A:550:LEU:HD13	1.93	0.51
1:A:837:PRO:HD3	1:A:989:TRP:CD2	2.44	0.51
1:A:596:LEU:HD12	1:A:600:GLU:O	2.10	0.51
1:A:605:THR:HG23	1:A:606:PRO:HD2	1.91	0.51
1:A:220:MET:O	1:A:224:THR:HG23	2.10	0.51
1:A:250:ASN:ND2	1:A:250:ASN:N	2.56	0.51
1:A:529:ILE:HD11	1:A:575:GLN:CD	2.31	0.51
1:A:800:THR:HG21	1:A:1073:GLY:CA	2.41	0.51
1:A:52:LYS:O	1:A:54:GLY:N	2.43	0.51
1:A:874:THR:HB	1:A:923:ASN:HD21	1.76	0.51
1:A:187:SER:O	1:A:189:GLU:N	2.43	0.51
1:A:375:ASN:CA	1:A:378:THR:HG22	2.39	0.51
1:A:649:HIS:HB2	1:A:650:PRO:HD2	1.93	0.51
1:A:377:ILE:HD11	1:A:592:GLU:HB3	1.93	0.51
1:A:604:HIS:CE1	1:A:1262:SER:HB3	2.46	0.51
1:A:74:LEU:HD21	1:A:96:VAL:HG13	1.93	0.51
1:A:134:ARG:HG3	1:A:259:PHE:CE1	2.45	0.51
1:A:15:ARG:CZ	1:A:38:ILE:HG21	2.41	0.51
1:A:453:PRO:C	1:A:454:ILE:HD12	2.31	0.51
1:A:712:ALA:O	1:A:715:THR:HB	2.11	0.51
1:A:66:ILE:H	1:A:66:ILE:HD13	1.75	0.51
1:A:923:ASN:O	1:A:927:GLN:HG3	2.11	0.51
1:A:1016:SER:O	1:A:1022:THR:HG21	2.11	0.50
1:A:35:GLU:O	1:A:38:ILE:HG12	2.11	0.50
1:A:108:VAL:HG22	1:A:112:LYS:HE3	1.92	0.50
1:A:15:ARG:NH2	1:A:38:ILE:HG21	2.26	0.50
1:A:307:HIS:HD2	1:A:390:VAL:HA	1.75	0.50
1:A:57:ALA:HA	1:A:79:GLN:HB3	1.93	0.50
2:G:2008:C:H2'	5:T:2501:GH3:O4'	2.11	0.50
1:A:297:VAL:HB	1:A:361:TYR:CD1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:TYR:CD1	1:A:410:VAL:HG21	2.46	0.50
1:A:13:ARG:HD2	1:A:20:MET:HE3	1.94	0.50
1:A:410:VAL:HG13	1:A:410:VAL:O	2.12	0.50
1:A:598:LYS:HD3	1:A:604:HIS:CB	2.41	0.50
1:A:785:VAL:CG2	1:A:912:THR:HB	2.41	0.50
1:A:862:HIS:CD2	1:A:864:SER:OG	2.64	0.50
1:A:930:ILE:HD11	1:A:1021:TYR:HB2	1.94	0.50
1:A:1239:ILE:HG22	1:A:1239:ILE:O	2.11	0.50
1:A:187:SER:O	1:A:190:VAL:HG12	2.11	0.50
1:A:1049:THR:HG22	1:A:1056:ILE:HB	1.93	0.50
1:A:1235:ILE:N	1:A:1235:ILE:HD12	2.26	0.50
1:A:9:VAL:CG1	1:A:23:CYS:HB3	2.41	0.49
1:A:1243:ASN:HD22	1:A:1243:ASN:N	2.10	0.49
1:A:369:HIS:O	1:A:373:VAL:HG23	2.12	0.49
1:A:13:ARG:C	1:A:15:ARG:H	2.15	0.49
1:A:276:VAL:HG11	1:A:352:VAL:HG11	1.93	0.49
1:A:747:ILE:O	1:A:747:ILE:HG12	2.12	0.49
1:A:871:GLN:HB2	1:A:922:TRP:CD1	2.47	0.49
1:A:1118:LEU:CD2	2:G:2005:C:H5"	2.42	0.49
1:A:109:GLU:OE2	1:A:112:LYS:HD2	2.13	0.49
1:A:191:VAL:HG13	1:A:220:MET:HE3	1.95	0.49
1:A:304:HIS:CE1	1:A:305:VAL:HG12	2.48	0.49
1:A:103:GLY:O	1:A:105:ILE:N	2.46	0.49
1:A:249:HIS:C	1:A:250:ASN:ND2	2.66	0.49
1:A:354:TYR:CE2	1:A:361:TYR:HB2	2.48	0.49
1:A:1023:PHE:O	1:A:1026:GLU:HG2	2.13	0.48
1:A:134:ARG:HH11	1:A:259:PHE:CB	2.26	0.48
1:A:75:GLU:HB3	1:A:134:ARG:HG2	1.94	0.48
1:A:714:ASN:HD21	1:A:1254:PHE:N	1.89	0.48
1:A:1074:PHE:CD2	1:A:1074:PHE:N	2.78	0.48
1:A:130:ILE:HG12	1:A:130:ILE:O	2.13	0.48
1:A:188:ALA:O	1:A:192:GLU:HB2	2.12	0.48
1:A:703:ASN:C	1:A:705:LEU:H	2.17	0.48
1:A:984:LEU:HD23	1:A:1029:ILE:HD12	1.94	0.48
1:A:957:GLU:O	1:A:961:THR:HB	2.14	0.48
1:A:752:ARG:H	1:A:763:ASN:ND2	2.12	0.48
1:A:117:GLU:O	1:A:120:VAL:HG22	2.14	0.47
1:A:252:GLU:OE2	1:A:253:VAL:N	2.46	0.47
1:A:134:ARG:NH1	1:A:259:PHE:HA	2.28	0.47
1:A:47:ILE:O	1:A:50:ALA:HB3	2.14	0.47
1:A:1173:ASN:HD22	1:A:1175:PHE:N	2.04	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1193:ARG:HG2	1:A:1194:ASP:N	2.30	0.47
1:A:20:MET:CE	1:A:20:MET:HA	2.44	0.47
1:A:80:THR:CG2	1:A:83:VAL:H	2.27	0.47
1:A:376:MET:HG3	1:A:410:VAL:HG22	1.95	0.47
1:A:629:PRO:HD2	1:A:632:VAL:HG13	1.96	0.47
1:A:948:GLN:HE21	1:A:1091:CYS:HB3	1.80	0.47
1:A:1173:ASN:ND2	1:A:1173:ASN:C	2.67	0.47
1:A:246:LEU:HD12	1:A:246:LEU:HA	1.82	0.47
1:A:198:GLN:HA	1:A:201:ILE:CD1	2.40	0.47
1:A:197:VAL:HG13	1:A:198:GLN:N	2.30	0.47
1:A:65:LYS:CG	1:A:101:VAL:HG21	2.40	0.47
1:A:626:ILE:HG22	1:A:645:VAL:HG22	1.97	0.47
1:A:824:MET:HE2	1:A:1040:ILE:HD12	1.97	0.47
1:A:23:CYS:O	1:A:27:LEU:HB2	2.15	0.46
1:A:372:TYR:C	1:A:372:TYR:CD1	2.88	0.46
1:A:413:PRO:HB2	1:A:414:TYR:HD1	1.77	0.46
1:A:596:LEU:CD1	1:A:600:GLU:HB2	2.45	0.46
2:G:2005:C:O2'	2:G:2006:C:H5'	2.14	0.46
1:A:562:LEU:N	1:A:562:LEU:HD12	2.31	0.46
1:A:4:ILE:HG22	1:A:5:THR:N	2.29	0.46
1:A:729:ASN:ND2	1:A:740:PHE:H	2.11	0.46
1:A:34:ILE:HG22	1:A:35:GLU:N	2.30	0.46
1:A:418:PHE:HD1	1:A:476:LEU:HD22	1.80	0.46
1:A:521:ILE:HD12	1:A:525:GLU:OE2	2.15	0.46
1:A:324:TYR:CG	1:A:357:PRO:HD3	2.51	0.46
1:A:324:TYR:CD2	1:A:357:PRO:HG3	2.51	0.46
1:A:493:LYS:HB3	1:A:494:PRO:HD2	1.98	0.46
1:A:1173:ASN:HD21	1:A:1175:PHE:H	1.58	0.46
1:A:194:GLU:HA	1:A:197:VAL:HG12	1.98	0.46
1:A:472:LYS:O	1:A:475:GLU:HB3	2.16	0.46
1:A:4:ILE:HG22	1:A:5:THR:HG22	1.98	0.46
1:A:840:GLU:CD	1:A:840:GLU:H	2.19	0.46
1:A:1262:SER:O	1:A:1264:ARG:N	2.48	0.46
1:A:442:LEU:O	1:A:447:PHE:HB2	2.15	0.46
1:A:272:PHE:O	1:A:275:GLU:HB3	2.16	0.46
1:A:203:MET:HG2	1:A:212:ALA:HB3	1.97	0.46
1:A:836:VAL:HG22	1:A:837:PRO:HD2	1.96	0.46
1:A:824:MET:CE	1:A:1040:ILE:HD12	2.46	0.45
1:A:715:THR:HG21	1:A:1149:PRO:HG3	1.97	0.45
1:A:430:LEU:HA	1:A:430:LEU:HD12	1.83	0.45
1:A:833:ILE:HA	1:A:833:ILE:HD12	1.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:2109:C:H2'	3:T:2110:C:C6	2.51	0.45
1:A:15:ARG:HH12	1:A:38:ILE:HD13	1.81	0.45
1:A:66:ILE:O	1:A:66:ILE:HG12	2.16	0.45
1:A:717:ILE:O	1:A:717:ILE:HD13	2.15	0.45
1:A:832:LEU:HG	1:A:833:ILE:HD13	1.98	0.45
1:A:441:LEU:O	1:A:442:LEU:C	2.54	0.45
1:A:874:THR:HG22	1:A:877:ALA:CB	2.46	0.45
1:A:418:PHE:CD1	1:A:476:LEU:HD22	2.52	0.45
1:A:60:GLY:HA3	1:A:77:ASN:HB2	1.99	0.45
1:A:260:GLU:HB3	1:A:263:GLU:HG3	1.99	0.45
1:A:1206:ASP:OD1	1:A:1210:ARG:HD2	2.17	0.45
1:A:372:TYR:CE1	1:A:376:MET:HB2	2.51	0.45
1:A:445:TYR:O	1:A:446:ASP:HB2	2.16	0.45
1:A:301:THR:HG23	1:A:365:ASP:OD2	2.17	0.45
1:A:49:ALA:HA	1:A:52:LYS:HB2	1.99	0.45
1:A:1145:ARG:HH11	1:A:1145:ARG:HB3	1.82	0.45
1:A:253:VAL:HG23	1:A:253:VAL:O	2.17	0.45
1:A:49:ALA:HB2	1:A:123:VAL:CG1	2.40	0.45
1:A:571:ILE:HG22	1:A:572:GLU:N	2.32	0.45
3:T:2109:C:H2'	3:T:2110:C:H6	1.81	0.45
1:A:502:VAL:HG21	1:A:571:ILE:HB	1.99	0.45
1:A:118:GLU:O	1:A:121:ALA:HB3	2.17	0.44
1:A:782:THR:HG23	1:A:784:ALA:HB3	1.99	0.44
1:A:80:THR:HG22	1:A:83:VAL:HG23	1.99	0.44
1:A:252:GLU:CD	1:A:253:VAL:H	2.21	0.44
1:A:320:LEU:HD12	1:A:355:ASP:O	2.17	0.44
1:A:728:ALA:O	1:A:732:LEU:HG	2.18	0.44
1:A:1124:TYR:CE1	1:A:1128:THR:HG21	2.52	0.44
1:A:614:GLN:HG3	1:A:621:ASP:HB3	1.99	0.44
1:A:733:LEU:HD12	1:A:733:LEU:HA	1.86	0.44
1:A:107:ASP:HB3	1:A:110:VAL:HG23	2.00	0.44
1:A:772:LYS:HE3	1:A:1105:TYR:CE1	2.52	0.44
1:A:181:ILE:HD12	1:A:253:VAL:O	2.18	0.44
1:A:765:LEU:HA	1:A:765:LEU:HD12	1.81	0.44
1:A:998:SER:HA	1:A:999:PRO:HD2	1.86	0.44
1:A:121:ALA:O	1:A:125:LYS:HG3	2.17	0.44
1:A:1236:ASP:C	1:A:1238:LEU:N	2.71	0.44
1:A:220:MET:HG2	1:A:220:MET:H	1.59	0.44
1:A:229:LEU:HD11	1:A:242:VAL:HG11	2.00	0.44
1:A:629:PRO:HD2	1:A:632:VAL:HG11	1.99	0.44
1:A:956:HIS:O	1:A:960:VAL:HG12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:GLU:CD	1:A:1241:ARG:HD3	2.39	0.44
1:A:12:LEU:HG	1:A:23:CYS:SG	2.57	0.44
1:A:836:VAL:CG2	1:A:837:PRO:HD2	2.48	0.44
1:A:147:GLN:HG3	1:A:149:GLY:O	2.18	0.44
1:A:210:GLU:HA	1:A:213:GLU:HB2	2.00	0.44
1:A:65:LYS:HG2	1:A:101:VAL:CG2	2.42	0.44
1:A:1057:LEU:N	1:A:1057:LEU:HD23	2.32	0.43
1:A:162:ASP:O	1:A:166:VAL:HG22	2.18	0.43
1:A:384:ASP:O	1:A:413:PRO:HD2	2.17	0.43
1:A:1003:LEU:HB3	1:A:1004:PRO:CD	2.48	0.43
1:A:868:ALA:HB2	1:A:1201:GLY:HA3	1.99	0.43
1:A:276:VAL:CG1	1:A:277:ALA:N	2.81	0.43
1:A:700:SER:O	1:A:1179:ARG:CD	2.63	0.43
1:A:773:TYR:CE2	1:A:775:ASP:HB3	2.54	0.43
1:A:21:MET:O	1:A:25:LYS:HG2	2.19	0.43
1:A:496:LEU:HA	1:A:577:LEU:O	2.19	0.43
1:A:936:ASP:O	1:A:939:ARG:HB2	2.18	0.43
1:A:1236:ASP:C	1:A:1238:LEU:H	2.21	0.43
1:A:806:ARG:N	1:A:807:PRO:CD	2.82	0.43
2:G:2001:G:H2'	2:G:2002:G:H8	1.83	0.43
1:A:152:ILE:HD13	1:A:258:ARG:NH1	2.33	0.43
1:A:52:LYS:C	1:A:54:GLY:N	2.72	0.43
1:A:971:ALA:O	1:A:972:ALA:C	2.57	0.43
1:A:1003:LEU:HB3	1:A:1004:PRO:HD2	2.00	0.43
1:A:134:ARG:HH11	1:A:259:PHE:CA	2.31	0.43
1:A:1019:ASN:CB	1:A:1022:THR:HG22	2.19	0.43
1:A:1035:ARG:NH2	6:A:3515:HOH:O	2.52	0.42
1:A:1093:LYS:HA	1:A:1093:LYS:HD3	1.78	0.42
1:A:1185:VAL:HG11	1:A:1261:CYS:SG	2.59	0.42
1:A:1154:ARG:HH11	1:A:1154:ARG:CG	2.12	0.42
1:A:1172:ILE:HA	1:A:1172:ILE:HD13	1.88	0.42
1:A:4:ILE:HG22	1:A:5:THR:CG2	2.50	0.42
1:A:1128:THR:O	1:A:1128:THR:CG2	2.65	0.42
1:A:165:LEU:HD22	1:A:165:LEU:HA	1.76	0.42
1:A:791:LEU:HD12	1:A:791:LEU:HA	1.69	0.42
1:A:194:GLU:O	1:A:197:VAL:HG12	2.19	0.42
1:A:200:ASP:O	1:A:201:ILE:C	2.58	0.42
1:A:305:VAL:HG13	1:A:306:ASP:H	1.85	0.42
1:A:61:VAL:HG13	1:A:89:PHE:HE1	1.83	0.42
1:A:906:VAL:O	1:A:913:ASP:HB3	2.19	0.42
1:A:1177:LYS:CA	1:A:1177:LYS:HE3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ASP:O	1:A:203:MET:N	2.53	0.42
1:A:246:LEU:HD21	1:A:253:VAL:HG13	2.00	0.42
1:A:628:LEU:HA	1:A:628:LEU:HD12	1.81	0.42
1:A:817:LEU:HD23	1:A:1067:GLU:HG2	2.02	0.42
1:A:837:PRO:HD3	1:A:989:TRP:CE2	2.55	0.42
1:A:93:ALA:HA	1:A:96:VAL:CG1	2.48	0.42
1:A:435:GLU:O	1:A:439:ARG:HG3	2.20	0.42
1:A:567:LYS:HD2	1:A:569:GLU:OE2	2.18	0.42
1:A:812:ASP:O	1:A:814:ASN:N	2.53	0.42
1:A:649:HIS:CB	1:A:650:PRO:CD	2.97	0.42
1:A:777:SER:O	1:A:779:GLY:N	2.52	0.42
1:A:586:HIS:CG	1:A:676:VAL:HG21	2.55	0.42
1:A:222:LYS:O	1:A:225:GLY:N	2.53	0.42
1:A:812:ASP:O	1:A:813:PHE:C	2.58	0.42
1:A:924:MET:HE1	1:A:928:LEU:CD1	2.50	0.42
1:A:1054:ASP:OD1	1:A:1091:CYS:N	2.44	0.41
1:A:579:LYS:HA	1:A:580:PRO:HD3	1.87	0.41
1:A:860:TYR:HA	1:A:865:PHE:CD1	2.55	0.41
1:A:465:GLY:HA2	1:A:470:GLU:OE2	2.19	0.41
1:A:1092:GLY:HA3	2:G:2007:A:H4'	2.01	0.41
1:A:235:VAL:CG1	1:A:608:PHE:HZ	2.33	0.41
1:A:304:HIS:ND1	1:A:305:VAL:HG12	2.36	0.41
1:A:38:ILE:HG13	1:A:39:GLU:N	2.34	0.41
1:A:712:ALA:HB1	1:A:1152:LEU:HD22	2.02	0.41
1:A:74:LEU:HD12	1:A:75:GLU:H	1.85	0.41
1:A:996:LEU:HD12	1:A:996:LEU:HA	1.77	0.41
1:A:1116:LEU:HD13	1:A:1148:LEU:HG	2.03	0.41
1:A:363:HIS:C	1:A:363:HIS:CD2	2.93	0.41
1:A:419:LEU:HD23	1:A:454:ILE:HG23	2.02	0.41
1:A:724:ALA:HB1	1:A:1106:ILE:HG21	2.03	0.41
1:A:521:ILE:O	1:A:552:GLU:HA	2.21	0.41
1:A:846:CYS:HB3	1:A:925:PHE:CE2	2.56	0.41
1:A:785:VAL:HG22	1:A:912:THR:HB	2.02	0.41
1:A:304:HIS:HB3	1:A:307:HIS:CG	2.56	0.41
1:A:500:GLU:CD	1:A:1210:ARG:NH1	2.75	0.41
1:A:658:ARG:NH1	1:A:672:VAL:HG11	2.35	0.41
1:A:64:THR:HB	1:A:147:GLN:NE2	2.36	0.41
1:A:165:LEU:O	1:A:169:ILE:HG23	2.21	0.41
1:A:275:GLU:O	1:A:275:GLU:OE2	2.39	0.41
1:A:10:LYS:HD3	1:A:433:LEU:HD11	2.03	0.41
1:A:944:ASP:OD2	1:A:944:ASP:C	2.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:TYR:O	1:A:199:LEU:HB2	2.21	0.41
1:A:797:CYS:HB2	1:A:1012:GLU:HB3	2.02	0.40
1:A:1057:LEU:H	1:A:1057:LEU:HD23	1.84	0.40
1:A:273:ALA:HA	1:A:352:VAL:HG12	2.04	0.40
1:A:294:LYS:HA	1:A:295:PRO:HD3	1.91	0.40
1:A:300:GLY:CA	1:A:383:MET:SD	3.07	0.40
1:A:596:LEU:HD13	1:A:600:GLU:HB2	2.02	0.40
1:A:901:ASN:C	1:A:901:ASN:ND2	2.73	0.40
1:A:199:LEU:O	1:A:203:MET:HB2	2.22	0.40
1:A:460:LEU:O	1:A:464:GLU:HG3	2.21	0.40
1:A:521:ILE:O	1:A:521:ILE:HG23	2.22	0.40
1:A:878:LEU:HD22	1:A:897:ILE:HD12	2.03	0.40
1:A:950:ILE:O	1:A:950:ILE:HD12	2.21	0.40
1:A:97:LEU:O	1:A:100:ALA:N	2.51	0.40
1:A:1003:LEU:HD12	1:A:1003:LEU:N	2.37	0.40
1:A:134:ARG:HH11	1:A:259:PHE:HA	1.85	0.40
1:A:1122:ASN:HD22	1:A:1122:ASN:HA	1.70	0.40
1:A:180:PHE:CD2	1:A:186:VAL:HG12	2.56	0.40
1:A:234:PHE:CE1	1:A:236:MET:HB2	2.56	0.40
1:A:874:THR:HG21	6:A:3505:HOH:O	2.20	0.40
1:A:172:HIS:CD2	1:A:172:HIS:C	2.95	0.40
1:A:34:ILE:N	1:A:34:ILE:HD12	2.35	0.40
2:G:2004:U:H2'	2:G:2005:C:C6	2.56	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	1193/1289 (93%)	1070 (90%)	100 (8%)	23 (2%)	8 15

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	ILE
1	A	104	LYS
1	A	250	ASN
1	A	381	ALA
1	A	806	ARG
1	A	810	SER
1	A	813	PHE
1	A	1263	SER
1	A	188	ALA
1	A	223	PHE
1	A	778	LEU
1	A	53	ALA
1	A	187	SER
1	A	273	ALA
1	A	324	TYR
1	A	325	GLY
1	A	535	THR
1	A	201	ILE
1	A	467	ALA
1	A	703	ASN
1	A	619	THR
1	A	209	LYS
1	A	780	ILE

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	995/1060 (94%)	851 (86%)	144 (14%)	3 5

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	24	LYS
1	A	40	ASN
1	A	64	THR

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Mol	Chain	Res	Type
1	A	66	ILE
1	A	76	VAL
1	A	80	THR
1	A	81	ASP
1	A	111	LEU
1	A	130	ILE
1	A	133	ARG
1	A	151	ARG
1	A	154	VAL
1	A	155	LEU
1	A	165	LEU
1	A	169	ILE
1	A	181	ILE
1	A	189	GLU
1	A	203	MET
1	A	205	SER
1	A	210	GLU
1	A	230	THR
1	A	237	GLU
1	A	245	LEU
1	A	246	LEU
1	A	250	ASN
1	A	254	THR
1	A	258	ARG
1	A	269	GLU
1	A	292	ARG
1	A	304	HIS
1	A	307	HIS
1	A	352	VAL
1	A	355	ASP
1	A	356	THR
1	A	364	VAL
1	A	371	ASP
1	A	387	ILE
1	A	390	VAL
1	A	399	GLN
1	A	401	ARG
1	A	406	LEU
1	A	410	VAL
1	A	419	LEU
1	A	440	GLU
1	A	452	THR

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Mol	Chain	Res	Type
1	A	480	LEU
1	A	491	ILE
1	A	508	ARG
1	A	516	VAL
1	A	522	LYS
1	A	529	ILE
1	A	530	VAL
1	A	535	THR
1	A	547	ARG
1	A	548	LYS
1	A	549	LEU
1	A	550	LEU
1	A	563	LEU
1	A	568	ARG
1	A	582	THR
1	A	593	VAL
1	A	604	HIS
1	A	614	GLN
1	A	619	THR
1	A	622	VAL
1	A	626	ILE
1	A	628	LEU
1	A	632	VAL
1	A	646	THR
1	A	672	VAL
1	A	676	VAL
1	A	715	THR
1	A	717	ILE
1	A	733	LEU
1	A	747	ILE
1	A	777	SER
1	A	778	LEU
1	A	781	ASP
1	A	782	THR
1	A	791	LEU
1	A	799	LEU
1	A	800	THR
1	A	804	LEU
1	A	809	TYR
1	A	812	ASP
1	A	813	PHE
1	A	833	ILE

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Mol	Chain	Res	Type
1	A	839	VAL
1	A	842	MET
1	A	843	LEU
1	A	847	ARG
1	A	854	THR
1	A	858	ARG
1	A	869	LEU
1	A	873	CYS
1	A	874	THR
1	A	894	ILE
1	A	898	SER
1	A	901	ASN
1	A	930	ILE
1	A	933	ILE
1	A	938	LEU
1	A	949	THR
1	A	950	ILE
1	A	960	VAL
1	A	961	THR
1	A	970	SER
1	A	984	LEU
1	A	996	LEU
1	A	1013	LYS
1	A	1014	ILE
1	A	1021	TYR
1	A	1022	THR
1	A	1033	LEU
1	A	1035	ARG
1	A	1040	ILE
1	A	1049	THR
1	A	1053	ASP
1	A	1075	THR
1	A	1076	THR
1	A	1077	ASN
1	A	1089	GLU
1	A	1099	VAL
1	A	1102	THR
1	A	1116	LEU
1	A	1128	THR
1	A	1145	ARG
1	A	1151	GLN
1	A	1152	LEU

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Mol	Chain	Res	Type
1	A	1154	ARG
1	A	1173	ASN
1	A	1177	LYS
1	A	1182	ILE
1	A	1194	ASP
1	A	1200	LEU
1	A	1204	LEU
1	A	1236	ASP
1	A	1237	GLN
1	A	1241	ARG
1	A	1250	SER
1	A	1251	THR
1	A	1257	GLN
1	A	1261	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	GLN
1	A	147	GLN
1	A	250	ASN
1	A	298	ASN
1	A	307	HIS
1	A	382	GLN
1	A	399	GLN
1	A	409	GLN
1	A	586	HIS
1	A	708	GLN
1	A	714	ASN
1	A	729	ASN
1	A	763	ASN
1	A	862	HIS
1	A	871	GLN
1	A	901	ASN
1	A	948	GLN
1	A	1077	ASN
1	A	1094	HIS
1	A	1121	ASN
1	A	1122	ASN
1	A	1151	GLN
1	A	1155	ASN
1	A	1173	ASN

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Mol	Chain	Res	Type
1	A	1237	GLN
1	A	1243	ASN
1	A	1257	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	G	6/8 (75%)	1 (16%)	0
3	T	11/12 (91%)	2 (18%)	0
All	All	17/20 (85%)	3 (17%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	G	2002	G
3	T	2102	U
3	T	2111	C

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GH3	T	2501	4	25,33,33	2.89	9 (36%)	30,52,52	2.22	8 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GH3	T	2501	4	-	5/18/34/34	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	T	2501	GH3	C2-N2	7.80	1.49	1.33
5	T	2501	GH3	C2'-C1'	-6.31	1.48	1.54
5	T	2501	GH3	C8-N7	-5.82	1.24	1.34
5	T	2501	GH3	O6-C6	5.55	1.38	1.24
5	T	2501	GH3	C6-C5	-2.67	1.36	1.41
5	T	2501	GH3	C6-N1	2.43	1.37	1.33
5	T	2501	GH3	C3'-C4'	-2.07	1.48	1.52
5	T	2501	GH3	C5-C4	2.06	1.46	1.40
5	T	2501	GH3	O2'-C2'	-2.03	1.39	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	T	2501	GH3	C1'-N9-C4	-8.30	112.06	126.64
5	T	2501	GH3	N3-C2-N1	-3.74	122.23	127.22
5	T	2501	GH3	O2G-PG-O3B	3.24	115.50	104.64
5	T	2501	GH3	C6-C5-C4	-3.14	117.80	120.80
5	T	2501	GH3	C6-N1-C2	2.86	120.47	115.93
5	T	2501	GH3	C2-N3-C4	2.70	118.44	115.36
5	T	2501	GH3	C5-C6-N1	-2.64	119.83	123.43
5	T	2501	GH3	PA-O3A-PB	-2.05	125.80	132.83

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	T	2501	GH3	PB-O3A-PA-O5'
5	T	2501	GH3	C5'-O5'-PA-O3A

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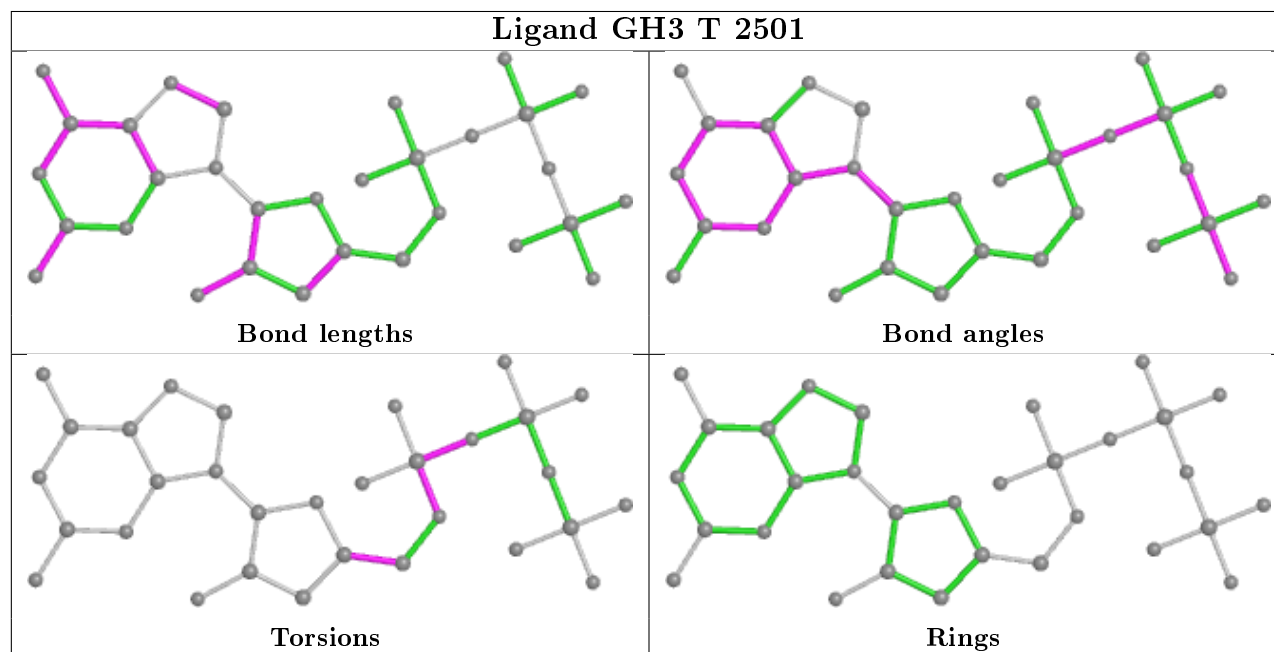
Mol	Chain	Res	Type	Atoms
5	T	2501	GH3	C5'-O5'-PA-O2A
5	T	2501	GH3	O4'-C4'-C5'-O5'
5	T	2501	GH3	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	T	2501	GH3	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	1203/1289 (93%)	-0.12	41 (3%) 45 38	20, 51, 100, 127	0
2	G	8/8 (100%)	-0.19	0 100 100	35, 52, 83, 84	0
3	T	12/12 (100%)	0.08	1 (8%) 11 8	32, 49, 91, 118	0
All	All	1223/1309 (93%)	-0.11	42 (3%) 45 38	20, 51, 100, 127	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	701	SER	7.0
1	A	191	VAL	6.0
1	A	703	ASN	5.5
3	T	2101	A	5.3
1	A	702	ARG	5.2
1	A	199	LEU	5.1
1	A	4	ILE	4.8
1	A	189	GLU	4.7
1	A	778	LEU	4.1
1	A	780	ILE	3.9
1	A	192	GLU	3.9
1	A	15	ARG	3.8
1	A	809	TYR	3.7
1	A	193	LYS	3.5
1	A	1235	ILE	3.5
1	A	812	ASP	3.4
1	A	200	ASP	3.3
1	A	197	VAL	3.2
1	A	190	VAL	3.1
1	A	161	ALA	3.0
1	A	202	ALA	3.0
1	A	8	LEU	2.9
1	A	700	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	291	GLU	2.9
1	A	284	HIS	2.7
1	A	43	LYS	2.6
1	A	204	GLN	2.6
1	A	5	THR	2.6
1	A	34	ILE	2.6
1	A	3	GLU	2.6
1	A	36	LEU	2.5
1	A	33	ASP	2.5
1	A	281	LYS	2.5
1	A	680	ALA	2.4
1	A	223	PHE	2.3
1	A	267	LYS	2.2
1	A	32	GLY	2.2
1	A	807	PRO	2.2
1	A	196	GLN	2.2
1	A	349	THR	2.1
1	A	489	ARG	2.1
1	A	195	TYR	2.1

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](#)

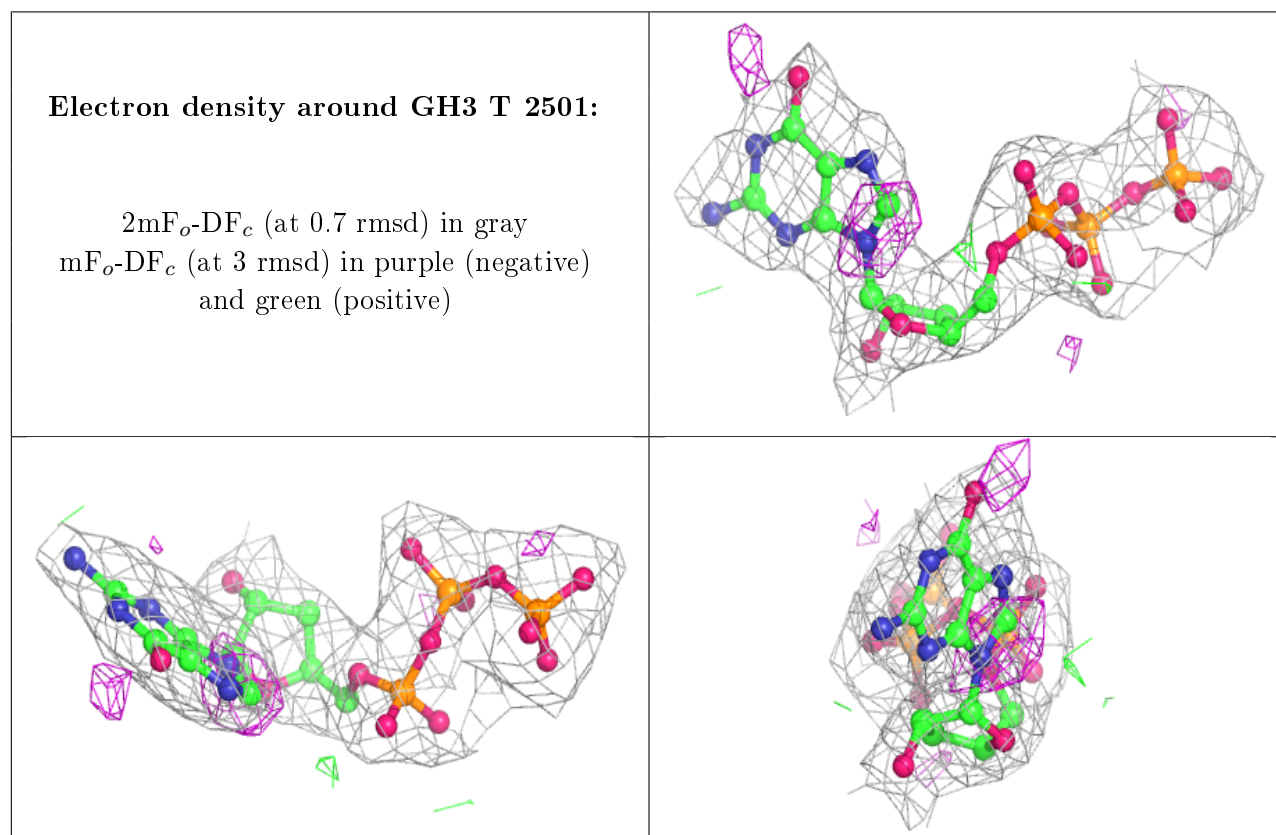
There are no carbohydrates in this entry.

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
4	CA	A	3002	1/1	0.92	0.39	61,61,61,61	0
4	CA	A	3001	1/1	0.98	0.21	33,33,33,33	0
5	GH3	T	2501	31/31	0.98	0.20	29,33,39,39	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.