



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2020 – 03:03 PM BST

PDB ID : 5C52  
Title : Probing the Structural and Molecular Basis of Nucleotide Selectivity by Human Mitochondrial DNA Polymerase gamma  
Authors : Sohl, C.D.; Szymanski, M.R.; Mislak, A.C.; Shumate, C.K.; Amiralaie, S.; Schinazi, R.F.; Anderson, K.S.; Yin, Y.W.  
Deposited on : 2015-06-19  
Resolution : 3.64 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 : 2.13  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13

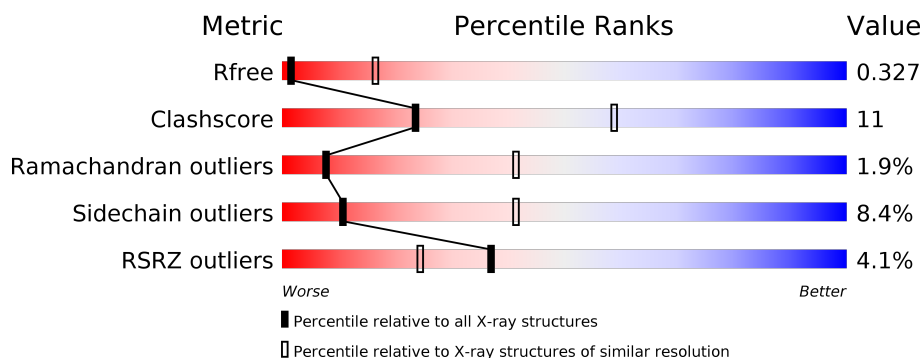
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.64 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	1341 (3.78-3.50)
Clashscore	141614	1439 (3.78-3.50)
Ramachandran outliers	138981	1391 (3.78-3.50)
Sidechain outliers	138945	1391 (3.78-3.50)
RSRZ outliers	127900	1242 (3.78-3.50)

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	1205	<div> <div>4%</div> <div> <div></div> <div>55%</div> <div>23%</div> <div>•</div> <div>18%</div> </div> </div>
2	B	485	<div> <div>%</div> <div> <div></div> <div>55%</div> <div>18%</div> <div>•</div> <div>25%</div> </div> </div>
2	C	485	<div> <div>4%</div> <div> <div></div> <div>55%</div> <div>15%</div> <div>•</div> <div>26%</div> </div> </div>
3	T	26	<div> <div>12%</div> <div> <div></div> <div>54%</div> <div>46%</div> </div> </div>
4	P	22	<div> <div></div> <div> <div></div> <div>68%</div> <div>27%</div> <div>5%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	1RY	A	1301	X	-	-	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14639 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 DNA polymerase subunit gamma-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	983	7799	4966	1371	1413	49	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLN	deletion	UNP P54098
A	?	-	GLN	deletion	UNP P54098
A	?	-	GLN	deletion	UNP P54098
A	?	-	GLN	deletion	UNP P54098
A	?	-	GLN	deletion	UNP P54098
A	?	-	GLN	deletion	UNP P54098
A	?	-	GLN	deletion	UNP P54098
A	?	-	GLN	deletion	UNP P54098
A	?	-	GLN	deletion	UNP P54098
A	?	-	GLN	deletion	UNP P54098

- Molecule 2 is a protein called DNA polymerase subunit gamma-2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	363	2943	1885	520	522	16	0	0	0
2	C	358	2887	1853	506	512	16	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	67	LEU	GLU	conflict	UNP Q9UHN1
C	67	LEU	GLU	conflict	UNP Q9UHN1

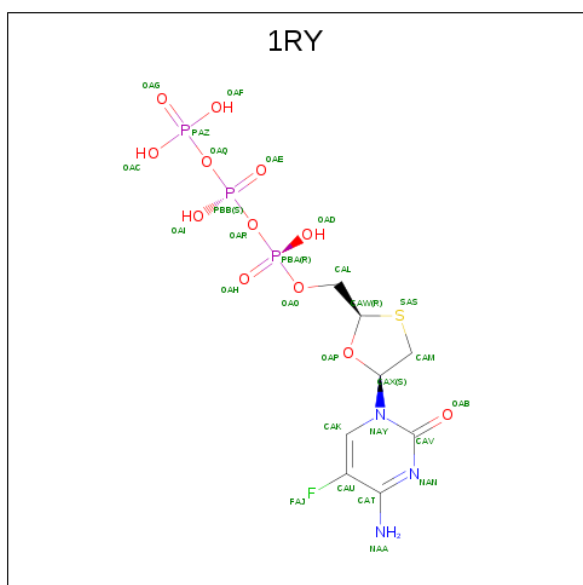
- Molecule 3 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	26	Total	C	N	O	P	0	0	0
			529	251	93	159	26			

- Molecule 4 is a DNA chain called DNA (5'-D(\*AP\*AP\*AP\*AP\*CP\*GP\*AP\*GP\*GP\*GP\*CP\*CP\*AP\*GP\*TP\*GP\*CP\*CP\*GP\*TP\*AP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	P	22	Total	C	N	O	P	0	0	0
			451	214	92	124	21			

- Molecule 5 is [[(2R,5S)-5-(4-azanyl-5-fluoranyl-2-oxidanylidene-pyrimidin-1-yl)-1,3-oxathiolan-2-yl]methoxy-oxidanyl-phosphoryl] phosphono hydrogen phosphate (three-letter code: 1RY) (formula: C<sub>8</sub>H<sub>13</sub>FN<sub>3</sub>O<sub>12</sub>P<sub>3</sub>S).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
5	A	1	Total	C	F	N	O	P	S	0	0
			28	8	1	3	12	3	1		

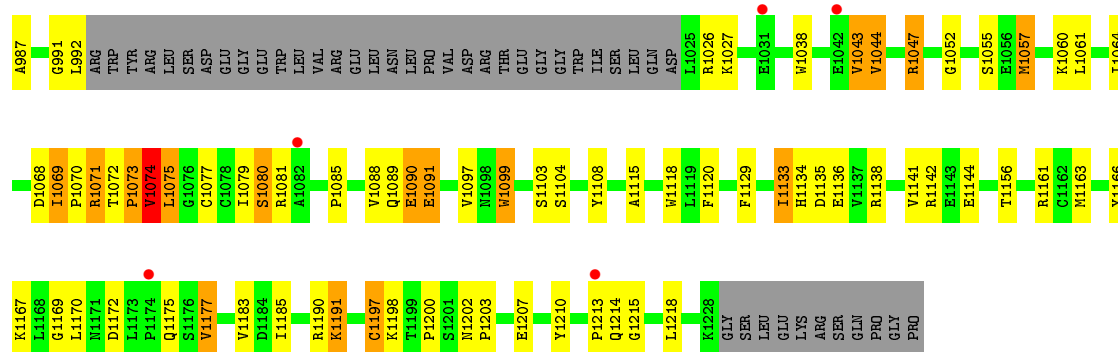
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Mg	0	0
			2	2		

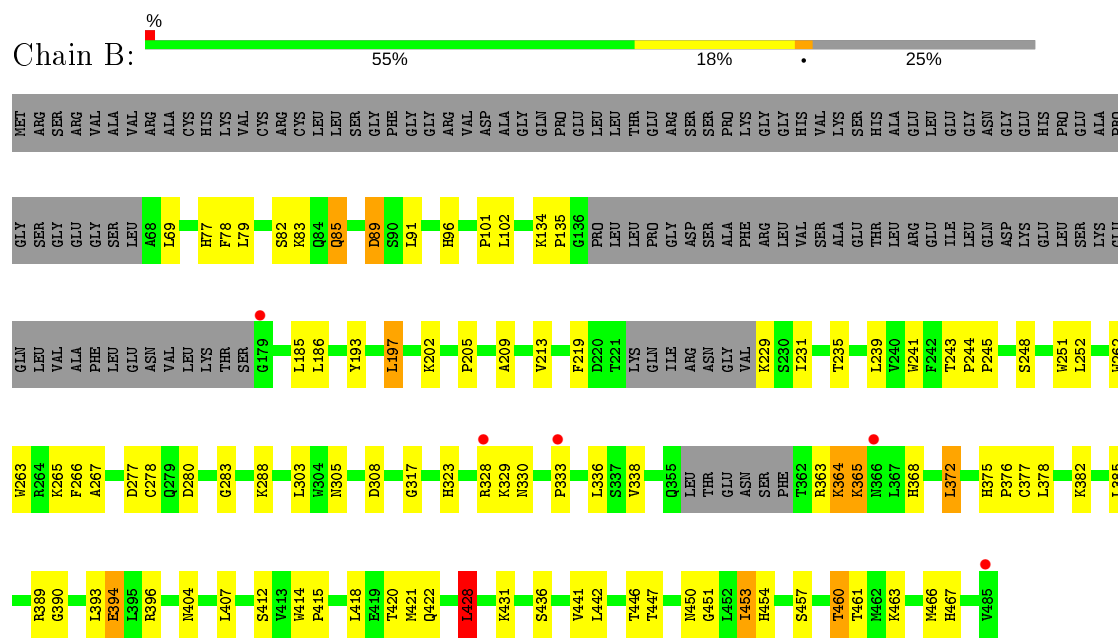


- Molecule 1: DNA polymerase subunit gamma-1

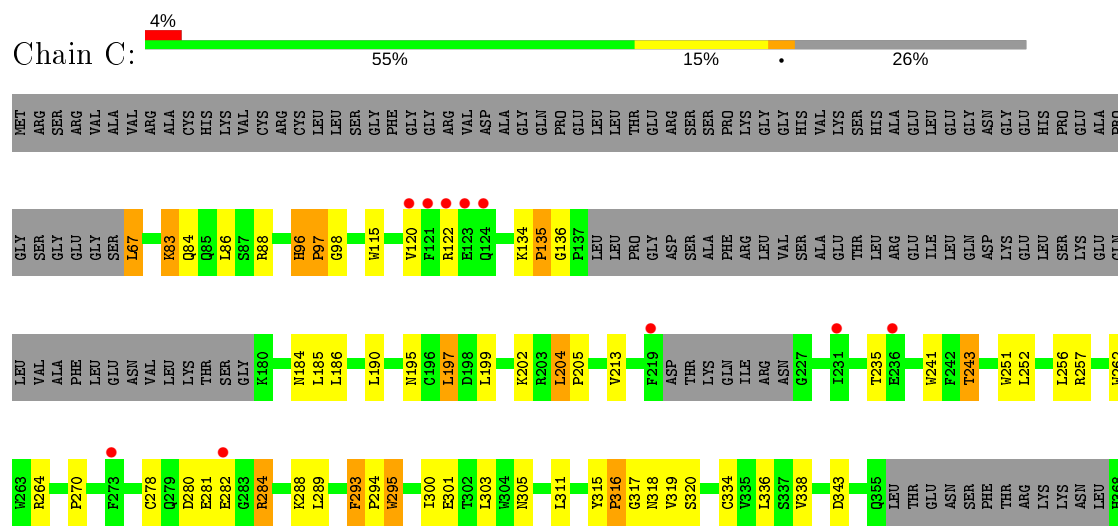


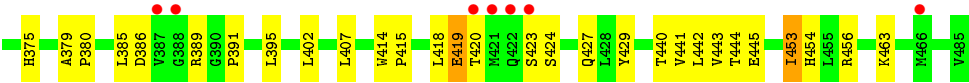


• Molecule 2: DNA polymerase subunit gamma-2, mitochondrial



• Molecule 2: DNA polymerase subunit gamma-2, mitochondrial

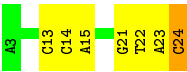




● Molecule 3: DNA (26-MER)



● Molecule 4: DNA (5'-D(\*AP\*AP\*AP\*AP\*CP\*GP\*AP\*GP\*GP\*GP\*CP\*CP\*AP\*GP\*TP\*GP\*CP\*CP\*GP\*TP\*AP\*C)-3')





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	217.28Å 217.28Å 165.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.21 – 3.64 51.21 – 3.64	Depositor EDS
% Data completeness (in resolution range)	98.2 (51.21-3.64) 81.3 (51.21-3.64)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.93 (at 3.67Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.311 , 0.314 0.313 , 0.327	Depositor DCC
$R_{free}$ test set	2000 reflections (4.47%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	137.7	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 29.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	14639	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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: 1RY, MG, DOC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.25	0/7999	0.45	3/10852 (0.0%)
2	B	0.23	0/3016	0.41	1/4074 (0.0%)
2	C	0.25	0/2960	0.45	3/4001 (0.1%)
3	T	0.51	0/591	0.89	0/909
4	P	0.50	0/488	0.77	0/752
All	All	0.27	0/15054	0.49	7/20588 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	135	PRO	CA-N-CD	-8.81	99.16	111.50
2	C	96	HIS	C-N-CD	-7.76	103.52	120.60
1	A	752	LEU	C-N-CD	-6.63	106.02	120.60
2	B	428	LEU	CA-CB-CG	5.28	127.45	115.30
1	A	752	LEU	C-N-CA	5.05	143.22	122.00
2	C	96	HIS	C-N-CA	5.05	143.22	122.00
1	A	488	LEU	CA-CB-CG	5.01	126.81	115.30

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	7799	0	7692	196	0
2	B	2943	0	2939	56	0
2	C	2887	0	2867	60	0
3	T	529	0	291	10	0
4	P	451	0	246	6	0
5	A	28	0	10	2	0
6	A	2	0	0	0	0
All	All	14639	0	14045	318	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 11.

All (318) 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)
5:A:1301:1RY:OAP	5:A:1301:1RY:CAW	1.68	1.16
2:C:134:LYS:HD2	2:C:135:PRO:HD3	1.33	1.07
2:C:135:PRO:HD2	2:C:136:GLY:H	1.24	0.99
2:C:134:LYS:CD	2:C:135:PRO:HD3	1.98	0.93
2:C:419:GLU:H	2:C:420:THR:HA	1.35	0.92
2:C:135:PRO:HD2	2:C:136:GLY:N	1.93	0.83
2:C:443:VAL:HG22	2:C:453:ILE:HD11	1.65	0.78
2:C:442:LEU:HB3	2:C:454:HIS:HB2	1.66	0.76
2:C:134:LYS:NZ	2:C:135:PRO:CD	2.48	0.75
2:C:134:LYS:HZ3	2:C:135:PRO:CD	2.00	0.75
2:C:134:LYS:NZ	2:C:135:PRO:HD2	2.01	0.74
1:A:850:ILE:HG22	3:T:6:DT:H4'	1.69	0.74
1:A:849:THR:HG22	1:A:850:ILE:HD13	1.70	0.73
2:C:135:PRO:CD	2:C:136:GLY:H	2.02	0.71
1:A:834:GLU:HG3	2:B:328:ARG:HH21	1.54	0.71
1:A:487:ASP:OD2	1:A:601:LYS:NZ	2.23	0.70
5:A:1301:1RY:H13	3:T:4:DG:H1	1.40	0.69
1:A:463:LEU:HD21	1:A:594:LEU:HD23	1.76	0.68
2:C:134:LYS:HZ2	2:C:135:PRO:HD2	1.57	0.68
1:A:938:THR:H	1:A:939:VAL:HA	1.58	0.68
1:A:856:GLU:OE1	1:A:859:TRP:N	2.25	0.67
1:A:911:HIS:NE2	1:A:1172:ASP:O	2.28	0.67
2:B:363:ARG:HD3	2:B:364:LYS:H	1.59	0.67
1:A:884:TYR:HA	1:A:1142:ARG:HA	1.76	0.67
2:C:419:GLU:N	2:C:420:THR:HA	2.06	0.66
1:A:243:ASP:HB3	1:A:279:ARG:HE	1.61	0.65
1:A:1161:ARG:HE	1:A:1177:VAL:HG22	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1108:TYR:OH	1:A:1161:ARG:NH1	2.29	0.65
1:A:978:ALA:HA	1:A:981:LYS:HD2	1.78	0.64
1:A:586:THR:HG1	1:A:590:SER:HG	1.44	0.64
2:C:135:PRO:CD	2:C:136:GLY:N	2.61	0.64
2:B:197:LEU:HD22	2:B:202:LYS:HA	1.80	0.63
1:A:1057:MET:N	1:A:1057:MET:SD	2.71	0.63
1:A:79:LEU:H	1:A:83:LEU:HG	1.64	0.63
1:A:1068:ASP:HA	1:A:1085:PRO:HG2	1.80	0.62
2:B:442:LEU:HB3	2:B:454:HIS:HB2	1.82	0.62
2:B:77:HIS:HE1	2:B:431:LYS:HG3	1.64	0.62
1:A:384:ASP:OD1	1:A:384:ASP:N	2.30	0.62
2:C:424:SER:HB3	2:C:427:GLN:HG2	1.81	0.62
2:C:83:LYS:HG2	2:C:84:GLN:HG2	1.82	0.61
2:B:83:LYS:HG2	2:B:85:GLN:H	1.65	0.61
1:A:963:GLU:HG3	1:A:981:LYS:HZ3	1.65	0.61
1:A:800:PHE:HB2	1:A:869:ARG:HE	1.65	0.60
1:A:230:GLU:OE2	1:A:386:ARG:NH1	2.33	0.60
1:A:977:GLU:HB3	1:A:981:LYS:HZ2	1.67	0.59
1:A:896:LEU:HD21	1:A:931:LEU:HD23	1.84	0.59
1:A:239:LEU:O	1:A:279:ARG:NH1	2.35	0.59
1:A:938:THR:N	1:A:939:VAL:HA	2.16	0.59
1:A:750:PHE:HD1	1:A:751:LYS:HG2	1.68	0.59
1:A:991:GLY:HA2	1:A:1052:GLY:HA2	1.84	0.58
1:A:861:THR:HG21	3:T:8:DC:H1'	1.84	0.58
1:A:744:ILE:HG23	1:A:745:PRO:HD3	1.85	0.58
1:A:502:LYS:HB3	1:A:503:VAL:HB	1.84	0.58
1:A:533:CYS:SG	1:A:534:SER:N	2.67	0.58
1:A:1142:ARG:NH1	1:A:1144:GLU:OE1	2.35	0.58
1:A:953:ARG:HA	1:A:957:ALA:HB2	1.85	0.58
1:A:752:LEU:HB2	1:A:753:PRO:HA	1.86	0.58
1:A:94:MET:HG3	1:A:1170:LEU:HD11	1.85	0.58
1:A:153:ALA:HB1	1:A:194:ALA:HB2	1.85	0.57
1:A:761:ASN:N	1:A:761:ASN:OD1	2.35	0.57
1:A:617:ARG:HB2	1:A:763:GLY:HA3	1.86	0.57
1:A:782:GLY:HA2	1:A:784:GLY:HA2	1.87	0.56
1:A:1069:ILE:O	1:A:1071:ARG:N	2.39	0.56
1:A:372:GLU:HG3	1:A:375:GLU:H	1.71	0.56
2:B:185:LEU:H	2:B:185:LEU:HD23	1.70	0.56
2:C:235:THR:OG1	2:C:343:ASP:OD1	2.24	0.56
2:B:77:HIS:CE1	2:B:431:LYS:HG3	2.40	0.56
1:A:134:ASN:ND2	1:A:1166:TYR:OH	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:457:SER:OG	2:B:460:THR:O	2.23	0.56
1:A:495:PHE:HB3	1:A:496:LYS:HB2	1.87	0.56
1:A:464:MET:HB2	1:A:589:PRO:HG2	1.88	0.56
1:A:196:VAL:HG22	1:A:215:ILE:HG12	1.88	0.56
1:A:743:ASP:OD1	1:A:743:ASP:N	2.39	0.56
2:B:365:LYS:H	2:B:365:LYS:HD2	1.70	0.55
1:A:593:SER:O	1:A:599:THR:OG1	2.16	0.55
2:C:278:CYS:SG	2:C:288:LYS:NZ	2.79	0.55
1:A:488:LEU:H	1:A:488:LEU:HD13	1.72	0.55
2:B:407:LEU:HD13	2:C:120:VAL:HG12	1.88	0.55
1:A:606:THR:HB	1:A:612:LEU:HD13	1.88	0.55
1:A:1079:ILE:HG12	1:A:1099:TRP:CZ3	2.42	0.54
1:A:1073:PRO:HA	1:A:1074:VAL:HG13	1.89	0.54
1:A:296:SER:HB2	1:A:847:ALA:HB3	1.90	0.54
1:A:466:LEU:HB3	1:A:602:LEU:HD21	1.89	0.54
1:A:1061:LEU:HB3	1:A:1097:VAL:HG13	1.88	0.54
2:C:134:LYS:CD	2:C:135:PRO:CD	2.81	0.54
1:A:817:PRO:HB2	1:A:818:ARG:HH21	1.72	0.54
1:A:866:ARG:HH21	1:A:869:ARG:HD2	1.72	0.54
1:A:93:GLU:HA	1:A:94:MET:HB2	1.88	0.54
2:B:209:ALA:HB2	2:B:239:LEU:HD13	1.89	0.54
2:C:190:LEU:HD22	2:C:311:LEU:HD13	1.90	0.54
2:B:82:SER:OG	2:C:195:ASN:OD1	2.25	0.54
2:B:278:CYS:SG	2:B:288:LYS:NZ	2.75	0.54
1:A:299:MET:HG2	1:A:848:GLY:HA2	1.90	0.53
2:B:372:LEU:HD13	2:B:436:SER:HB2	1.90	0.53
4:P:14:DC:H2'	4:P:15:DA:C8	2.42	0.53
1:A:1089:GLN:N	1:A:1090:GLU:HA	2.24	0.53
1:A:869:ARG:HB2	1:A:872:SER:HB2	1.90	0.53
2:C:197:LEU:HD12	2:C:202:LYS:HG2	1.90	0.53
2:C:264:ARG:HG3	2:C:270:PRO:HB3	1.90	0.53
1:A:831:TYR:H	1:A:832:ASP:HA	1.74	0.53
3:T:9:DG:H2'	3:T:10:DG:C8	2.43	0.53
2:B:404:ASN:HA	2:B:407:LEU:HG	1.90	0.53
1:A:212:ALA:HB3	1:A:223:TRP:HB3	1.90	0.53
1:A:963:GLU:HG3	1:A:981:LYS:NZ	2.24	0.53
1:A:887:VAL:HG22	1:A:1185:ILE:HG23	1.89	0.52
2:B:241:TRP:HB3	2:B:336:LEU:HB3	1.89	0.52
1:A:1213:PRO:O	1:A:1214:GLN:NE2	2.43	0.52
1:A:135:LEU:H	1:A:135:LEU:HD23	1.73	0.52
1:A:864:ASN:HB3	1:A:1191:LYS:HD3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:262:TRP:HA	2:B:265:LYS:HE2	1.91	0.51
1:A:1200:PRO:O	1:A:1202:ASN:N	2.42	0.51
1:A:162:LEU:HG	1:A:401:TRP:CZ3	2.46	0.51
2:C:375:HIS:O	2:C:379:ALA:N	2.41	0.51
1:A:1060:LYS:HE2	1:A:1064:ILE:HD11	1.93	0.51
1:A:851:THR:OG1	1:A:851:THR:O	2.29	0.51
1:A:864:ASN:O	1:A:872:SER:OG	2.24	0.51
1:A:178:TYR:O	1:A:219:ALA:HB1	2.10	0.51
3:T:16:DG:H1	4:P:13:DC:H42	1.59	0.51
1:A:149:PRO:HB3	1:A:262:GLN:N	2.26	0.50
2:B:428:LEU:HA	2:B:431:LYS:HB3	1.92	0.50
1:A:1072:THR:OG1	1:A:1072:THR:O	2.19	0.50
2:C:429:TYR:HE1	2:C:463:LYS:HZ3	1.59	0.50
1:A:1115:ALA:HB3	1:A:1156:THR:HG23	1.94	0.50
2:B:447:THR:HG21	2:B:453:ILE:HA	1.94	0.50
1:A:1133:ILE:HG12	1:A:1136:GLU:HB3	1.93	0.49
1:A:86:GLN:HG2	1:A:88:PHE:H	1.76	0.49
1:A:977:GLU:HB3	1:A:981:LYS:NZ	2.26	0.49
2:B:382:LYS:H	2:B:412:SER:HB2	1.77	0.49
1:A:869:ARG:NH1	4:P:22:DT:OP1	2.46	0.49
1:A:87:ILE:HD13	1:A:127:LEU:HD22	1.94	0.49
1:A:243:ASP:N	1:A:243:ASP:OD1	2.36	0.49
1:A:275:ARG:NH2	1:A:433:SER:O	2.42	0.49
1:A:566:LEU:HD13	1:A:566:LEU:H	1.76	0.49
2:B:219:PHE:HA	2:B:229:LYS:N	2.27	0.49
1:A:1072:THR:HB	1:A:1077:CYS:N	2.28	0.49
1:A:1074:VAL:HB	1:A:1167:LYS:HB3	1.94	0.49
1:A:435:LEU:HG	1:A:842:PRO:HG3	1.95	0.49
1:A:828:HIS:CG	1:A:829:PRO:HD2	2.48	0.49
1:A:107:LEU:O	1:A:112:LEU:N	2.43	0.49
2:B:213:VAL:HA	2:B:235:THR:HA	1.95	0.49
2:C:418:LEU:N	2:C:419:GLU:HA	2.28	0.49
2:C:184:ASN:OD1	2:C:185:LEU:N	2.40	0.49
1:A:268:GLY:HA2	1:A:403:THR:HG21	1.95	0.48
1:A:818:ARG:H	1:A:818:ARG:HE	1.61	0.48
2:C:241:TRP:HD1	2:C:336:LEU:HD22	1.78	0.48
1:A:475:SER:HA	1:A:476:GLY:HA2	1.49	0.48
1:A:850:ILE:HD12	1:A:851:THR:HA	1.95	0.48
1:A:851:THR:HG21	1:A:1103:SER:HB2	1.96	0.48
1:A:163:PRO:HG3	1:A:219:ALA:HA	1.96	0.48
2:B:79:LEU:HG	2:B:102:LEU:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:428:LEU:HD13	2:B:428:LEU:H	1.78	0.48
4:P:23:DA:H2'	4:P:24:DOC:H6	1.96	0.48
2:B:418:LEU:HD22	2:C:204:LEU:HD12	1.96	0.48
1:A:614:TYR:HE1	1:A:765:PRO:HG3	1.79	0.47
1:A:299:MET:HG3	1:A:849:THR:HG23	1.94	0.47
2:B:441:VAL:HG23	2:B:453:ILE:HG13	1.96	0.47
2:C:205:PRO:HB3	2:C:243:THR:HA	1.95	0.47
2:C:252:LEU:HD22	2:C:305:ASN:HB2	1.95	0.47
1:A:1136:GLU:HG2	1:A:1138:ARG:HD3	1.97	0.47
2:B:78:PHE:HD2	2:C:199:LEU:HD13	1.79	0.47
1:A:887:VAL:HG13	1:A:1185:ILE:HG12	1.96	0.47
2:C:293:PHE:H	2:C:294:PRO:HA	1.79	0.47
2:C:389:ARG:HD3	2:C:395:LEU:HD11	1.97	0.47
2:C:444:THR:OG1	2:C:445:GLU:OE2	2.33	0.47
2:C:134:LYS:NZ	2:C:135:PRO:HD3	2.29	0.47
2:C:444:THR:OG1	2:C:445:GLU:N	2.48	0.47
1:A:856:GLU:H	1:A:860:LEU:HD12	1.80	0.47
2:B:446:THR:O	2:B:450:ASN:ND2	2.48	0.47
1:A:1088:VAL:HG12	1:A:1090:GLU:HA	1.96	0.47
1:A:765:PRO:HA	1:A:766:PHE:HA	1.58	0.46
1:A:607:TRP:HA	1:A:778:THR:HG23	1.97	0.46
1:A:831:TYR:N	1:A:832:ASP:HA	2.31	0.46
1:A:562:ARG:HD2	1:A:563:PRO:HD2	1.98	0.46
2:C:303:LEU:HD22	2:C:338:VAL:HG22	1.97	0.46
1:A:804:ALA:O	1:A:808:ILE:HG12	2.16	0.46
1:A:636:THR:OG1	1:A:637:GLY:N	2.49	0.46
1:A:1044:VAL:HG22	1:A:1047:ARG:HD2	1.98	0.46
1:A:888:GLY:HA3	1:A:1138:ARG:HD2	1.97	0.46
2:B:421:MET:HA	2:B:422:GLN:HB3	1.97	0.46
1:A:426:GLY:O	1:A:430:MET:HB2	2.16	0.45
1:A:288:ARG:HA	1:A:288:ARG:HE	1.81	0.45
1:A:800:PHE:HB2	1:A:869:ARG:HH21	1.81	0.45
1:A:892:ASP:HA	1:A:893:SER:HA	1.69	0.45
2:C:134:LYS:CE	2:C:135:PRO:HD3	2.45	0.45
2:B:229:LYS:HE2	2:B:229:LYS:HB3	1.82	0.45
2:C:315:TYR:N	2:C:316:PRO:HD3	2.31	0.45
1:A:831:TYR:HE1	1:A:834:GLU:HA	1.81	0.45
1:A:155:ASN:O	1:A:159:GLN:HG2	2.17	0.45
1:A:939:VAL:HA	1:A:940:GLY:HA3	1.72	0.45
1:A:608:ASP:OD1	1:A:778:THR:OG1	2.31	0.45
2:B:78:PHE:HB3	2:B:101:PRO:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:293:PHE:HB3	2:C:295:TRP:H	1.82	0.45
1:A:262:GLN:HB2	1:A:263:GLU:HG2	1.98	0.45
1:A:897:TRP:CD1	1:A:1177:VAL:HG21	2.52	0.45
2:C:134:LYS:HZ3	2:C:135:PRO:CG	2.29	0.45
1:A:898:ILE:HD13	1:A:1104:SER:HB2	1.99	0.45
1:A:1214:GLN:HA	1:A:1215:GLY:HA3	1.65	0.45
1:A:1133:ILE:O	1:A:1135:ASP:N	2.50	0.44
1:A:850:ILE:HA	1:A:851:THR:HA	1.68	0.44
1:A:262:GLN:HA	1:A:263:GLU:HA	1.53	0.44
1:A:778:THR:HA	1:A:779:LEU:HA	1.57	0.44
1:A:910:MET:HG3	1:A:911:HIS:H	1.81	0.44
1:A:963:GLU:HA	1:A:981:LYS:HE2	2.00	0.44
2:C:67:LEU:N	2:C:88:ARG:HH21	2.15	0.44
2:B:266:PHE:HA	2:B:375:HIS:CD2	2.52	0.44
2:C:213:VAL:HG22	2:C:235:THR:HG22	1.98	0.44
1:A:1085:PRO:HB3	1:A:1090:GLU:HG2	1.98	0.44
1:A:152:GLU:O	1:A:156:LEU:HG	2.18	0.44
1:A:433:SER:HB2	1:A:842:PRO:HG2	2.00	0.44
2:B:252:LEU:HD13	2:B:336:LEU:HD11	2.00	0.44
2:C:317:GLY:HA3	2:C:318:ASN:HA	1.61	0.44
1:A:808:ILE:HD12	1:A:874:LEU:HG	2.00	0.44
2:B:89:ASP:N	2:B:89:ASP:OD2	2.50	0.44
1:A:247:LEU:H	1:A:247:LEU:HD13	1.83	0.44
1:A:891:VAL:HG11	1:A:894:GLN:HB3	1.98	0.44
2:B:393:LEU:HA	2:B:394:GLU:HA	1.71	0.44
1:A:353:VAL:HG13	1:A:355:SER:H	1.82	0.43
2:B:193:TYR:OH	2:B:333:PRO:HG3	2.18	0.43
1:A:420:HIS:HB3	1:A:1075:LEU:HD13	1.99	0.43
1:A:828:HIS:O	1:A:830:ASP:N	2.44	0.43
2:C:134:LYS:HG3	2:C:135:PRO:CD	2.48	0.43
2:C:284:ARG:CZ	2:C:284:ARG:HA	2.49	0.43
1:A:110:HIS:HB3	1:A:111:GLY:HA2	1.99	0.43
1:A:133:ASP:N	1:A:133:ASP:OD2	2.50	0.43
1:A:536:GLU:HG3	2:C:257:ARG:HH12	1.83	0.43
1:A:803:ASN:HA	3:T:10:DG:H4'	2.00	0.43
1:A:463:LEU:HB3	1:A:592:LEU:HD12	2.00	0.43
1:A:490:TRP:HA	1:A:570:PRO:HB3	2.01	0.43
1:A:755:LYS:HD2	1:A:758:ASN:HD22	1.84	0.43
1:A:953:ARG:HG3	1:A:957:ALA:HB2	2.00	0.43
4:P:22:DT:H2'	4:P:23:DA:C8	2.54	0.43
1:A:493:GLN:HG2	1:A:574:ARG:NH2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:973:LEU:HD22	1:A:976:GLN:H	1.83	0.43
2:C:389:ARG:HD2	2:C:445:GLU:HB3	2.01	0.43
1:A:987:ALA:HA	1:A:1055:SER:HB3	2.00	0.43
2:B:323:HIS:HB3	2:B:330:ASN:HB2	2.01	0.43
1:A:606:THR:HG21	1:A:612:LEU:HB2	2.00	0.43
1:A:91:GLY:HA2	1:A:92:GLY:HA3	1.58	0.43
2:C:199:LEU:HD12	2:C:199:LEU:HA	1.86	0.43
3:T:14:DT:H2''	3:T:15:DG:C8	2.54	0.43
2:B:134:LYS:HA	2:B:135:PRO:HD3	1.90	0.43
2:B:197:LEU:HD23	2:B:197:LEU:HA	1.82	0.43
1:A:1163:MET:SD	1:A:1167:LYS:HE2	2.59	0.42
1:A:480:LYS:HD3	1:A:646:VAL:HG11	2.01	0.42
1:A:459:MET:HB2	1:A:794:ILE:HG21	2.00	0.42
1:A:1136:GLU:OE2	1:A:1138:ARG:NH1	2.52	0.42
1:A:209:PRO:HG3	1:A:277:HIS:CD2	2.53	0.42
1:A:856:GLU:HA	1:A:857:PRO:HD3	1.87	0.42
2:B:205:PRO:HB2	2:B:241:TRP:CZ2	2.55	0.42
2:B:303:LEU:HG	2:B:338:VAL:HB	2.01	0.42
2:B:385:LEU:HA	2:B:441:VAL:HG13	2.01	0.42
1:A:1197:CYS:SG	1:A:1200:PRO:HG2	2.59	0.42
1:A:97:GLU:HA	1:A:100:VAL:HG22	2.00	0.42
1:A:82:GLY:HA2	1:A:1175:GLN:NE2	2.34	0.42
2:B:389:ARG:N	2:B:390:GLY:HA3	2.35	0.42
2:B:453:ILE:HD13	2:B:466:MET:O	2.20	0.42
1:A:225:SER:HB3	1:A:227:ARG:NH2	2.34	0.42
1:A:314:ALA:O	1:A:316:LYS:N	2.53	0.42
1:A:849:THR:HA	1:A:850:ILE:HA	1.82	0.42
1:A:963:GLU:HA	1:A:981:LYS:CE	2.50	0.42
2:B:248:SER:HB3	2:B:305:ASN:HD21	1.83	0.42
3:T:1:DA:H5''	3:T:2:DG:C8	2.55	0.42
1:A:1047:ARG:H	1:A:1047:ARG:HG3	1.62	0.42
1:A:873:GLU:O	1:A:877:MET:HG2	2.20	0.42
1:A:942:SER:HA	1:A:943:ARG:HA	1.58	0.42
1:A:209:PRO:HG3	1:A:277:HIS:CG	2.55	0.42
1:A:631:LEU:HB3	1:A:633:LYS:NZ	2.35	0.42
1:A:799:SER:HA	1:A:802:ARG:HH12	1.84	0.42
1:A:818:ARG:H	1:A:818:ARG:NE	2.17	0.42
2:C:134:LYS:HG3	2:C:135:PRO:HD2	2.01	0.42
1:A:497:GLN:OE1	1:A:559:LEU:HB3	2.20	0.42
2:C:318:ASN:O	2:C:320:SER:N	2.53	0.42
4:P:21:DG:H2'	4:P:22:DT:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:612:LEU:HA	1:A:612:LEU:HD12	1.72	0.42
1:A:976:GLN:O	1:A:980:GLU:HG2	2.20	0.41
2:C:414:TRP:HA	2:C:415:PRO:HD3	1.85	0.41
1:A:1090:GLU:O	1:A:1091:GLU:HG2	2.20	0.41
1:A:562:ARG:HH11	1:A:563:PRO:HD2	1.85	0.41
2:C:280:ASP:N	2:C:280:ASP:OD1	2.52	0.41
1:A:483:PRO:HG2	1:A:484:TRP:CE3	2.56	0.41
1:A:79:LEU:HD13	1:A:80:SER:H	1.85	0.41
1:A:1183:VAL:HB	1:A:1214:GLN:HB3	2.02	0.41
3:T:10:DG:H2'	3:T:11:DC:C6	2.55	0.41
1:A:599:THR:N	1:A:600:PRO:HD2	2.35	0.41
2:B:375:HIS:CG	2:B:376:PRO:HD2	2.56	0.41
2:C:385:LEU:HB3	2:C:441:VAL:HB	2.01	0.41
1:A:973:LEU:H	1:A:973:LEU:HD13	1.85	0.41
2:B:414:TRP:HA	2:B:415:PRO:HD3	1.89	0.41
1:A:1079:ILE:HD12	1:A:1080:SER:OG	2.21	0.41
1:A:163:PRO:O	1:A:220:TRP:NE1	2.52	0.41
2:C:289:LEU:HB2	2:C:301:GLU:HB3	2.02	0.41
1:A:1064:ILE:HG22	1:A:1071:ARG:HB3	2.02	0.41
1:A:353:VAL:HG22	1:A:354:ASN:H	1.86	0.41
1:A:594:LEU:N	1:A:596:MET:H	2.19	0.41
2:B:265:LYS:C	2:B:267:ALA:H	2.23	0.41
2:B:280:ASP:HB3	2:B:283:GLY:H	1.86	0.41
2:B:454:HIS:ND1	2:B:463:LYS:HE3	2.36	0.41
2:B:91:LEU:HD23	2:B:96:HIS:HB3	2.02	0.41
1:A:891:VAL:HG13	1:A:1161:ARG:HH12	1.86	0.41
1:A:908:ALA:HB3	1:A:913:CYS:SG	2.60	0.41
2:B:420:THR:HG23	2:B:421:MET:HG2	2.02	0.41
1:A:185:VAL:O	1:A:187:VAL:HG23	2.20	0.41
1:A:642:SER:HA	1:A:643:ALA:HA	1.66	0.41
2:B:243:THR:HG1	2:B:251:TRP:HD1	1.64	0.41
2:C:96:HIS:HB3	2:C:97:PRO:C	2.41	0.41
1:A:556:THR:HA	1:A:559:LEU:HD13	2.03	0.40
1:A:973:LEU:HD21	1:A:976:GLN:HG3	2.03	0.40
2:B:454:HIS:CE1	2:B:463:LYS:HE3	2.56	0.40
1:A:499:LYS:H	1:A:499:LYS:HG3	1.60	0.40
2:C:440:THR:OG1	2:C:456:ARG:HB3	2.20	0.40
1:A:1169:GLY:HA2	1:A:1170:LEU:HA	1.75	0.40
1:A:616:GLU:HB2	1:A:617:ARG:HD3	2.04	0.40
1:A:236:THR:O	1:A:815:TRP:HD1	2.04	0.40
1:A:880:ALA:HA	1:A:881:PRO:HD3	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:244:PRO:HA	2:B:245:PRO:HD3	1.89	0.40
3:T:11:DC:H2"	3:T:12:DA:H8	1.86	0.40
1:A:272:SER:OG	1:A:844:VAL:O	2.30	0.40
2:C:407:LEU:HD23	2:C:407:LEU:HA	1.92	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	969/1205 (80%)	827 (85%)	120 (12%)	22 (2%)	6	37
2	B	355/485 (73%)	325 (92%)	27 (8%)	3 (1%)	19	58
2	C	350/485 (72%)	324 (93%)	19 (5%)	7 (2%)	7	40
All	All	1674/2175 (77%)	1476 (88%)	166 (10%)	32 (2%)	8	41

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	749	PHE
1	A	752	LEU
1	A	1070	PRO
1	A	1177	VAL
2	C	97	PRO
2	C	423	SER
1	A	767	ALA
1	A	1080	SER
1	A	1134	HIS
2	C	98	GLY
1	A	315	ALA
1	A	642	SER
1	A	743	ASP

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Mol	Chain	Res	Type
1	A	1073	PRO
1	A	1091	GLU
1	A	1207	GLU
2	C	316	PRO
2	C	319	VAL
2	C	380	PRO
2	C	391	PRO
1	A	618	HIS
1	A	927	ARG
2	B	308	ASP
1	A	560	PRO
1	A	610	PHE
1	A	765	PRO
1	A	1074	VAL
2	B	317	GLY
2	B	451	GLY
1	A	95	PRO
1	A	1203	PRO
1	A	1043	VAL

### 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	823/1017 (81%)	745 (90%)	78 (10%)	8	36
2	B	325/426 (76%)	303 (93%)	22 (7%)	16	49
2	C	317/426 (74%)	294 (93%)	23 (7%)	14	46
All	All	1465/1869 (78%)	1342 (92%)	123 (8%)	11	41

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	LEU
1	A	81	ARG
1	A	101	ARG

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Mol	Chain	Res	Type
1	A	118	VAL
1	A	130	LEU
1	A	133	ASP
1	A	195	LEU
1	A	197	PHE
1	A	227	ARG
1	A	236	THR
1	A	245	ILE
1	A	247	LEU
1	A	292	LEU
1	A	304	LEU
1	A	311	LEU
1	A	316	LYS
1	A	384	ASP
1	A	488	LEU
1	A	499	LYS
1	A	558	LEU
1	A	565	HIS
1	A	566	LEU
1	A	596	MET
1	A	613	HIS
1	A	617	ARG
1	A	639	THR
1	A	640	LEU
1	A	641	GLU
1	A	655	LEU
1	A	743	ASP
1	A	744	ILE
1	A	748	TRP
1	A	749	PHE
1	A	751	LYS
1	A	761	ASN
1	A	762	VAL
1	A	768	LYS
1	A	774	MET
1	A	779	LEU
1	A	816	LEU
1	A	818	ARG
1	A	821	LEU
1	A	841	LEU
1	A	851	THR
1	A	892	ASP

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Mol	Chain	Res	Type
1	A	913	CYS
1	A	921	LEU
1	A	927	ARG
1	A	941	ILE
1	A	964	ARG
1	A	973	LEU
1	A	977	GLU
1	A	992	LEU
1	A	1026	ARG
1	A	1027	LYS
1	A	1038	TRP
1	A	1043	VAL
1	A	1044	VAL
1	A	1047	ARG
1	A	1057	MET
1	A	1069	ILE
1	A	1071	ARG
1	A	1074	VAL
1	A	1075	LEU
1	A	1081	ARG
1	A	1090	GLU
1	A	1099	TRP
1	A	1118	TRP
1	A	1120	PHE
1	A	1129	PHE
1	A	1133	ILE
1	A	1141	VAL
1	A	1190	ARG
1	A	1191	LYS
1	A	1197	CYS
1	A	1198	LYS
1	A	1210	TYR
1	A	1218	LEU
2	B	69	LEU
2	B	85	GLN
2	B	89	ASP
2	B	186	LEU
2	B	197	LEU
2	B	231	ILE
2	B	263	TRP
2	B	277	ASP
2	B	329	LYS

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Mol	Chain	Res	Type
2	B	364	LYS
2	B	365	LYS
2	B	368	HIS
2	B	372	LEU
2	B	377	CYS
2	B	378	LEU
2	B	394	GLU
2	B	396	ARG
2	B	428	LEU
2	B	453	ILE
2	B	460	THR
2	B	461	THR
2	B	467	HIS
2	C	67	LEU
2	C	83	LYS
2	C	86	LEU
2	C	115	TRP
2	C	122	ARG
2	C	186	LEU
2	C	197	LEU
2	C	204	LEU
2	C	243	THR
2	C	251	TRP
2	C	256	LEU
2	C	262	TRP
2	C	281	GLU
2	C	282	GLU
2	C	284	ARG
2	C	293	PHE
2	C	295	TRP
2	C	300	ILE
2	C	334	CYS
2	C	386	ASP
2	C	402	LEU
2	C	419	GLU
2	C	453	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1175	GLN
2	B	355	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
4	DOC	P	24	3,4	14,19,20	3.53	8 (57%)	13,26,29	2.63	5 (38%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DOC	P	24	3,4	-	0/4/18/19	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	24	DOC	C2'-C1'	-8.85	1.31	1.51
4	P	24	DOC	O4'-C4'	5.93	1.56	1.44
4	P	24	DOC	C3'-C4'	-4.27	1.29	1.52
4	P	24	DOC	C4-N4	3.27	1.44	1.35
4	P	24	DOC	C3'-C2'	3.04	1.62	1.54
4	P	24	DOC	O4'-C1'	2.82	1.48	1.42
4	P	24	DOC	C5'-C4'	2.56	1.58	1.50
4	P	24	DOC	C2-N3	-2.14	1.33	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	24	DOC	C4'-O4'-C1'	-5.28	104.83	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	24	DOC	C2-N3-C4	4.88	121.28	116.34
4	P	24	DOC	C3'-C2'-C1'	4.82	108.36	102.78
4	P	24	DOC	N4-C4-N3	2.61	120.62	116.49
4	P	24	DOC	C5-C4-N3	-2.07	119.33	121.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	P	24	DOC	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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	1RY	A	1301	6	22,29,29	3.80	7 (31%)	28,45,45	3.03	12 (42%)

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	1RY	A	1301	6	1/1/5/5	6/19/31/31	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1301	1RY	CAW-SAS	-13.19	1.35	1.81
5	A	1301	1RY	OAP-CAW	8.52	1.68	1.44
5	A	1301	1RY	CAM-SAS	-4.89	1.66	1.81
5	A	1301	1RY	CAX-NAY	-3.27	1.39	1.49
5	A	1301	1RY	CAT-NAA	3.19	1.42	1.34
5	A	1301	1RY	CAL-CAW	2.89	1.60	1.51
5	A	1301	1RY	CAV-NAN	-2.80	1.32	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1301	1RY	CAW-OAP-CAX	-7.82	96.08	112.59
5	A	1301	1RY	CAM-SAS-CAW	6.30	104.80	88.24
5	A	1301	1RY	CAV-NAN-CAT	6.18	123.48	116.02
5	A	1301	1RY	FAJ-CAU-CAT	4.26	124.46	119.60
5	A	1301	1RY	NAA-CAT-NAN	4.07	122.79	117.03
5	A	1301	1RY	CAK-NAY-CAX	-3.80	110.69	119.24
5	A	1301	1RY	PBB-OAQ-PAZ	-3.65	120.32	132.83
5	A	1301	1RY	OAP-CAX-CAM	-3.58	100.95	109.29
5	A	1301	1RY	CAM-CAX-NAY	3.52	123.54	112.58
5	A	1301	1RY	PBA-OAR-PBB	-2.69	123.59	132.83
5	A	1301	1RY	CAX-CAM-SAS	-2.47	98.15	104.03
5	A	1301	1RY	CAU-CAK-NAY	2.47	122.06	119.77

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	1301	1RY	CAX

All (6) torsion outliers are listed below:

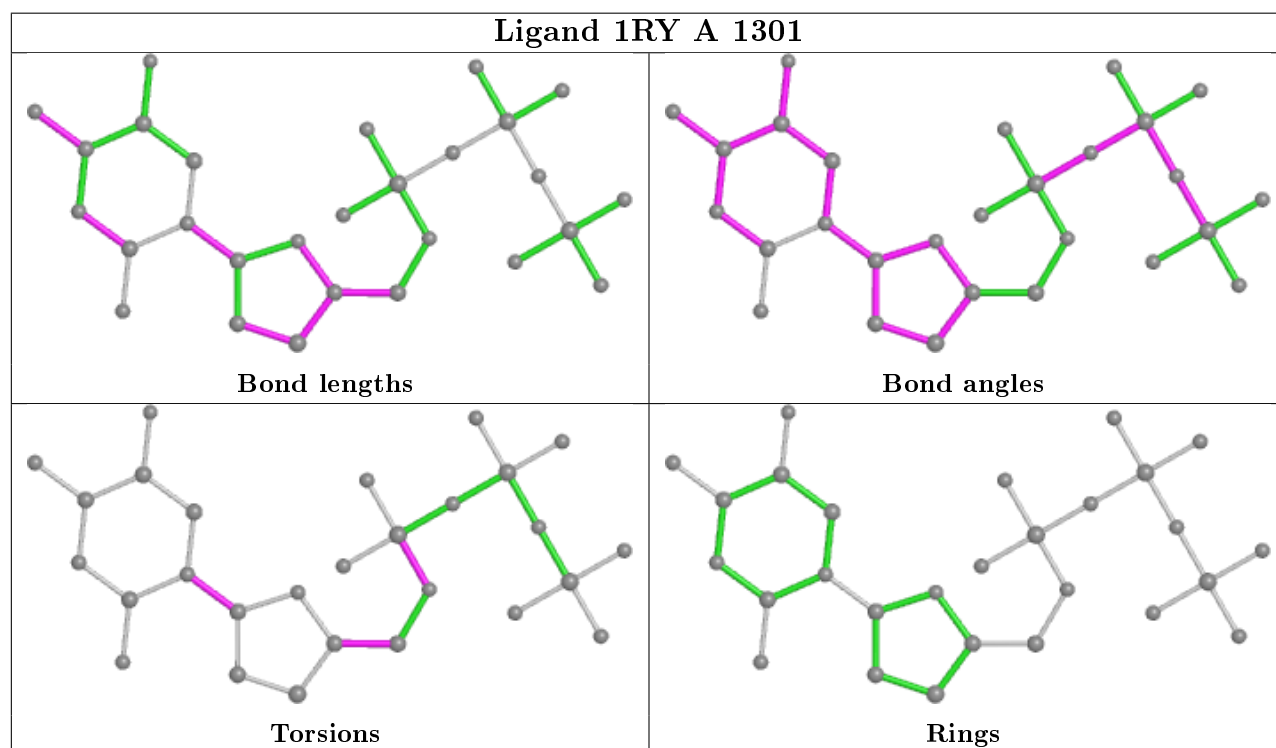
Mol	Chain	Res	Type	Atoms
5	A	1301	1RY	CAL-OAO-PBA-OAR
5	A	1301	1RY	CAL-OAO-PBA-OAH
5	A	1301	1RY	CAL-OAO-PBA-OAD
5	A	1301	1RY	OAO-CAL-CAW-OAP
5	A	1301	1RY	OAO-CAL-CAW-SAS
5	A	1301	1RY	OAP-CAX-NAY-CAK

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1301	1RY	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	983/1205 (81%)	0.21	46 (4%) 31 20	68, 92, 132, 164	0
2	B	363/485 (74%)	0.10	5 (1%) 75 62	69, 82, 122, 162	0
2	C	358/485 (73%)	0.22	17 (4%) 31 20	69, 87, 123, 162	0
3	T	26/26 (100%)	0.45	3 (11%) 4 3	110, 120, 129, 132	0
4	P	21/22 (95%)	0.31	0 100 100	111, 119, 130, 132	0
All	All	1751/2223 (78%)	0.19	71 (4%) 37 24	68, 88, 131, 164	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	630	ASN	9.8
1	A	746	GLY	9.3
1	A	747	CYS	8.3
1	A	745	PRO	8.0
1	A	632	ALA	6.0
1	A	744	ILE	5.4
1	A	173	GLU	5.4
2	C	121	PHE	4.8
1	A	622	TYR	4.2
1	A	631	LEU	4.1
2	C	219	PHE	4.1
2	C	120	VAL	3.8
1	A	506	GLU	3.6
2	C	387	VAL	3.6
1	A	634	LEU	3.6
1	A	764	SER	3.4
1	A	504	LYS	3.3
1	A	639	THR	3.3
1	A	633	LYS	3.2
2	C	423	SER	3.2

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Mol	Chain	Res	Type	RSRZ
2	C	422	GLN	3.2
2	C	123	GLU	3.2
1	A	507	PRO	3.1
1	A	508	ALA	3.0
1	A	215	ILE	3.0
2	C	122	ARG	2.9
1	A	759	SER	2.9
2	C	420	THR	2.9
1	A	172	ALA	2.9
1	A	230	GLU	2.8
1	A	124	GLU	2.8
1	A	193	ARG	2.8
2	C	282	GLU	2.7
1	A	563	PRO	2.7
2	C	466	MET	2.7
1	A	376	LEU	2.7
2	C	421	MET	2.6
1	A	765	PRO	2.6
2	C	388	GLY	2.6
1	A	1031	GLU	2.5
1	A	942	SER	2.5
1	A	210	THR	2.5
2	B	328	ARG	2.5
2	B	366	ASN	2.5
1	A	640	LEU	2.4
3	T	25	DT	2.4
2	C	124	GLN	2.3
1	A	595	GLN	2.3
2	B	485	VAL	2.3
1	A	741	ASP	2.3
1	A	912	GLY	2.3
2	C	236	GLU	2.3
1	A	214	ALA	2.3
2	C	273	PHE	2.2
1	A	1082	ALA	2.2
2	B	333	PRO	2.2
3	T	23	DT	2.2
1	A	771	LEU	2.2
1	A	171	TRP	2.2
2	C	231	ILE	2.2
1	A	918	TRP	2.1
1	A	509	THR	2.1

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Mol	Chain	Res	Type	RSRZ
3	T	22	DG	2.1
1	A	84	HIS	2.1
1	A	497	GLN	2.1
1	A	865	ALA	2.1
1	A	1174	PRO	2.1
1	A	1042	GLU	2.0
1	A	1213	PRO	2.0
2	B	179	GLY	2.0
1	A	211	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> )	Q<0.9
4	DOC	P	24	18/19	0.83	0.33	107,111,116,116	0

## 6.3 Carbohydrates [i](#)

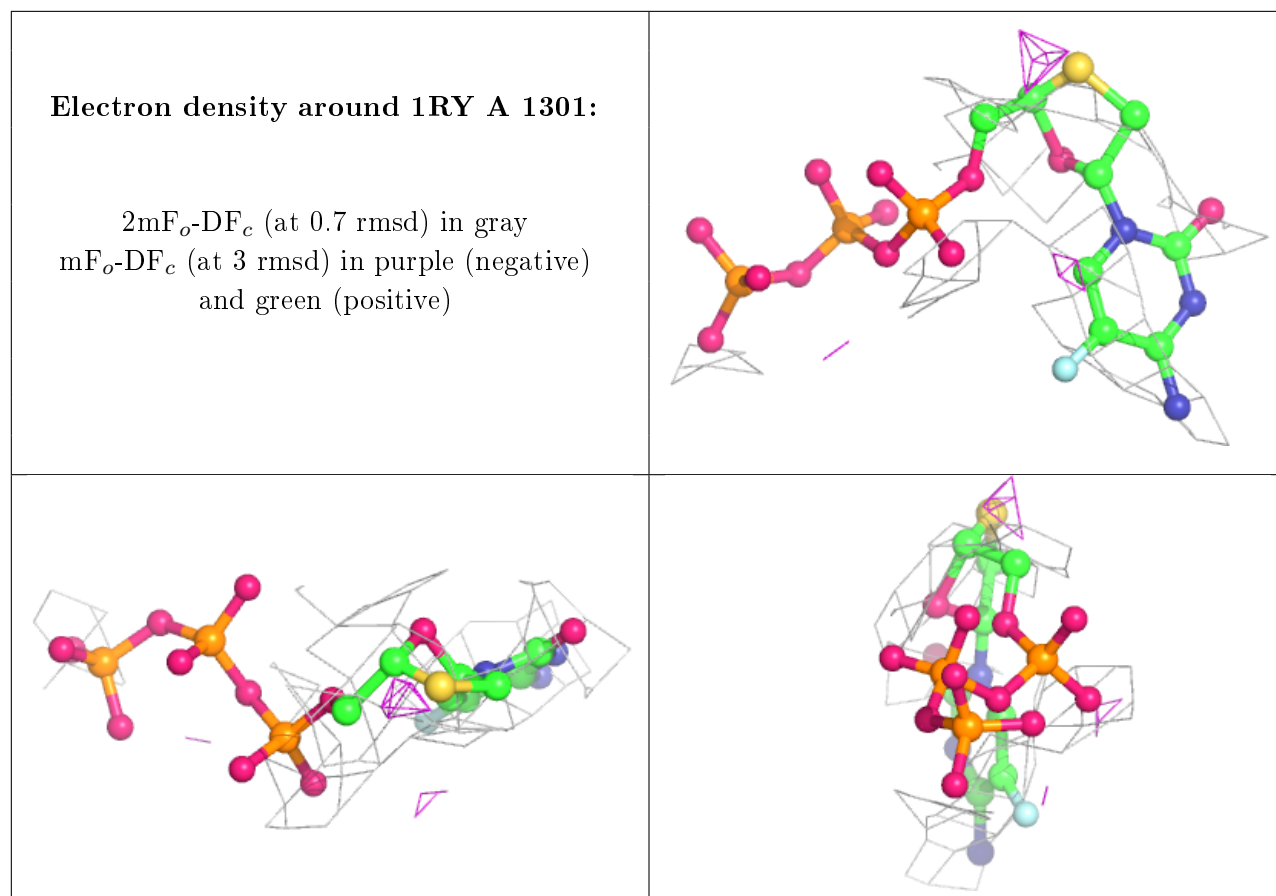
There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	MG	A	1302	1/1	0.84	0.44	84,84,84,84	0
5	1RY	A	1301	28/28	0.90	0.36	137,137,137,137	0
6	MG	A	1303	1/1	0.98	0.42	83,83,83,83	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.