



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 01:30 pm BST

PDB ID : 3AVX  
Title : Structure of viral RNA polymerase complex 5  
Authors : Takeshita, D.; Tomita, K.  
Deposited on : 2011-03-08  
Resolution : 2.41 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.

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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 : 2.11  
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

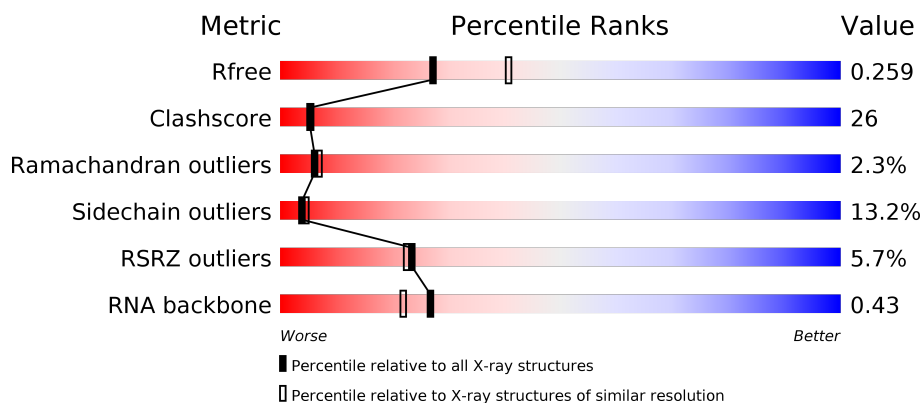
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.41 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)
RNA backbone	3102	1174 (2.80-2.00)

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  $\geq 3$ , 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	1289	<div> <div>5%</div> <div> <div>51%</div> <div>35%</div> <div>7%</div> <div>7%</div> </div> </div>
2	G	9	<div> <div>11%</div> <div> <div>11%</div> <div>44%</div> <div>33%</div> <div>11%</div> </div> </div>
3	T	13	<div> <div>15%</div> <div> <div>23%</div> <div>46%</div> <div>31%</div> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9888 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

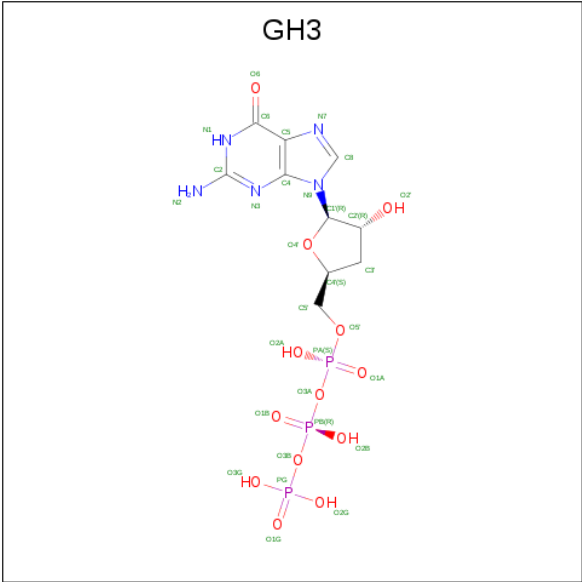
- Molecule 2 is a RNA chain called RNA (5'-R(\*GP\*GP\*GP\*UP\*CP\*CP\*AP\*UP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	9	Total	C	N	O	P	0	0	0
			187	85	33	61	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	13	Total	C	N	O	P	0	0	0
			276	125	54	85	12			

- Molecule 4 is 3'-DEOXY-GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GH3) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



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

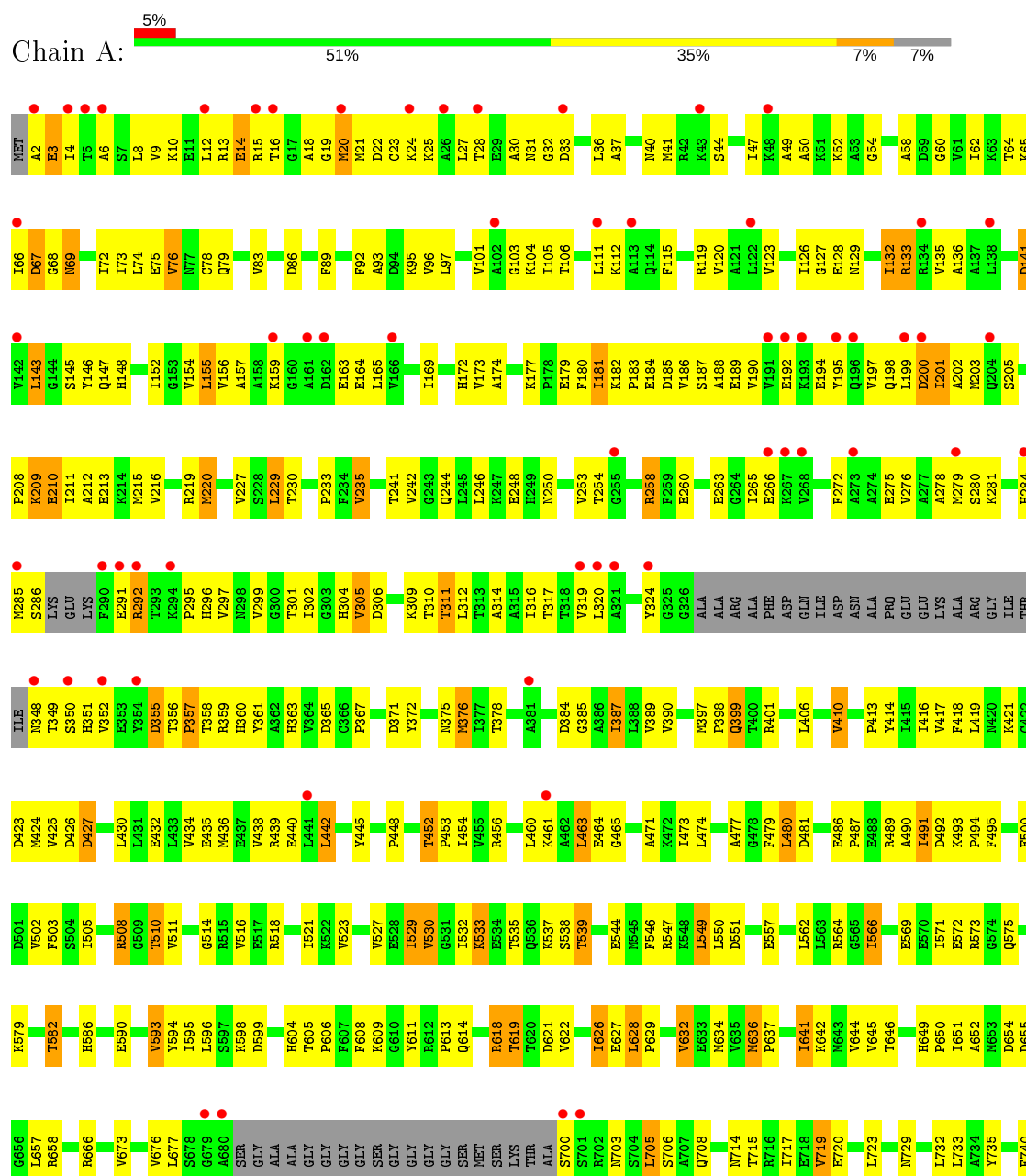
- Molecule 6 is water.

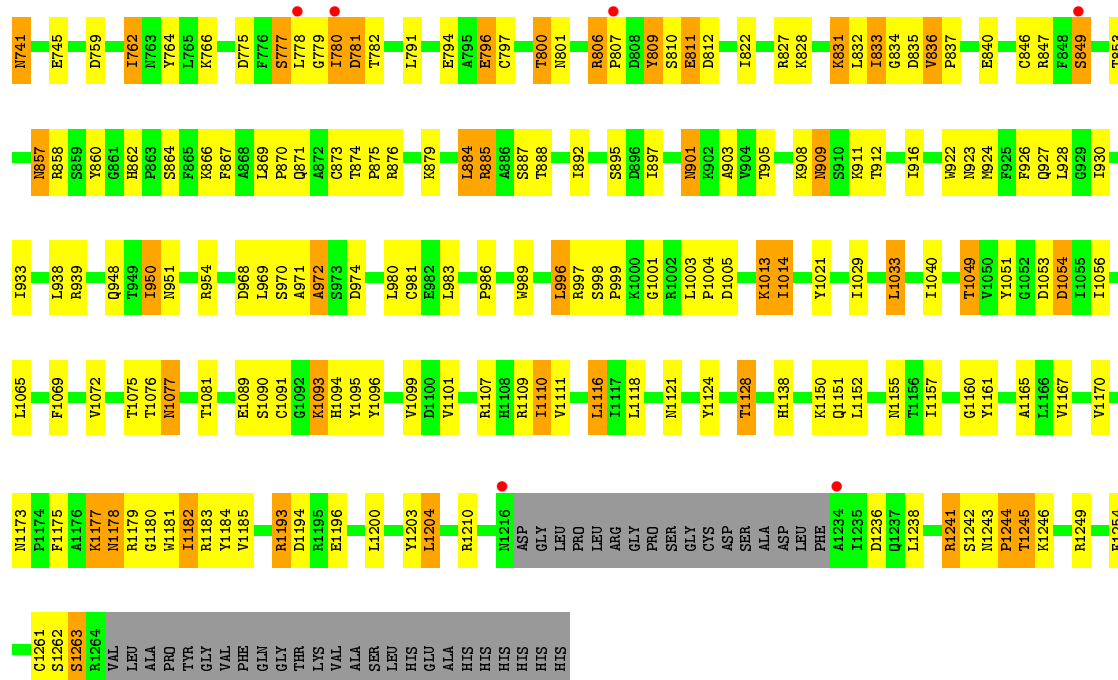
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	96	Total	O	0	0
			96	96		
6	G	2	Total	O	0	0
			2	2		
6	T	7	Total	O	0	0
			7	7		

### 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\*UP\*C)-3')



- Molecule 3: RNA (5'-R(\*AP\*AP\*CP\*GP\*AP\*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, $\alpha$ , $\beta$ , $\gamma$	139.31Å 256.58Å 101.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.93 – 2.41 48.15 – 2.41	Depositor EDS
% Data completeness (in resolution range)	99.4 (19.93-2.41) 99.4 (48.15-2.41)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.80 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.230 , 0.276 0.216 , 0.259	Depositor DCC
$R_{free}$ test set	3561 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.7	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 49.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9888	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% of the height of the origin peak. No significant pseudotranslation is detected.*

<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 ⓘ

### 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	0.51	2/9456 (0.0%)	0.64	0/12787
2	G	0.66	0/208	1.27	3/322 (0.9%)
3	T	0.76	0/309	1.27	3/480 (0.6%)
All	All	0.52	2/9973 (0.0%)	0.70	6/13589 (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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	981	CYS	CB-SG	-5.75	1.72	1.81
1	A	846	CYS	CB-SG	-5.58	1.72	1.81

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2009	C	O4'-C1'-N1	9.00	115.40	108.20
3	T	2103	C	C6-N1-C2	-7.34	117.36	120.30
3	T	2106	U	C6-N1-C2	-5.79	117.53	121.00
2	G	2008	U	N3-C2-O2	-5.24	118.53	122.20
3	T	2106	U	N3-C2-O2	-5.20	118.56	122.20
2	G	2009	C	C6-N1-C2	-5.13	118.25	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	495	0
2	G	187	0	97	10	0
3	T	276	0	144	11	0
4	A	31	0	11	2	0
5	A	2	0	0	0	0
6	A	96	0	0	5	0
6	G	2	0	0	0	0
6	T	7	0	0	0	0
All	All	9888	0	9525	509	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 26.

All (509) 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:491:ILE:HD12	1:A:491:ILE:H	1.17	1.06
1:A:723:LEU:HD23	1:A:1110:ILE:HG12	1.43	0.99
1:A:356:THR:HG22	1:A:358:THR:H	1.28	0.98
1:A:1241:ARG:HG2	1:A:1241:ARG:HH11	1.26	0.98
1:A:950:ILE:HD13	1:A:951:ASN:H	1.30	0.97
1:A:1193:ARG:HH22	1:A:1249:ARG:HH21	1.13	0.96
1:A:611:TYR:HB3	1:A:626:ILE:HD11	1.46	0.96
1:A:65:LYS:HD3	1:A:101:VAL:HG21	1.47	0.94
1:A:658:ARG:HG2	1:A:658:ARG:HH11	1.32	0.93
1:A:618:ARG:HG2	1:A:618:ARG:HH21	1.29	0.93
1:A:399:GLN:HE21	1:A:399:GLN:H	0.98	0.93
1:A:714:ASN:HD21	1:A:1254:PHE:H	1.09	0.91
1:A:152:ILE:HG12	1:A:260:GLU:HG3	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:810:SER:O	1:A:811:GLU:HB2	1.69	0.91
1:A:916:ILE:HD13	3:T:2103:C:C6	2.06	0.90
1:A:74:LEU:HD21	1:A:96:VAL:HG13	1.53	0.89
1:A:729:ASN:HD21	1:A:740:PHE:H	1.20	0.88
1:A:579:LYS:O	1:A:582:THR:HB	1.72	0.88
3:T:2112:C:H5'	3:T:2113:A:OP2	1.75	0.86
1:A:968:ASP:H	1:A:1081:THR:HG22	1.40	0.86
1:A:857:ASN:H	1:A:857:ASN:HD22	1.24	0.85
1:A:1155:ASN:ND2	1:A:1173:ASN:HD21	1.75	0.84
1:A:44:SER:O	1:A:47:ILE:HG22	1.76	0.84
1:A:442:LEU:HD23	1:A:452:THR:HG21	1.60	0.84
1:A:547:ARG:HA	1:A:888:THR:HG22	1.61	0.83
2:G:2001:G:H2'	2:G:2002:G:C8	2.14	0.83
1:A:399:GLN:NE2	1:A:399:GLN:H	1.76	0.82
1:A:1241:ARG:CG	1:A:1241:ARG:HH11	1.93	0.82
1:A:448:PRO:O	1:A:452:THR:HG22	1.80	0.82
1:A:1193:ARG:NH2	1:A:1249:ARG:HH21	1.76	0.81
1:A:309:LYS:HB3	1:A:389:VAL:HG21	1.62	0.80
1:A:12:LEU:HD22	1:A:27:LEU:HD13	1.65	0.79
2:G:2001:G:H2'	2:G:2002:G:H8	1.47	0.79
1:A:212:ALA:O	1:A:216:VAL:HG23	1.81	0.79
1:A:49:ALA:HA	1:A:52:LYS:HB2	1.66	0.78
1:A:780:ILE:H	1:A:780:ILE:HD12	1.48	0.78
1:A:909:ASN:HD22	1:A:911:LYS:H	1.30	0.78
1:A:491:ILE:CD1	1:A:491:ILE:H	1.91	0.78
1:A:1157:ILE:HG22	1:A:1185:VAL:HG21	1.66	0.77
1:A:729:ASN:ND2	1:A:740:PHE:H	1.82	0.76
1:A:3:GLU:HB2	1:A:426:ASP:HB3	1.67	0.76
1:A:618:ARG:HH21	1:A:618:ARG:CG	1.99	0.76
1:A:862:HIS:HD2	1:A:864:SER:H	1.35	0.75
1:A:120:VAL:HA	1:A:123:VAL:HG12	1.67	0.75
1:A:93:ALA:HA	1:A:96:VAL:HG12	1.69	0.74
1:A:1121:ASN:HD21	1:A:1167:VAL:H	1.34	0.74
1:A:626:ILE:HG22	1:A:645:VAL:HG22	1.68	0.74
1:A:951:ASN:OD1	1:A:1049:THR:HG23	1.87	0.74
1:A:874:THR:HG21	6:A:3513:HOH:O	1.86	0.74
1:A:609:LYS:HZ2	1:A:628:LEU:H	1.34	0.74
1:A:930:ILE:HD11	1:A:1021:TYR:CB	2.18	0.74
1:A:1124:TYR:O	1:A:1128:THR:HB	1.88	0.73
1:A:510:THR:HG21	1:A:566:ILE:O	1.88	0.73
1:A:76:VAL:HG11	1:A:93:ALA:HB1	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:ASN:HA	1:A:378:THR:HG22	1.70	0.73
1:A:1077:ASN:O	1:A:1081:THR:HG23	1.88	0.73
1:A:195:TYR:HA	1:A:220:MET:HE1	1.70	0.73
1:A:1054:ASP:OD1	1:A:1090:SER:OG	2.06	0.72
1:A:296:HIS:CD2	1:A:360:HIS:HD2	2.07	0.72
1:A:700:SER:O	1:A:1177:LYS:HG3	1.90	0.72
1:A:372:TYR:CE1	1:A:410:VAL:HG21	2.25	0.71
1:A:658:ARG:NH1	1:A:658:ARG:HG2	2.05	0.71
1:A:700:SER:N	1:A:1179:ARG:HG2	2.04	0.71
1:A:539:THR:HG23	1:A:564:ARG:HB3	1.71	0.71
1:A:950:ILE:HD13	1:A:951:ASN:N	2.04	0.71
1:A:858:ARG:HG3	1:A:858:ARG:HH11	1.54	0.71
1:A:182:LYS:HB3	1:A:184:GLU:OE2	1.91	0.70
1:A:320:LEU:HD12	1:A:355:ASP:O	1.91	0.70
1:A:806:ARG:HG2	1:A:806:ARG:O	1.92	0.70
1:A:930:ILE:HD11	1:A:1021:TYR:HB2	1.74	0.70
1:A:924:MET:HE3	1:A:928:LEU:HG	1.72	0.70
1:A:181:ILE:HD12	1:A:253:VAL:O	1.93	0.69
1:A:21:MET:HE3	1:A:425:VAL:HG22	1.74	0.69
1:A:33:ASP:HB2	1:A:36:LEU:HB3	1.74	0.69
1:A:1241:ARG:HG2	1:A:1241:ARG:NH1	2.00	0.69
1:A:79:GLN:HE21	1:A:128:GLU:HA	1.58	0.68
1:A:714:ASN:ND2	1:A:1254:PHE:H	1.89	0.68
1:A:419:LEU:HD23	1:A:454:ILE:HG23	1.75	0.68
1:A:210:GLU:CD	1:A:210:GLU:H	1.94	0.68
1:A:73:ILE:HB	1:A:155:LEU:HD22	1.75	0.68
1:A:198:GLN:HE21	1:A:201:ILE:HD12	1.57	0.68
1:A:65:LYS:CD	1:A:101:VAL:HG21	2.23	0.68
1:A:954:ARG:NH1	1:A:1049:THR:HB	2.09	0.68
1:A:1049:THR:HG22	1:A:1056:ILE:HB	1.75	0.67
1:A:103:GLY:O	1:A:105:ILE:HG13	1.94	0.67
1:A:126:ILE:HG22	1:A:128:GLU:H	1.60	0.67
1:A:296:HIS:CD2	1:A:360:HIS:CD2	2.83	0.67
1:A:1157:ILE:HG12	1:A:1165:ALA:HB3	1.76	0.67
4:A:2501:GH3:O4'	2:G:2009:C:H2'	1.95	0.67
1:A:924:MET:CE	1:A:928:LEU:HG	2.25	0.66
1:A:194:GLU:HG3	1:A:220:MET:SD	2.36	0.66
1:A:1155:ASN:HD22	1:A:1173:ASN:HD21	1.39	0.66
1:A:764:TYR:OH	1:A:1094:HIS:HD2	1.78	0.66
1:A:198:GLN:NE2	1:A:201:ILE:HD12	2.10	0.66
1:A:549:LEU:HD23	1:A:550:LEU:H	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:GLN:HE21	1:A:129:ASN:H	1.42	0.65
1:A:1193:ARG:HH22	1:A:1249:ARG:NH2	1.92	0.65
1:A:423:ASP:OD2	1:A:424:MET:HG3	1.96	0.65
1:A:930:ILE:HD11	1:A:1021:TYR:CG	2.32	0.65
1:A:12:LEU:HG	1:A:23:CYS:SG	2.37	0.65
1:A:874:THR:HG23	1:A:875:PRO:HD2	1.78	0.65
1:A:372:TYR:HE1	1:A:410:VAL:HG21	1.62	0.65
1:A:295:PRO:HG2	1:A:359:ARG:HG2	1.77	0.65
1:A:997:ARG:NH1	6:A:3550:HOH:O	2.31	0.64
1:A:58:ALA:HB2	1:A:265:ILE:HG21	1.78	0.64
1:A:348:ASN:HA	1:A:351:HIS:CE1	2.32	0.64
1:A:324:TYR:CD1	1:A:357:PRO:HD3	2.32	0.64
1:A:508:ARG:HD3	1:A:562:LEU:HD21	1.80	0.64
1:A:862:HIS:CD2	1:A:864:SER:H	2.15	0.64
1:A:495:PHE:CE2	1:A:521:ILE:HB	2.33	0.63
1:A:1160:GLY:O	3:T:2109:A:H4'	1.97	0.63
1:A:75:GLU:HG2	1:A:133:ARG:HE	1.64	0.63
1:A:316:ILE:O	1:A:320:LEU:HB2	1.99	0.63
1:A:79:GLN:NE2	1:A:128:GLU:HA	2.12	0.63
1:A:421:LYS:HE2	1:A:460:LEU:HD21	1.81	0.63
1:A:4:ILE:HD11	1:A:24:LYS:HG3	1.80	0.63
1:A:529:ILE:HD11	1:A:575:GLN:CD	2.18	0.63
1:A:794:GLU:OE1	1:A:1013:LYS:NZ	2.30	0.63
1:A:1110:ILE:HG13	1:A:1110:ILE:O	1.97	0.63
1:A:1121:ASN:ND2	1:A:1167:VAL:H	1.95	0.63
1:A:796:GLU:O	1:A:800:THR:HG22	1.98	0.63
1:A:281:LYS:HA	1:A:284:HIS:HD2	1.64	0.63
1:A:566:ILE:HG21	1:A:571:ILE:HD11	1.80	0.63
1:A:797:CYS:HA	1:A:800:THR:HG23	1.80	0.62
1:A:183:PRO:HD3	1:A:230:THR:HB	1.81	0.62
1:A:491:ILE:HD12	1:A:491:ILE:N	2.02	0.62
1:A:547:ARG:NH1	1:A:887:SER:HB2	2.14	0.62
1:A:1238:LEU:HD23	1:A:1238:LEU:H	1.64	0.62
1:A:181:ILE:HG12	1:A:182:LYS:HG3	1.81	0.62
1:A:969:LEU:HD21	1:A:1069:PHE:CD2	2.35	0.61
1:A:546:PHE:O	1:A:888:THR:HG22	2.01	0.61
1:A:523:VAL:HG13	1:A:551:ASP:O	2.01	0.61
1:A:723:LEU:HD23	1:A:1110:ILE:CG1	2.25	0.61
1:A:76:VAL:HG11	1:A:93:ALA:CB	2.31	0.61
1:A:1236:ASP:HA	1:A:1238:LEU:HD23	1.82	0.60
1:A:833:ILE:HG23	1:A:989:TRP:NE1	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:847:ARG:NH1	3:T:2105:A:OP1	2.34	0.60
1:A:435:GLU:O	1:A:439:ARG:HG3	2.01	0.60
1:A:658:ARG:CG	1:A:658:ARG:HH11	2.09	0.60
1:A:997:ARG:HD2	1:A:1014:ILE:O	2.02	0.60
1:A:529:ILE:HD11	1:A:575:GLN:OE1	2.01	0.59
1:A:417:VAL:HB	1:A:454:ILE:HG12	1.83	0.59
1:A:590:GLU:HG3	1:A:677:LEU:HD11	1.83	0.59
1:A:143:LEU:HB2	1:A:156:VAL:O	2.02	0.59
1:A:609:LYS:NZ	1:A:628:LEU:H	2.00	0.59
1:A:530:VAL:HG22	1:A:652:ALA:HB2	1.83	0.59
1:A:141:ASP:OD2	1:A:159:LYS:HG3	2.03	0.58
1:A:853:THR:HG23	1:A:866:LYS:HE2	1.84	0.58
1:A:974:ASP:HA	1:A:1013:LYS:HE3	1.86	0.58
1:A:292:ARG:HD2	1:A:292:ARG:N	2.19	0.58
1:A:432:GLU:CG	1:A:456:ARG:HH22	2.17	0.58
1:A:951:ASN:OD1	1:A:1049:THR:CG2	2.52	0.58
1:A:120:VAL:HA	1:A:123:VAL:CG1	2.32	0.58
1:A:66:ILE:HD12	1:A:66:ILE:O	2.04	0.58
1:A:968:ASP:N	1:A:1081:THR:HG22	2.14	0.57
1:A:546:PHE:CD2	1:A:888:THR:HG21	2.39	0.57
1:A:627:GLU:HG2	1:A:644:VAL:HB	1.86	0.57
1:A:92:PHE:HZ	1:A:132:ILE:HD11	1.68	0.57
1:A:1077:ASN:HD22	1:A:1077:ASN:C	2.08	0.57
1:A:265:ILE:HG22	1:A:266:GLU:H	1.68	0.57
1:A:292:ARG:HD2	1:A:292:ARG:H	1.70	0.57
1:A:79:GLN:HE21	1:A:128:GLU:CA	2.18	0.56
1:A:764:TYR:OH	1:A:1094:HIS:CD2	2.57	0.56
1:A:836:VAL:HG22	1:A:837:PRO:HD2	1.87	0.56
1:A:511:VAL:HB	1:A:562:LEU:HD23	1.86	0.56
1:A:546:PHE:O	1:A:888:THR:CG2	2.53	0.56
1:A:1243:ASN:HB3	1:A:1244:PRO:HD2	1.85	0.56
1:A:187:SER:HB3	1:A:190:VAL:HB	1.87	0.56
1:A:372:TYR:C	1:A:372:TYR:CD1	2.78	0.56
1:A:195:TYR:OH	1:A:213:GLU:HG3	2.06	0.56
1:A:916:ILE:HD13	3:T:2103:C:N1	2.20	0.56
1:A:23:CYS:O	1:A:27:LEU:HB2	2.06	0.56
1:A:279:MET:HG2	1:A:314:ALA:HB2	1.88	0.56
1:A:432:GLU:HG2	1:A:456:ARG:HH22	1.70	0.56
4:A:2501:GH3:N2	3:T:2103:C:O2	2.36	0.56
1:A:806:ARG:H	1:A:807:PRO:HD3	1.71	0.56
1:A:948:GLN:HG2	1:A:1051:TYR:CZ	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:GLN:NE2	1:A:129:ASN:H	2.03	0.55
1:A:272:PHE:O	1:A:275:GLU:HB3	2.06	0.55
1:A:779:GLY:C	1:A:781:ASP:H	2.09	0.55
1:A:732:LEU:HD21	1:A:766:LYS:HB2	1.89	0.55
1:A:169:ILE:O	1:A:173:VAL:HG23	2.07	0.55
1:A:126:ILE:HG22	1:A:128:GLU:N	2.21	0.55
1:A:618:ARG:NH2	1:A:618:ARG:CG	2.62	0.55
1:A:163:GLU:HG2	1:A:164:GLU:H	1.72	0.54
1:A:208:PRO:HG2	1:A:211:ILE:HG12	1.89	0.54
1:A:463:LEU:HD12	1:A:464:GLU:N	2.22	0.54
1:A:604:HIS:CE1	1:A:1262:SER:HB3	2.42	0.54
1:A:413:PRO:HB2	1:A:414:TYR:CD1	2.41	0.54
1:A:741:ASN:OD1	1:A:745:GLU:HB2	2.08	0.54
1:A:629:PRO:HG2	1:A:632:VAL:HG11	1.88	0.54
1:A:211:ILE:O	1:A:215:MET:HG3	2.07	0.54
1:A:37:ALA:HA	1:A:40:ASN:HD22	1.73	0.54
1:A:874:THR:HG22	1:A:876:ARG:H	1.73	0.54
2:G:2007:A:H3'	2:G:2008:U:H5''	1.90	0.54
1:A:714:ASN:HD21	1:A:1254:PHE:N	1.93	0.54
1:A:181:ILE:HD12	1:A:253:VAL:HG23	1.90	0.54
1:A:187:SER:HB3	1:A:190:VAL:CG1	2.38	0.54
1:A:65:LYS:HB2	1:A:97:LEU:HD11	1.90	0.54
1:A:79:GLN:HE21	1:A:129:ASN:N	2.06	0.54
1:A:312:LEU:O	1:A:316:ILE:HG13	2.08	0.53
1:A:604:HIS:HE1	1:A:1262:SER:HB3	1.73	0.53
1:A:305:VAL:HG13	1:A:306:ASP:H	1.73	0.53
1:A:586:HIS:CG	1:A:676:VAL:HG21	2.44	0.53
1:A:296:HIS:HD2	1:A:360:HIS:HB3	1.74	0.53
1:A:285:MET:O	1:A:286:SER:HB2	2.07	0.53
1:A:304:HIS:NE2	1:A:305:VAL:HG12	2.24	0.53
1:A:305:VAL:HG13	1:A:306:ASP:N	2.23	0.53
1:A:276:VAL:HG11	1:A:352:VAL:HG22	1.90	0.53
1:A:356:THR:HG23	1:A:357:PRO:HD2	1.91	0.53
1:A:416:ILE:HG12	1:A:453:PRO:HG2	1.91	0.53
1:A:500:GLU:CD	1:A:1210:ARG:HH12	2.12	0.52
1:A:276:VAL:HG23	1:A:314:ALA:HA	1.90	0.52
1:A:401:ARG:CG	1:A:445:TYR:OH	2.58	0.52
1:A:1091:CYS:HA	2:G:2009:C:H5'	1.91	0.52
1:A:115:PHE:O	1:A:119:ARG:HB2	2.09	0.52
1:A:495:PHE:HA	1:A:518:ARG:O	2.09	0.52
1:A:6:ALA:HB1	1:A:9:VAL:CG2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:ILE:HG13	1:A:529:ILE:O	2.09	0.52
1:A:187:SER:O	1:A:190:VAL:HG12	2.09	0.52
1:A:189:GLU:HA	1:A:192:GLU:CG	2.39	0.52
1:A:2:ALA:HA	1:A:427:ASP:HA	1.91	0.52
1:A:229:LEU:HD22	1:A:242:VAL:HG11	1.91	0.52
1:A:901:ASN:ND2	1:A:1001:GLY:HA2	2.25	0.52
1:A:132:ILE:H	1:A:132:ILE:HD12	1.73	0.52
1:A:181:ILE:HG23	1:A:185:ASP:OD1	2.10	0.52
1:A:187:SER:C	1:A:189:GLU:H	2.13	0.52
1:A:349:THR:HG22	1:A:349:THR:O	2.10	0.52
1:A:19:GLY:O	1:A:23:CYS:HB2	2.09	0.52
1:A:828:LYS:O	1:A:831:LYS:HG3	2.10	0.52
3:T:2108:G:O2'	3:T:2109:A:H5'	2.10	0.52
1:A:25:LYS:O	1:A:28:THR:HG22	2.10	0.52
1:A:608:PHE:CE1	1:A:634:MET:HB2	2.46	0.51
1:A:705:LEU:HD11	1:A:1175:PHE:CD2	2.45	0.51
1:A:658:ARG:CG	1:A:658:ARG:NH1	2.68	0.51
1:A:951:ASN:HB3	1:A:1090:SER:OG	2.10	0.51
1:A:954:ARG:HD3	1:A:1049:THR:HG21	1.91	0.51
1:A:210:GLU:CD	1:A:210:GLU:N	2.64	0.51
1:A:544:GLU:HB3	1:A:549:LEU:HG	1.93	0.51
1:A:24:LYS:HD2	1:A:430:LEU:HD22	1.92	0.51
1:A:546:PHE:CE2	1:A:888:THR:HG21	2.46	0.51
1:A:37:ALA:HA	1:A:40:ASN:ND2	2.26	0.51
1:A:732:LEU:CD2	1:A:766:LYS:HB2	2.41	0.51
1:A:923:ASN:O	1:A:927:GLN:HG3	2.11	0.51
1:A:67:ASP:O	1:A:69:ASN:N	2.44	0.51
1:A:950:ILE:CD1	1:A:951:ASN:N	2.73	0.51
1:A:278:ALA:O	1:A:281:LYS:HB3	2.11	0.51
1:A:629:PRO:HD3	1:A:642:LYS:O	2.11	0.51
1:A:735:TYR:CG	1:A:762:ILE:HG13	2.46	0.51
1:A:154:VAL:HG12	1:A:258:ARG:CB	2.41	0.50
1:A:301:THR:HG23	1:A:365:ASP:OD2	2.10	0.50
1:A:49:ALA:CA	1:A:52:LYS:HB2	2.40	0.50
1:A:871:GLN:HB2	1:A:922:TRP:CD1	2.47	0.50
1:A:1243:ASN:HB3	1:A:1244:PRO:CD	2.42	0.50
1:A:33:ASP:CB	1:A:36:LEU:HB3	2.39	0.50
1:A:885:ARG:O	1:A:885:ARG:HG3	2.12	0.50
1:A:495:PHE:CE1	1:A:521:ILE:HD12	2.46	0.50
1:A:306:ASP:HB3	1:A:310:THR:HG21	1.93	0.50
1:A:60:GLY:HA2	1:A:78:CYS:SG	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:ILE:HG22	1:A:266:GLU:N	2.26	0.50
1:A:304:HIS:CD2	1:A:305:VAL:H	2.29	0.50
1:A:461:LYS:HA	1:A:464:GLU:HG2	1.93	0.50
1:A:356:THR:HG21	1:A:481:ASP:CG	2.31	0.49
1:A:897:ILE:O	1:A:897:ILE:HG23	2.12	0.49
1:A:92:PHE:CZ	1:A:132:ILE:HD11	2.47	0.49
1:A:598:LYS:CG	1:A:604:HIS:HA	2.43	0.49
1:A:83:VAL:O	1:A:86:ASP:HB3	2.12	0.49
1:A:179:GLU:HB2	1:A:227:VAL:HG22	1.93	0.49
1:A:605:THR:HG23	1:A:606:PRO:HD2	1.93	0.49
1:A:627:GLU:CG	1:A:644:VAL:HB	2.43	0.49
1:A:857:ASN:HD21	1:A:860:TYR:HD1	1.60	0.49
1:A:1013:LYS:HB3	1:A:1013:LYS:NZ	2.27	0.49
1:A:1093:LYS:HB3	1:A:1095:TYR:CE2	2.48	0.49
1:A:135:VAL:HG22	1:A:136:ALA:N	2.28	0.49
2:G:2002:G:H2'	2:G:2003:G:C8	2.47	0.49
1:A:834:GLY:O	1:A:986:PRO:HG2	2.13	0.49
3:T:2102:A:N3	3:T:2102:A:H2'	2.26	0.49
1:A:244:GLN:O	1:A:248:GLU:HG3	2.13	0.49
1:A:909:ASN:ND2	1:A:911:LYS:H	2.04	0.48
1:A:356:THR:HG21	1:A:481:ASP:OD2	2.13	0.48
1:A:387:ILE:O	1:A:387:ILE:HG13	2.12	0.48
1:A:521:ILE:HD11	1:A:527:VAL:HG11	1.95	0.48
1:A:67:ASP:C	1:A:69:ASN:H	2.17	0.48
1:A:105:ILE:HD12	1:A:111:LEU:HD13	1.96	0.48
1:A:285:MET:HG3	1:A:286:SER:N	2.28	0.48
1:A:421:LYS:HG2	1:A:460:LEU:CD2	2.43	0.48
2:G:2002:G:H2'	2:G:2003:G:H8	1.77	0.48
1:A:203:MET:SD	1:A:209:LYS:HA	2.54	0.48
1:A:629:PRO:HG2	1:A:632:VAL:CG1	2.43	0.48
1:A:64:THR:HG22	1:A:73:ILE:HG13	1.95	0.48
1:A:857:ASN:N	1:A:857:ASN:HD22	1.98	0.48
1:A:154:VAL:HG12	1:A:258:ARG:HB2	1.95	0.48
1:A:806:ARG:N	1:A:807:PRO:CD	2.77	0.48
1:A:8:LEU:CD1	1:A:10:LYS:HE2	2.44	0.48
1:A:903:ALA:O	1:A:1004:PRO:HD3	2.13	0.48
1:A:49:ALA:HB2	1:A:123:VAL:HG11	1.96	0.48
1:A:202:ALA:HB3	1:A:212:ALA:HB1	1.95	0.48
1:A:311:THR:O	1:A:314:ALA:HB3	2.14	0.48
1:A:419:LEU:HD23	1:A:454:ILE:CG2	2.42	0.48
1:A:598:LYS:HG3	1:A:604:HIS:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:ASP:O	1:A:413:PRO:HG2	2.14	0.48
1:A:41:MET:HA	1:A:44:SER:HG	1.78	0.48
1:A:840:GLU:CD	1:A:840:GLU:H	2.15	0.48
1:A:20:MET:CG	1:A:430:LEU:HG	2.44	0.47
1:A:1151:GLN:O	1:A:1175:PHE:HE1	1.96	0.47
1:A:177:LYS:HD3	1:A:258:ARG:NH2	2.29	0.47
1:A:74:LEU:HD23	1:A:97:LEU:HB2	1.96	0.47
1:A:879:LYS:HG2	6:A:3509:HOH:O	2.14	0.47
1:A:948:GLN:HE21	1:A:1091:CYS:HB3	1.79	0.47
1:A:971:ALA:O	1:A:972:ALA:C	2.52	0.47
1:A:105:ILE:HG22	1:A:106:THR:N	2.29	0.47
1:A:24:LYS:HD2	1:A:430:LEU:CD2	2.45	0.47
1:A:998:SER:HA	1:A:999:PRO:HD2	1.68	0.47
1:A:14:GLU:O	1:A:14:GLU:HG2	2.15	0.47
1:A:538:SER:HB2	1:A:566:ILE:HG13	1.96	0.47
1:A:649:HIS:HB2	1:A:650:PRO:HD2	1.96	0.47
1:A:573:ARG:NH2	1:A:619:THR:O	2.48	0.47
1:A:908:LYS:HB3	1:A:912:THR:O	2.15	0.47
1:A:477:ALA:HA	1:A:480:LEU:HD22	1.97	0.47
1:A:505:ILE:HD11	1:A:1203:TYR:CD1	2.49	0.47
1:A:857:ASN:ND2	6:A:3586:HOH:O	2.47	0.47
1:A:299:VAL:HA	1:A:385:GLY:O	2.14	0.47
1:A:1110:ILE:HD11	1:A:1116:LEU:HG	1.97	0.47
1:A:571:ILE:HG22	1:A:572:GLU:N	2.30	0.47
1:A:867:PHE:HB3	1:A:1204:LEU:HD12	1.96	0.47
1:A:867:PHE:CD2	1:A:1204:LEU:HD13	2.50	0.47
1:A:909:ASN:HD22	1:A:911:LYS:N	2.05	0.47
1:A:389:VAL:O	1:A:389:VAL:HG23	2.15	0.46
1:A:52:LYS:C	1:A:54:GLY:H	2.18	0.46
1:A:777:SER:OG	1:A:778:LEU:HD12	2.14	0.46
1:A:199:LEU:O	1:A:203:MET:HG2	2.15	0.46
1:A:291:GLU:H	1:A:292:ARG:NH2	2.12	0.46
1:A:486:GLU:HA	1:A:487:PRO:HD3	1.84	0.46
1:A:502:VAL:HG11	1:A:571:ILE:HB	1.97	0.46
1:A:822:ILE:HD11	1:A:1072:VAL:HG12	1.98	0.46
1:A:1161:TYR:CZ	1:A:1261:CYS:HB2	2.51	0.46
1:A:1182:ILE:HG12	1:A:1184:TYR:CE2	2.50	0.46
1:A:401:ARG:HG3	1:A:445:TYR:OH	2.15	0.46
1:A:916:ILE:CD1	3:T:2103:C:C6	2.91	0.46
1:A:157:ALA:O	1:A:254:THR:N	2.49	0.46
1:A:954:ARG:HH11	1:A:1049:THR:HB	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1157:ILE:O	1:A:1167:VAL:HA	2.14	0.46
1:A:503:PHE:HB2	1:A:511:VAL:HG12	1.97	0.46
1:A:614:GLN:NE2	1:A:621:ASP:HB3	2.31	0.46
1:A:980:LEU:HD22	1:A:1072:VAL:HB	1.97	0.46
1:A:460:LEU:H	1:A:460:LEU:CD1	2.29	0.46
1:A:20:MET:HG3	1:A:430:LEU:HG	1.97	0.46
1:A:120:VAL:CA	1:A:123:VAL:HG12	2.43	0.46
1:A:195:TYR:CA	1:A:220:MET:HE1	2.42	0.46
1:A:285:MET:O	1:A:286:SER:CB	2.64	0.46
1:A:279:MET:HG2	1:A:314:ALA:CB	2.46	0.46
1:A:372:TYR:CE1	1:A:376:MET:HB2	2.50	0.46
1:A:319:VAL:HG12	1:A:474:LEU:HD21	1.98	0.46
1:A:779:GLY:C	1:A:781:ASP:N	2.68	0.46
1:A:78:CYS:HB3	1:A:89:PHE:CE2	2.50	0.46
1:A:1185:VAL:HG22	1:A:1261:CYS:SG	2.56	0.46
1:A:593:VAL:HG22	1:A:641:ILE:CG2	2.46	0.46
1:A:119:ARG:HH11	1:A:119:ARG:HG2	1.81	0.45
1:A:4:ILE:HD11	1:A:24:LYS:CG	2.44	0.45
1:A:495:PHE:CZ	1:A:521:ILE:HD12	2.52	0.45
1:A:884:LEU:O	1:A:887:SER:OG	2.31	0.45
1:A:1193:ARG:NH2	1:A:1249:ARG:NH2	2.57	0.45
1:A:4:ILE:HG12	1:A:24:LYS:NZ	2.31	0.45
1:A:950:ILE:CD1	1:A:951:ASN:H	2.14	0.45
1:A:145:SER:HB3	1:A:155:LEU:HD12	1.99	0.45
1:A:227:VAL:HG22	1:A:227:VAL:O	2.17	0.45
1:A:280:SER:O	1:A:284:HIS:N	2.50	0.45
1:A:858:ARG:NH1	1:A:858:ARG:HG3	2.25	0.45
1:A:514:GLY:HA2	1:A:1210:ARG:HH11	1.82	0.45
1:A:180:PHE:CD2	1:A:186:VAL:HG12	2.52	0.45
1:A:399:GLN:HE21	1:A:399:GLN:N	1.84	0.45
1:A:618:ARG:NH2	1:A:618:ARG:HG2	2.10	0.45
1:A:72:ILE:CG2	1:A:101:VAL:HG22	2.46	0.45
1:A:924:MET:HE1	1:A:928:LEU:HD11	1.99	0.45
1:A:187:SER:HB3	1:A:190:VAL:CB	2.46	0.45
1:A:729:ASN:HD22	1:A:729:ASN:HA	1.60	0.45
1:A:968:ASP:H	1:A:1081:THR:CG2	2.19	0.45
1:A:281:LYS:HA	1:A:284:HIS:CD2	2.47	0.45
1:A:64:THR:CG2	1:A:73:ILE:HG13	2.47	0.45
1:A:939:ARG:HB2	1:A:939:ARG:HE	1.44	0.45
1:A:65:LYS:HB3	1:A:101:VAL:HG21	1.98	0.45
1:A:10:LYS:O	1:A:14:GLU:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:VAL:CG1	1:A:608:PHE:HZ	2.29	0.45
1:A:537:LYS:HE2	1:A:537:LYS:HB3	1.65	0.45
1:A:609:LYS:HD2	1:A:609:LYS:HA	1.74	0.45
1:A:1180:GLY:O	1:A:1181:TRP:HB2	2.17	0.44
1:A:1204:LEU:HA	1:A:1204:LEU:HD23	1.78	0.44
1:A:857:ASN:ND2	1:A:857:ASN:H	2.03	0.44
1:A:924:MET:CE	1:A:928:LEU:CG	2.93	0.44
1:A:187:SER:HB3	1:A:190:VAL:HG12	1.98	0.44
1:A:233:PRO:HA	1:A:241:THR:HA	1.98	0.44
1:A:514:GLY:HA2	1:A:1210:ARG:NH1	2.32	0.44
1:A:806:ARG:H	1:A:807:PRO:CD	2.30	0.44
1:A:806:ARG:N	1:A:807:PRO:HD3	2.32	0.44
1:A:291:GLU:HG2	1:A:291:GLU:O	2.18	0.44
1:A:146:TYR:OH	1:A:148:HIS:HB2	2.17	0.44
1:A:375:ASN:HA	1:A:378:THR:CG2	2.44	0.44
1:A:708:GLN:HB3	1:A:1151:GLN:HE22	1.81	0.44
1:A:112:LYS:HB2	1:A:112:LYS:NZ	2.32	0.44
1:A:133:ARG:NH1	1:A:263:GLU:O	2.43	0.44
1:A:926:PHE:HB3	1:A:996:LEU:HD21	1.98	0.44
1:A:997:ARG:O	6:A:3513:HOH:O	2.21	0.44
1:A:1118:LEU:HD11	2:G:2006:C:H4'	1.99	0.44
1:A:1236:ASP:HA	1:A:1238:LEU:CD2	2.47	0.44
1:A:312:LEU:HD22	1:A:418:PHE:CD2	2.53	0.44
1:A:471:ALA:HA	1:A:474:LEU:HG	2.00	0.44
1:A:181:ILE:CD1	1:A:253:VAL:HG23	2.47	0.44
1:A:924:MET:HE1	1:A:928:LEU:CG	2.48	0.44
1:A:1003:LEU:CD1	1:A:1003:LEU:N	2.81	0.44
1:A:434:VAL:O	1:A:438:VAL:HG12	2.18	0.44
1:A:416:ILE:HD13	1:A:479:PHE:HB3	2.00	0.44
1:A:1177:LYS:HD3	1:A:1178:ASN:N	2.33	0.43
1:A:65:LYS:HB3	1:A:101:VAL:CG2	2.48	0.43
1:A:436:MET:O	1:A:440:GLU:HG2	2.19	0.43
1:A:1245:THR:O	1:A:1246:LYS:HE2	2.19	0.43
1:A:594:TYR:HE2	1:A:596:LEU:HD13	1.83	0.43
1:A:741:ASN:ND2	1:A:741:ASN:H	2.16	0.43
1:A:1262:SER:HB2	1:A:1263:SER:H	1.63	0.43
1:A:884:LEU:HD13	1:A:892:ILE:HG12	1.99	0.43
1:A:324:TYR:CG	1:A:357:PRO:HD3	2.53	0.43
1:A:494:PRO:O	1:A:518:ARG:HG3	2.18	0.43
1:A:614:GLN:HE21	1:A:621:ASP:HB3	1.82	0.43
1:A:304:HIS:CD2	1:A:305:VAL:N	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:719:VAL:HG13	1:A:720:GLU:N	2.34	0.43
1:A:924:MET:HB3	1:A:924:MET:HE2	1.88	0.43
1:A:723:LEU:CD2	1:A:1110:ILE:HG12	2.32	0.43
1:A:532:ILE:HD12	1:A:532:ILE:N	2.34	0.43
1:A:538:SER:OG	1:A:539:THR:N	2.49	0.43
1:A:590:GLU:HG2	1:A:644:VAL:HG22	2.00	0.43
1:A:309:LYS:CB	1:A:389:VAL:HG21	2.42	0.43
1:A:489:ARG:HD2	1:A:492:ASP:OD2	2.19	0.43
1:A:533:LYS:HE2	1:A:533:LYS:HB3	1.77	0.43
1:A:595:ILE:HG22	1:A:637:PRO:HA	2.00	0.43
1:A:1096:TYR:O	1:A:1099:VAL:HG13	2.19	0.43
1:A:1118:LEU:HD12	1:A:1118:LEU:HA	1.89	0.43
1:A:1093:LYS:HA	1:A:1093:LYS:HD2	1.66	0.42
1:A:13:ARG:C	1:A:15:ARG:H	2.21	0.42
2:G:2007:A:H5'	2:G:2008:U:OP2	2.19	0.42
1:A:365:ASP:O	1:A:367:PRO:HD3	2.18	0.42
1:A:62:ILE:O	1:A:147:GLN:NE2	2.46	0.42
1:A:276:VAL:CG2	1:A:314:ALA:HA	2.49	0.42
1:A:301:THR:HG22	1:A:363:HIS:NE2	2.34	0.42
1:A:657:LEU:H	1:A:673:VAL:HG22	1.84	0.42
1:A:20:MET:CE	1:A:20:MET:HA	2.49	0.42
1:A:636:MET:HG2	1:A:636:MET:H	1.69	0.42
1:A:735:TYR:CD1	1:A:762:ILE:HG13	2.54	0.42
1:A:1170:VAL:HG23	1:A:1185:VAL:HG11	2.00	0.42
1:A:199:LEU:HA	1:A:216:VAL:HG21	2.02	0.42
1:A:200:ASP:O	1:A:203:MET:N	2.53	0.42
1:A:208:PRO:HG2	1:A:211:ILE:CG1	2.49	0.42
1:A:220:MET:HE2	1:A:220:MET:HB2	1.86	0.42
1:A:4:ILE:HG12	1:A:24:LYS:HE2	2.02	0.42
1:A:500:GLU:CD	1:A:1210:ARG:NH1	2.73	0.42
1:A:1150:LYS:HB3	1:A:1150:LYS:HE2	1.73	0.42
1:A:870:PRO:O	1:A:895:SER:HB3	2.19	0.42
1:A:700:SER:N	1:A:1179:ARG:CG	2.78	0.42
1:A:1241:ARG:HA	1:A:1241:ARG:HD3	1.82	0.42
1:A:197:VAL:HG13	1:A:198:GLN:N	2.35	0.42
1:A:297:VAL:HB	1:A:361:TYR:CD1	2.55	0.42
1:A:740:PHE:HD2	1:A:745:GLU:HG3	1.85	0.42
1:A:1029:ILE:O	1:A:1033:LEU:HD22	2.20	0.42
1:A:16:THR:HG22	1:A:18:ALA:HB2	2.01	0.42
1:A:490:ALA:HA	1:A:493:LYS:HE3	2.02	0.42
1:A:47:ILE:O	1:A:50:ALA:HB3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:649:HIS:HB2	1:A:650:PRO:CD	2.49	0.42
1:A:546:PHE:CD2	1:A:888:THR:CG2	3.03	0.41
1:A:950:ILE:CG1	1:A:951:ASN:N	2.83	0.41
2:G:2005:C:H2'	2:G:2006:C:O5'	2.20	0.41
1:A:1193:ARG:HH21	1:A:1193:ARG:HB2	1.85	0.41
1:A:410:VAL:HG13	1:A:410:VAL:O	2.19	0.41
1:A:930:ILE:CD1	1:A:1021:TYR:CB	2.95	0.41
1:A:1121:ASN:HD21	1:A:1167:VAL:N	2.10	0.41
1:A:185:ASP:O	1:A:186:VAL:C	2.59	0.41
1:A:27:LEU:HA	1:A:27:LEU:HD12	1.90	0.41
1:A:777:SER:OG	1:A:778:LEU:N	2.52	0.41
1:A:901:ASN:HD22	1:A:901:ASN:C	2.22	0.41
1:A:189:GLU:CD	1:A:192:GLU:HG3	2.40	0.41
1:A:20:MET:O	1:A:24:LYS:HB3	2.21	0.41
1:A:95:LYS:C	1:A:97:LEU:H	2.24	0.41
1:A:874:THR:HG22	1:A:876:ARG:N	2.35	0.41
1:A:372:TYR:CD1	1:A:410:VAL:HG21	2.55	0.41
1:A:319:VAL:HB	1:A:473:ILE:HG21	2.01	0.41
1:A:828:LYS:HD3	1:A:828:LYS:HA	1.84	0.41
1:A:163:GLU:H	1:A:163:GLU:CD	2.24	0.41
1:A:397:MET:HB3	1:A:398:PRO:HD2	2.03	0.41
1:A:930:ILE:CD1	1:A:1021:TYR:HB2	2.47	0.41
1:A:775:ASP:OD2	1:A:1109:ARG:HD3	2.21	0.41
1:A:1177:LYS:HD3	1:A:1178:ASN:H	1.86	0.41
1:A:174:ALA:O	1:A:258:ARG:NH1	2.51	0.41
1:A:594:TYR:CE2	1:A:596:LEU:HD13	2.56	0.41
1:A:797:CYS:O	1:A:801:ASN:HB2	2.20	0.41
1:A:809:TYR:CD1	1:A:811:GLU:O	2.73	0.41
1:A:126:ILE:HG22	1:A:127:GLY:N	2.35	0.41
1:A:143:LEU:C	1:A:143:LEU:HD12	2.42	0.41
1:A:197:VAL:O	1:A:201:ILE:HG13	2.21	0.41
1:A:516:VAL:HG12	1:A:557:GLU:O	2.20	0.41
1:A:145:SER:HB3	1:A:155:LEU:CD1	2.51	0.41
1:A:30:ALA:O	1:A:32:GLY:N	2.54	0.41
1:A:74:LEU:HD21	1:A:96:VAL:CG1	2.37	0.41
1:A:867:PHE:HB3	1:A:1204:LEU:CD1	2.50	0.41
1:A:996:LEU:HD12	1:A:996:LEU:HA	1.83	0.41
3:T:2110:C:H2'	3:T:2111:C:O4'	2.21	0.41
1:A:172:HIS:CD2	1:A:172:HIS:C	2.94	0.40
1:A:229:LEU:CD2	1:A:242:VAL:HG11	2.50	0.40
1:A:495:PHE:CD2	1:A:521:ILE:HB	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:954:ARG:HH11	1:A:1049:THR:CG2	2.34	0.40
1:A:356:THR:HG21	1:A:481:ASP:OD1	2.22	0.40
3:T:2108:G:C2'	3:T:2109:A:H5'	2.51	0.40
1:A:208:PRO:O	1:A:209:LYS:C	2.59	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%)	1078 (90%)	88 (7%)	27 (2%)	<b>6</b> <b>7</b>

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	811	GLU
1	A	1263	SER
1	A	68	GLY
1	A	69	ASN
1	A	104	LYS
1	A	133	ARG
1	A	188	ALA
1	A	305	VAL
1	A	465	GLY
1	A	780	ILE
1	A	806	ARG
1	A	972	ALA
1	A	3	GLU
1	A	641	ILE
1	A	14	GLU
1	A	209	LYS

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Mol	Chain	Res	Type
1	A	427	ASP
1	A	777	SER
1	A	141	ASP
1	A	219	ARG
1	A	350	SER
1	A	132	ILE
1	A	201	ILE
1	A	613	PRO
1	A	1244	PRO
1	A	357	PRO

### 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%)	864 (87%)	131 (13%)	<b>4</b> <b>4</b>

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	MET
1	A	22	ASP
1	A	67	ASP
1	A	76	VAL
1	A	143	LEU
1	A	155	LEU
1	A	165	LEU
1	A	181	ILE
1	A	200	ASP
1	A	205	SER
1	A	210	GLU
1	A	220	MET
1	A	229	LEU
1	A	235	VAL
1	A	246	LEU
1	A	250	ASN

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Mol	Chain	Res	Type
1	A	258	ARG
1	A	292	ARG
1	A	302	ILE
1	A	311	THR
1	A	317	THR
1	A	355	ASP
1	A	371	ASP
1	A	376	MET
1	A	387	ILE
1	A	390	VAL
1	A	399	GLN
1	A	406	LEU
1	A	410	VAL
1	A	442	LEU
1	A	452	THR
1	A	463	LEU
1	A	480	LEU
1	A	491	ILE
1	A	508	ARG
1	A	510	THR
1	A	529	ILE
1	A	530	VAL
1	A	533	LYS
1	A	535	THR
1	A	539	THR
1	A	549	LEU
1	A	566	ILE
1	A	569	GLU
1	A	582	THR
1	A	593	VAL
1	A	599	ASP
1	A	618	ARG
1	A	619	THR
1	A	622	VAL
1	A	626	ILE
1	A	628	LEU
1	A	632	VAL
1	A	636	MET
1	A	646	THR
1	A	651	ILE
1	A	654	ASP
1	A	655	ASP

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Mol	Chain	Res	Type
1	A	666	ARG
1	A	703	ASN
1	A	705	LEU
1	A	706	SER
1	A	715	THR
1	A	717	ILE
1	A	719	VAL
1	A	733	LEU
1	A	741	ASN
1	A	759	ASP
1	A	762	ILE
1	A	781	ASP
1	A	782	THR
1	A	791	LEU
1	A	796	GLU
1	A	800	THR
1	A	809	TYR
1	A	812	ASP
1	A	827	ARG
1	A	831	LYS
1	A	832	LEU
1	A	833	ILE
1	A	835	ASP
1	A	836	VAL
1	A	849	SER
1	A	857	ASN
1	A	869	LEU
1	A	873	CYS
1	A	884	LEU
1	A	885	ARG
1	A	901	ASN
1	A	905	THR
1	A	909	ASN
1	A	933	ILE
1	A	938	LEU
1	A	950	ILE
1	A	970	SER
1	A	983	LEU
1	A	996	LEU
1	A	1005	ASP
1	A	1013	LYS
1	A	1014	ILE

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Mol	Chain	Res	Type
1	A	1033	LEU
1	A	1040	ILE
1	A	1049	THR
1	A	1053	ASP
1	A	1054	ASP
1	A	1065	LEU
1	A	1075	THR
1	A	1076	THR
1	A	1077	ASN
1	A	1089	GLU
1	A	1093	LYS
1	A	1101	VAL
1	A	1107	ARG
1	A	1110	ILE
1	A	1111	VAL
1	A	1116	LEU
1	A	1128	THR
1	A	1138	HIS
1	A	1152	LEU
1	A	1177	LYS
1	A	1178	ASN
1	A	1182	ILE
1	A	1183	ARG
1	A	1193	ARG
1	A	1194	ASP
1	A	1196	GLU
1	A	1200	LEU
1	A	1204	LEU
1	A	1241	ARG
1	A	1242	SER
1	A	1245	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	79	GLN
1	A	198	GLN
1	A	284	HIS
1	A	296	HIS
1	A	304	HIS
1	A	360	HIS

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Mol	Chain	Res	Type
1	A	375	ASN
1	A	382	GLN
1	A	399	GLN
1	A	409	GLN
1	A	604	HIS
1	A	614	GLN
1	A	703	ASN
1	A	714	ASN
1	A	729	ASN
1	A	857	ASN
1	A	862	HIS
1	A	901	ASN
1	A	909	ASN
1	A	948	GLN
1	A	1077	ASN
1	A	1094	HIS
1	A	1121	ASN
1	A	1151	GLN
1	A	1155	ASN
1	A	1191	HIS
1	A	1243	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	G	7/9 (77%)	3 (42%)	0
3	T	12/13 (92%)	3 (25%)	0
All	All	19/22 (86%)	6 (31%)	0

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	G	2006	C
2	G	2007	A
2	G	2008	U
3	T	2102	A
3	T	2110	C
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
4	GH3	A	2501	5	25,33,33	2.74	12 (48%)	30,52,52	2.25	9 (30%)

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
4	GH3	A	2501	5	-	6/18/34/34	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2501	GH3	O6-C6	6.44	1.40	1.24
4	A	2501	GH3	C8-N7	-6.10	1.23	1.34
4	A	2501	GH3	C2'-C1'	-5.33	1.49	1.54
4	A	2501	GH3	O2'-C2'	-3.25	1.36	1.43
4	A	2501	GH3	C2-N2	3.23	1.40	1.33
4	A	2501	GH3	PG-O1G	2.96	1.60	1.50
4	A	2501	GH3	C3'-C2'	-2.63	1.45	1.52
4	A	2501	GH3	C5'-C4'	-2.62	1.42	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2501	GH3	PG-O2G	-2.56	1.45	1.54
4	A	2501	GH3	C3'-C4'	-2.45	1.47	1.52
4	A	2501	GH3	C5-C4	2.44	1.47	1.40
4	A	2501	GH3	C6-N1	2.39	1.37	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2501	GH3	N3-C2-N1	-5.85	119.41	127.22
4	A	2501	GH3	C2-N3-C4	4.85	120.89	115.36
4	A	2501	GH3	C4-C5-N7	-4.48	104.73	109.40
4	A	2501	GH3	C6-N1-C2	4.30	122.76	115.93
4	A	2501	GH3	C5-C6-N1	-3.41	118.77	123.43
4	A	2501	GH3	C3'-C4'-C5'	-3.10	107.00	113.11
4	A	2501	GH3	O4'-C4'-C5'	2.53	113.68	109.52
4	A	2501	GH3	C6-C5-C4	-2.45	118.46	120.80
4	A	2501	GH3	N2-C2-N3	2.02	121.08	117.79

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2501	GH3	C5'-O5'-PA-O3A
4	A	2501	GH3	C5'-O5'-PA-O1A
4	A	2501	GH3	O4'-C4'-C5'-O5'
4	A	2501	GH3	C3'-C4'-C5'-O5'
4	A	2501	GH3	PA-O3A-PB-O1B
4	A	2501	GH3	C5'-O5'-PA-O2A

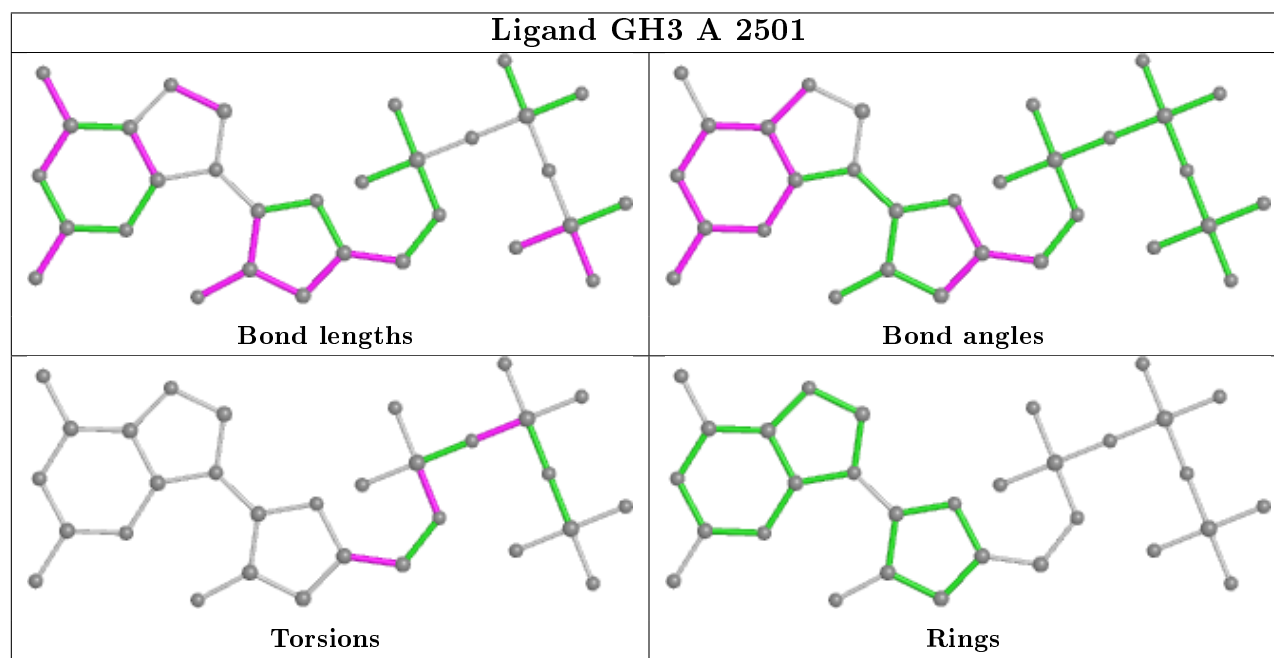
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2501	GH3	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, 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	1203/1289 (93%)	0.19	67 (5%) 24 23	23, 65, 121, 153	0
2	G	9/9 (100%)	-0.37	1 (11%) 5 4	51, 64, 93, 109	0
3	T	13/13 (100%)	0.18	2 (15%) 2 1	47, 66, 106, 110	0
All	All	1225/1311 (93%)	0.19	70 (5%) 23 22	23, 65, 121, 153	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	680	ALA	7.5
1	A	290	PHE	7.3
1	A	6	ALA	6.7
3	T	2113	A	6.3
1	A	268	VAL	6.3
1	A	700	SER	6.2
1	A	807	PRO	5.9
1	A	320	LEU	5.5
1	A	5	THR	5.4
1	A	780	ILE	5.1
1	A	16	THR	4.9
1	A	1234	ALA	4.5
1	A	267	LYS	4.3
2	G	2001	G	4.2
1	A	292	ARG	4.1
1	A	193	LYS	4.0
1	A	15	ARG	3.9
1	A	200	ASP	3.8
1	A	113	ALA	3.8
1	A	199	LEU	3.8
3	T	2101	A	3.8
1	A	102	ALA	3.7
1	A	111	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	26	ALA	3.7
1	A	204	GLN	3.4
1	A	284	HIS	3.4
1	A	701	SER	3.4
1	A	255	GLY	3.3
1	A	28	THR	3.3
1	A	266	GLU	3.3
1	A	279	MET	3.3
1	A	134	ARG	3.2
1	A	350	SER	3.1
1	A	191	VAL	3.1
1	A	2	ALA	3.0
1	A	4	ILE	3.0
1	A	122	LEU	2.9
1	A	196	GLN	2.9
1	A	12	LEU	2.9
1	A	381	ALA	2.8
1	A	192	GLU	2.7
1	A	348	ASN	2.7
1	A	319	VAL	2.7
1	A	24	LYS	2.7
1	A	294	LYS	2.6
1	A	33	ASP	2.6
1	A	273	ALA	2.5
1	A	291	GLU	2.5
1	A	849	SER	2.5
1	A	142	VAL	2.4
1	A	20	MET	2.4
1	A	778	LEU	2.4
1	A	166	VAL	2.4
1	A	352	VAL	2.4
1	A	324	TYR	2.4
1	A	66	ILE	2.3
1	A	138	LEU	2.3
1	A	321	ALA	2.2
1	A	48	LYS	2.2
1	A	679	GLY	2.2
1	A	43	LYS	2.2
1	A	195	TYR	2.1
1	A	159	LYS	2.1
1	A	354	TYR	2.1
1	A	461	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	285	MET	2.1
1	A	1216	ASN	2.1
1	A	161	ALA	2.1
1	A	441	LEU	2.1
1	A	162	ASP	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](#)

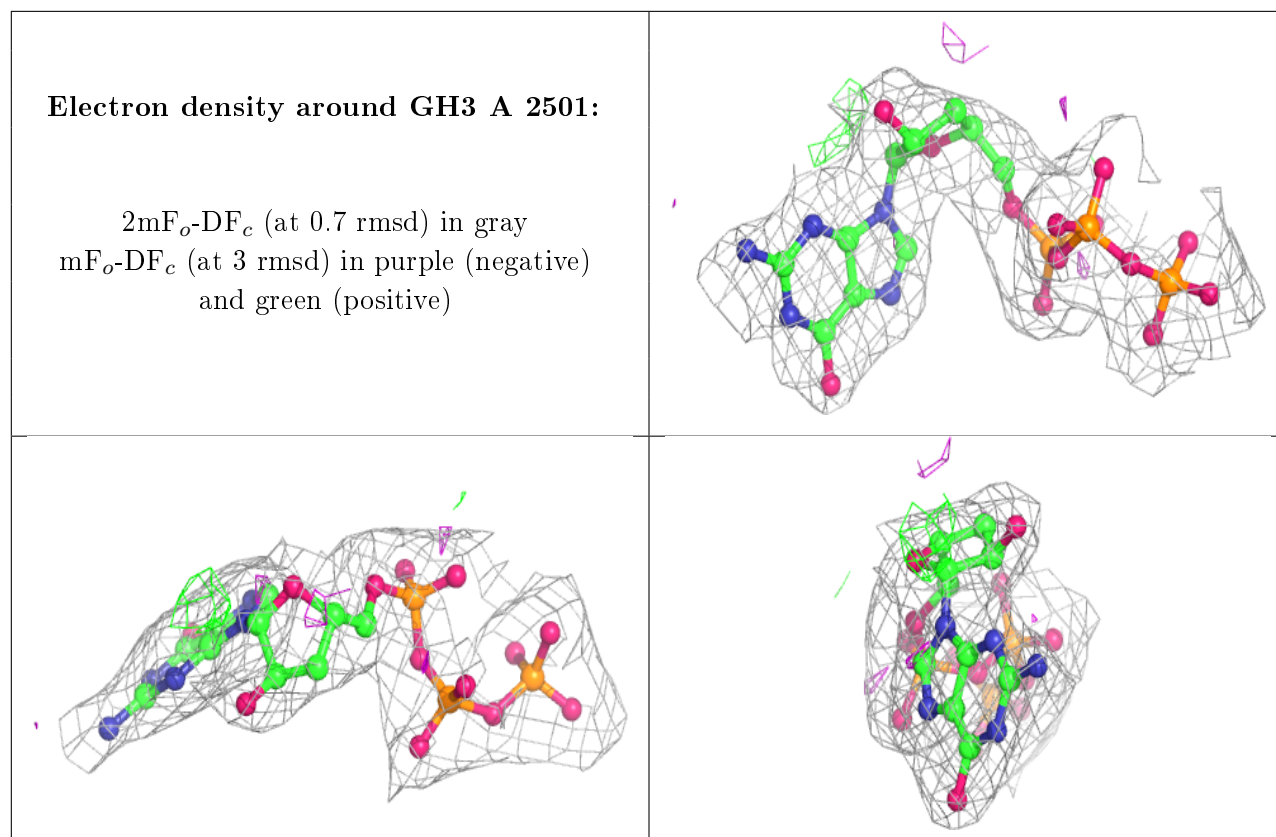
There are no carbohydrates in this entry.

## 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, 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
5	CA	A	3002	1/1	0.88	0.27	79,79,79,79	0
4	GH3	A	2501	31/31	0.97	0.12	36,47,53,54	0
5	CA	A	3001	1/1	0.98	0.17	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.