



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:21 PM UTC

PDB ID : 5C52 / pdb_00005c52
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

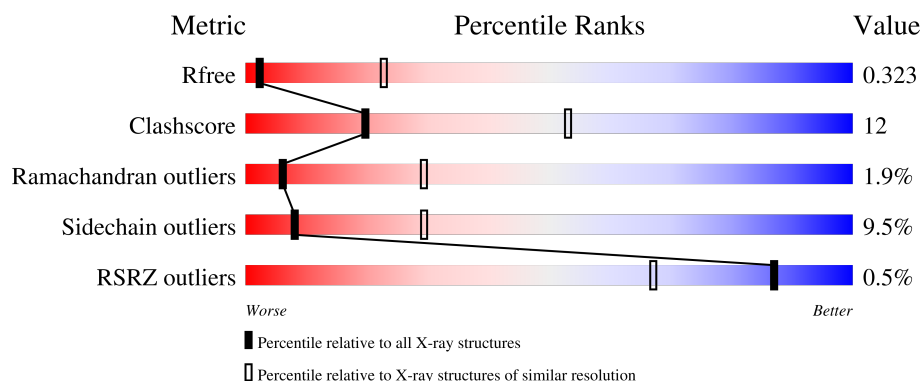
1 Overall quality at a glance

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}	180053	1132 (3.76-3.52)
Clashscore	190562	1014 (3.74-3.54)
Ramachandran outliers	187476	1123 (3.76-3.52)
Sidechain outliers	187428	1121 (3.76-3.52)
RSRZ outliers	180081	1130 (3.76-3.52)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1205	
2	B	485	
2	C	485	
3	T	26	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	P	22	68% 27% 5%

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
1	A	983	Total	C	N	O	S	0	0	0
			7799	4966	1371	1413	49			

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
2	B	363	Total	C	N	O	S	0	0	0
			2943	1885	520	522	16			
2	C	358	Total	C	N	O	S	0	0	0
			2887	1853	506	512	16			

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

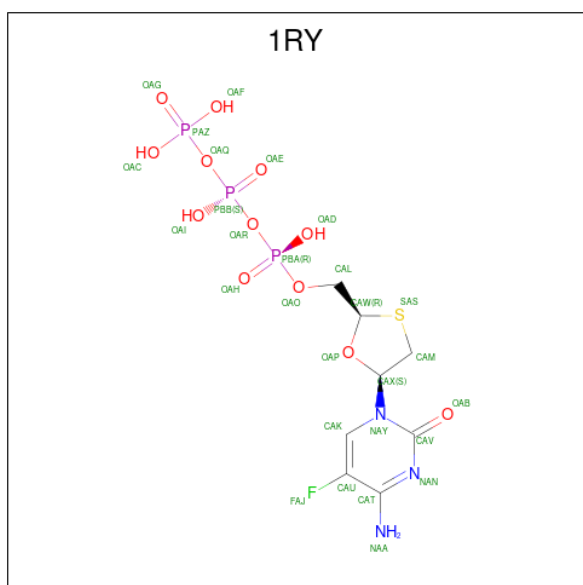
- Molecule 3 is a DNA chain called DNA (26-MER).

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 (CCD ID: 1RY) (formula: C₈H₁₃FN₃O₁₂P₃S).



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		

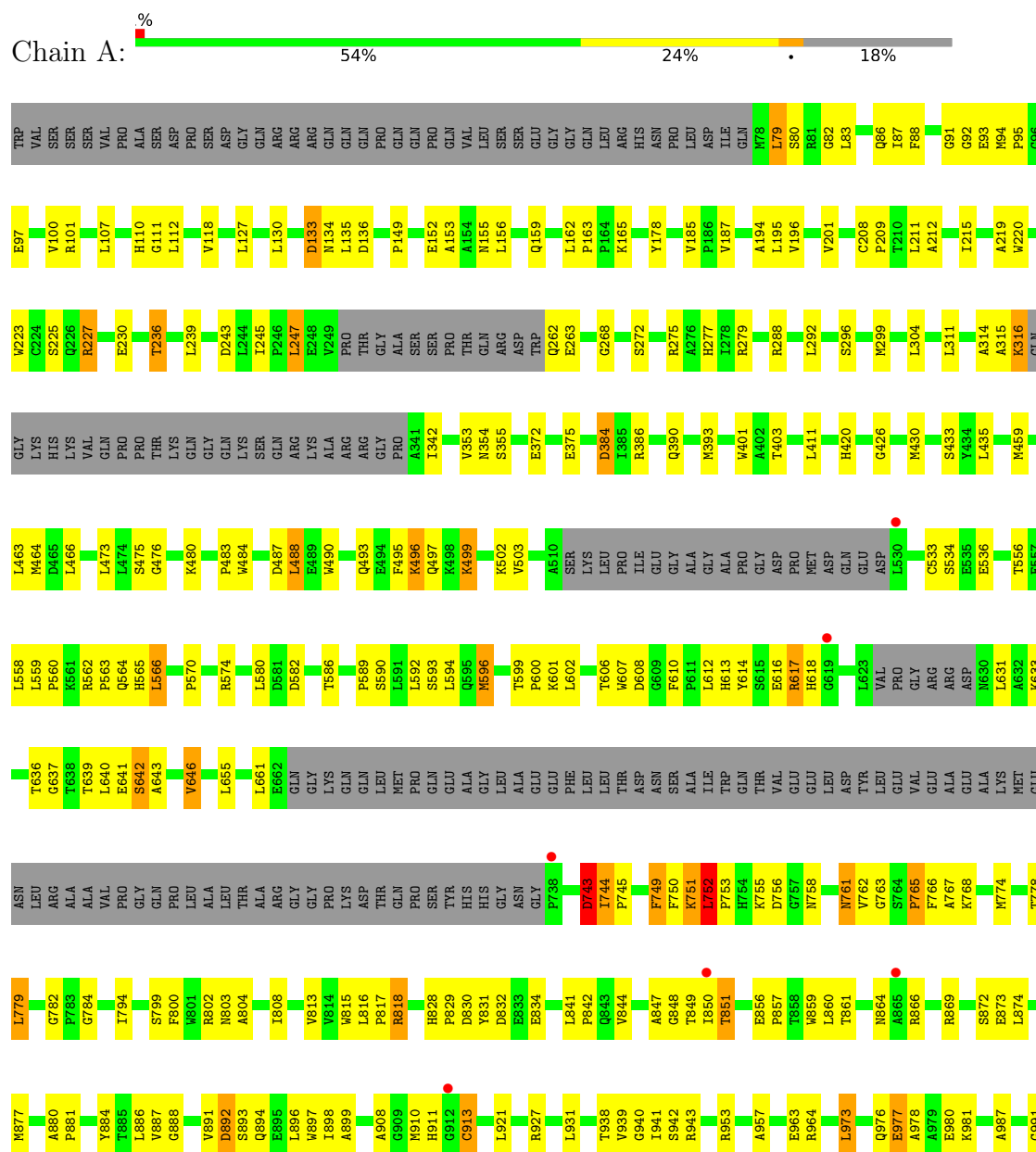
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

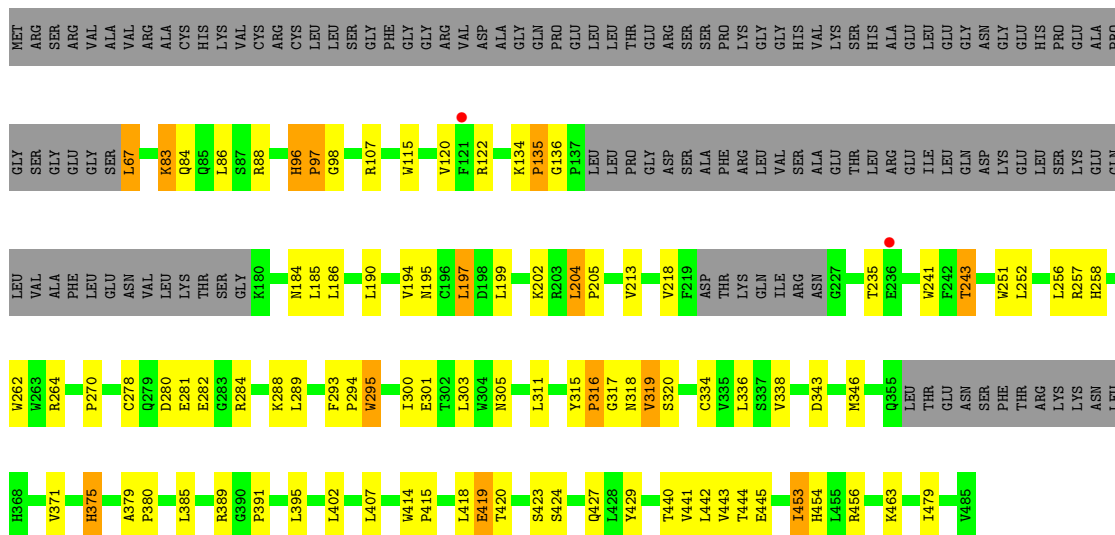
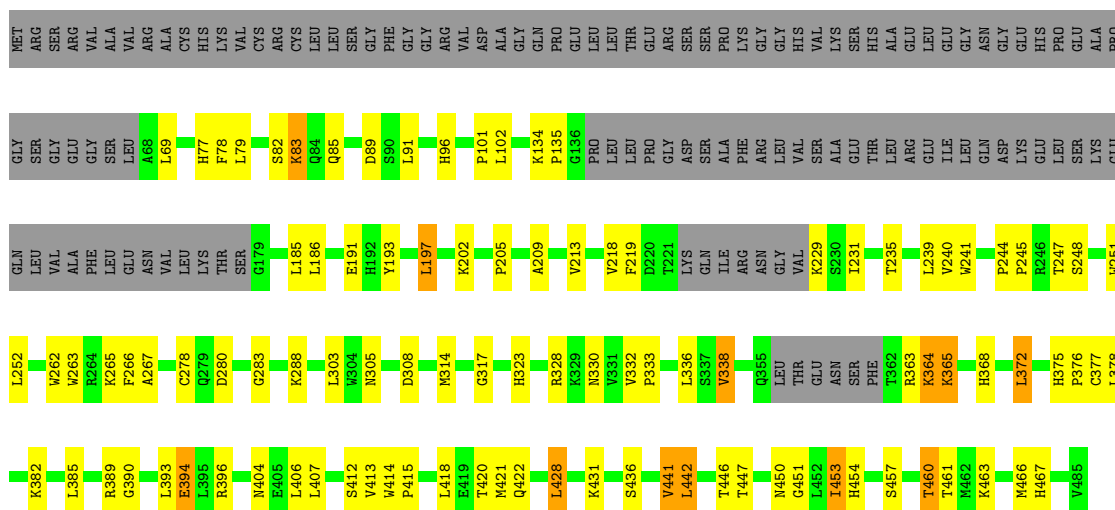
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Mg	0	0
			2	2		

3 Residue-property plots

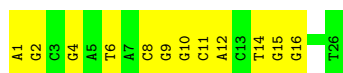
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: DNA polymerase subunit gamma-1





Chain T:  54% 46%



- 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')

Chain P:  68% 27% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 3.67Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.311 , 0.314 0.315 , 0.323	Depositor DCC
R_{free} test set	2000 reflections (4.47%)	wwPDB-VP
Wilson B-factor (Å ²)	137.7	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 123.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	14639	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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: DOC, MG, 1RY

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	0.32	0/7999	0.77	12/10852 (0.1%)
2	B	0.29	0/3016	0.74	0/4074
2	C	0.29	0/2960	0.77	6/4001 (0.1%)
3	T	0.19	0/591	0.33	0/909
4	P	0.17	0/488	0.28	0/752
All	All	0.30	0/15054	0.74	18/20588 (0.1%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	135	PRO	CA-N-CD	-9.17	99.16	112.00
1	A	1069	ILE	CA-C-N	8.60	130.59	119.84
1	A	1069	ILE	C-N-CA	8.60	130.59	119.84
2	C	96	HIS	C-N-CD	-7.76	103.52	120.60
2	C	96	HIS	CA-C-N	6.76	143.22	127.00
2	C	96	HIS	C-N-CA	6.76	143.22	127.00
1	A	752	LEU	CA-C-N	6.76	143.22	127.00
1	A	752	LEU	C-N-CA	6.76	143.22	127.00
1	A	752	LEU	C-N-CD	-6.63	106.02	120.60
1	A	1054	GLU	CB-CA-C	-6.24	109.39	116.63
1	A	165	LYS	CA-C-N	5.36	123.58	119.66
1	A	165	LYS	C-N-CA	5.36	123.58	119.66
2	C	375	HIS	CA-C-N	5.35	124.80	119.24
2	C	375	HIS	C-N-CA	5.35	124.80	119.24
1	A	208	CYS	CA-C-N	5.34	125.35	119.90
1	A	208	CYS	C-N-CA	5.34	125.35	119.90
1	A	582	ASP	CA-C-N	5.07	124.73	119.56
1	A	582	ASP	C-N-CA	5.07	124.73	119.56

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	203	0
2	B	2943	0	2939	58	0
2	C	2887	0	2867	61	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	328	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 12.

All (328) 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:211:LEU:HD22	1:A:393:MET:HE2	1.71	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:SD	1:A:1057:MET:N	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:977:GLU:HB3	1:A:981:LYS:HZ2	1.66	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:963:GLU:HG3	1:A:981:LYS:HZ3	1.66	0.59
1:A:896:LEU:HD21	1:A:931:LEU:HD23	1.84	0.59
2:B:278:CYS:SG	2:B:288:LYS:NZ	2.75	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:861:THR:HG21	3:T:8:DC:H1'	1.84	0.58
1:A:991:GLY:HA2	1:A:1052:GLY:HA2	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:899:ALA:HB1	1:A:1057:MET:HE3	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:953:ARG:HA	1:A:957:ALA:HB2	1.85	0.58
1:A:94:MET:HG3	1:A:1170:LEU:HD11	1.85	0.58
1:A:752:LEU:HB2	1:A:753:PRO:HA	1.86	0.58
1:A:153:ALA:HB1	1:A:194:ALA:HB2	1.85	0.57
1:A:761:ASN:OD1	1:A:761:ASN:N	2.35	0.57
1:A:136:ASP:HA	1:A:1163:MET:HE1	1.86	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:372:GLU:HG3	1:A:375:GLU:H	1.71	0.56
1:A:1069:ILE:O	1:A:1071:ARG:N	2.39	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:C:278:CYS:SG	2:C:288:LYS:NZ	2.79	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
2:B:457:SER:OG	2:B:460:THR:O	2.23	0.56
1:A:464:MET:HB2	1:A:589:PRO:HG2	1.88	0.56
1:A:495:PHE:HB3	1:A:496:LYS:HB2	1.87	0.56
1:A:196:VAL:HG22	1:A:215:ILE:HG12	1.88	0.56
1:A:743:ASP:N	1:A:743:ASP:OD1	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
1:A:488:LEU:HD13	1:A:488:LEU:H	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:296:SER:HB2	1:A:847:ALA:HB3	1.90	0.54
1:A:1073:PRO:HA	1:A:1074:VAL:HG13	1.89	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:93:GLU:HA	1:A:94:MET:HB2	1.88	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
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
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:869:ARG:HB2	1:A:872:SER:HB2	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1089:GLN:N	1:A:1090:GLU:HA	2.24	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:HD23	1:A:135:LEU:H	1.73	0.52
1:A:864:ASN:HB3	1:A:1191:LYS:HD3	1.91	0.52
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:851:THR:O	1:A:851:THR:OG1	2.29	0.51
1:A:864:ASN:O	1:A:872:SER:OG	2.24	0.51
1:A:1060:LYS:HE2	1:A:1064:ILE:HD11	1.93	0.51
2:C:107:ARG:HB2	2:C:346:MET:HE2	1.93	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:O	1:A:1072:THR:OG1	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:86:GLN:HG2	1:A:88:PHE:H	1.76	0.49
1:A:1133:ILE:HG12	1:A:1136:GLU:HB3	1.93	0.49
1:A:869:ARG:NH1	4:P:22:DT:OP1	2.46	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:87:ILE:HD13	1:A:127:LEU:HD22	1.94	0.49
1:A:243:ASP:OD1	1:A:243:ASP:N	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:435:LEU:HG	1:A:842:PRO:HG3	1.95	0.49
1:A:1072:THR:HB	1:A:1077:CYS:N	2.28	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1074:VAL:HB	1:A:1167:LYS:HB3	1.94	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
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:299:MET:HG3	1:A:849:THR:HG23	1.94	0.47
1:A:614:TYR:HE1	1:A:765:PRO:HG3	1.79	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:B:191:GLU:HA	2:B:314:MET:HE1	1.96	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:265:LYS:C	2:B:267:ALA:H	2.23	0.45
1:A:288:ARG:HE	1:A:288:ARG:HA	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:96:HIS:HB3	2:C:97:PRO:C	2.41	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
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:586:THR:OG1	1:A:590:SER:OG	2.23	0.44
1:A:850:ILE:HA	1:A:851:THR:HA	1.68	0.44
1:A:1133:ILE:O	1:A:1135:ASP:N	2.50	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: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
1:A:1085:PRO:HB3	1:A:1090:GLU:HG2	1.98	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:OD2	2:B:89:ASP:N	2.50	0.44
1:A:247:LEU:HD13	1:A:247:LEU:H	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:891:VAL:HG11	1:A:894:GLN:HB3	1.98	0.44
2:B:363:ARG:C	2:B:364:LYS:HG3	2.42	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
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:91:GLY:HA2	1:A:92:GLY:HA3	1.58	0.43
1:A:606:THR:HG21	1:A:612:LEU:HB2	2.00	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:459:MET:HB2	1:A:794:ILE:HG21	2.00	0.42
1:A:480:LYS:HD3	1:A:646:VAL:HG11	2.01	0.42
1:A:1163:MET:SD	1:A:1167:LYS:HE2	2.59	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
1:A:1136:GLU:OE2	1:A:1138:ARG:NH1	2.52	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1047:ARG:H	1:A:1047:ARG:HG3	1.62	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:94:MET:HE3	1:A:94:MET:HB3	1.97	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
1:A:612:LEU:HD12	1:A:612:LEU:HA	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:562:ARG:HH11	1:A:563:PRO:HD2	1.85	0.41
1:A:1090:GLU:O	1:A:1091:GLU:HG2	2.20	0.41
2:C:280:ASP:N	2:C:280:ASP:OD1	2.52	0.41
1:A:79:LEU:HD13	1:A:80:SER:H	1.85	0.41
1:A:483:PRO:HG2	1:A:484:TRP:CE3	2.56	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:272:SER:OG	1:A:844:VAL:O	2.30	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:564:GLN:H	1:A:564:GLN:CD	2.28	0.41
1:A:973:LEU:HD13	1:A:973:LEU:H	1.85	0.41
2:B:247:THR:HG1	2:B:251:TRP:CD1	2.38	0.41
2:B:414:TRP:HA	2:B:415:PRO:HD3	1.89	0.41
1:A:163:PRO:O	1:A:220:TRP:NE1	2.52	0.41
1:A:1079:ILE:HD12	1:A:1080:SER:OG	2.21	0.41
1:A:1090:GLU:CD	1:A:1096:ARG:HH11	2.28	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:289:LEU:HB2	2:C:301:GLU: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
1:A:1064:ILE:HG22	1:A:1071:ARG:HB3	2.02	0.41
2:B:91:LEU:HD23	2:B:96:HIS:HB3	2.02	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
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
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:236:THR:O	1:A:815:TRP:HD1	2.04	0.40
1:A:459:MET:HE2	1:A:459:MET:HB3	1.94	0.40
1:A:616:GLU:HB2	1:A:617:ARG:HD3	2.04	0.40
1:A:1169:GLY:HA2	1:A:1170:LEU:HA	1.75	0.40
1:A:880:ALA:HA	1:A:881:PRO:HD3	1.95	0.40
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
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%)	5 26

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	355/485 (73%)	325 (92%)	27 (8%)	3 (1%)	16	45
2	C	350/485 (72%)	324 (93%)	19 (5%)	7 (2%)	6	28
All	All	1674/2175 (77%)	1476 (88%)	166 (10%)	32 (2%)	6	29

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
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%)	737 (90%)	86 (10%)	7	27
2	B	325/426 (76%)	298 (92%)	27 (8%)	10	33
2	C	317/426 (74%)	291 (92%)	26 (8%)	10	33
All	All	1465/1869 (78%)	1326 (90%)	139 (10%)	8	29

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	LEU
1	A	101	ARG
1	A	118	VAL
1	A	130	LEU
1	A	133	ASP
1	A	195	LEU
1	A	201	VAL
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	342	ILE
1	A	384	ASP
1	A	390	GLN
1	A	411	LEU
1	A	473	LEU
1	A	488	LEU
1	A	496	LYS
1	A	499	LYS
1	A	558	LEU
1	A	565	HIS
1	A	566	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	580	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	646	VAL
1	A	655	LEU
1	A	661	LEU
1	A	743	ASP
1	A	744	ILE
1	A	749	PHE
1	A	751	LYS
1	A	756	ASP
1	A	761	ASN
1	A	762	VAL
1	A	768	LYS
1	A	774	MET
1	A	779	LEU
1	A	813	VAL
1	A	816	LEU
1	A	818	ARG
1	A	841	LEU
1	A	851	THR
1	A	886	LEU
1	A	892	ASP
1	A	913	CYS
1	A	921	LEU
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	1060	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1069	ILE
1	A	1071	ARG
1	A	1074	VAL
1	A	1081	ARG
1	A	1099	TRP
1	A	1102	GLN
1	A	1118	TRP
1	A	1120	PHE
1	A	1129	PHE
1	A	1133	ILE
1	A	1141	VAL
1	A	1151	LEU
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	83	LYS
2	B	186	LEU
2	B	197	LEU
2	B	218	VAL
2	B	231	ILE
2	B	240	VAL
2	B	263	TRP
2	B	332	VAL
2	B	338	VAL
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	406	LEU
2	B	413	VAL
2	B	428	LEU
2	B	441	VAL
2	B	442	LEU
2	B	453	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	194	VAL
2	C	197	LEU
2	C	204	LEU
2	C	218	VAL
2	C	243	THR
2	C	251	TRP
2	C	256	LEU
2	C	258	HIS
2	C	262	TRP
2	C	281	GLU
2	C	282	GLU
2	C	295	TRP
2	C	300	ILE
2	C	319	VAL
2	C	334	CYS
2	C	371	VAL
2	C	402	LEU
2	C	419	GLU
2	C	453	ILE
2	C	479	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	HIS
1	A	146	GLN
1	A	388	ASN
1	A	828	HIS
1	A	1175	GLN
1	A	1214	GLN
2	B	85	GLN
2	B	96	HIS
2	B	305	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	318	ASN
2	B	355	GLN
2	C	201	ASN
2	C	210	GLN
2	C	409	ASN

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	4,3	16,19,20	3.62	9 (56%)	20,26,29	1.87	2 (10%)

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	4,3	-	0/7/18/19	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	24	DOC	C2'-C1'	-9.25	1.31	1.52
4	P	24	DOC	O4'-C4'	6.12	1.56	1.44
4	P	24	DOC	C4-N4	4.50	1.44	1.33
4	P	24	DOC	C3'-C4'	-4.43	1.29	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	24	DOC	C2-N1	-3.32	1.33	1.40
4	P	24	DOC	C3'-C2'	3.04	1.62	1.54
4	P	24	DOC	C6-C5	2.89	1.41	1.35
4	P	24	DOC	O4'-C1'	2.82	1.48	1.42
4	P	24	DOC	C5'-C4'	2.48	1.58	1.50

All (2) 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
4	P	24	DOC	C3'-C2'-C1'	4.76	108.36	102.87

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 oligosaccharides 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	28,29,29	3.80	10 (35%)	40,45,45	3.23	15 (37%)

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	9/22/31/31	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1301	1RY	CAW-SAS	-14.22	1.35	1.81
5	A	1301	1RY	OAP-CAW	9.18	1.68	1.43
5	A	1301	1RY	CAM-SAS	-5.15	1.66	1.81
5	A	1301	1RY	CAK-CAU	3.41	1.38	1.33
5	A	1301	1RY	CAT-CAU	-3.39	1.40	1.42
5	A	1301	1RY	CAX-NAY	-3.33	1.39	1.48
5	A	1301	1RY	CAT-NAA	3.15	1.42	1.34
5	A	1301	1RY	CAL-CAW	3.14	1.60	1.51
5	A	1301	1RY	CAK-NAY	-2.95	1.33	1.38
5	A	1301	1RY	CAV-NAY	-2.92	1.33	1.40

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1301	1RY	FAJ-CAU-CAT	10.01	124.46	118.09
5	A	1301	1RY	CAW-OAP-CAX	-8.06	96.08	112.68
5	A	1301	1RY	CAX-NAY-CAV	6.86	129.60	117.83
5	A	1301	1RY	CAM-SAS-CAW	6.60	104.80	88.41
5	A	1301	1RY	CAX-NAY-CAK	-5.98	110.69	120.74
5	A	1301	1RY	OAP-CAX-CAM	-3.86	100.95	109.26
5	A	1301	1RY	CAM-CAX-NAY	3.76	123.54	112.69
5	A	1301	1RY	OAP-CAX-NAY	3.73	114.49	107.86
5	A	1301	1RY	CAK-CAU-CAT	-3.71	117.57	120.25
5	A	1301	1RY	FAJ-CAU-CAK	-3.59	117.96	120.99
5	A	1301	1RY	CAU-CAT-NAN	-3.48	117.32	119.59
5	A	1301	1RY	OAB-CAV-NAN	-3.21	117.27	122.33
5	A	1301	1RY	CAX-CAM-SAS	-2.63	98.15	104.08
5	A	1301	1RY	NAA-CAT-NAN	2.36	122.79	118.51
5	A	1301	1RY	OAB-CAV-NAY	2.03	122.87	118.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	1301	1RY	CAX

All (9) torsion outliers are listed below:

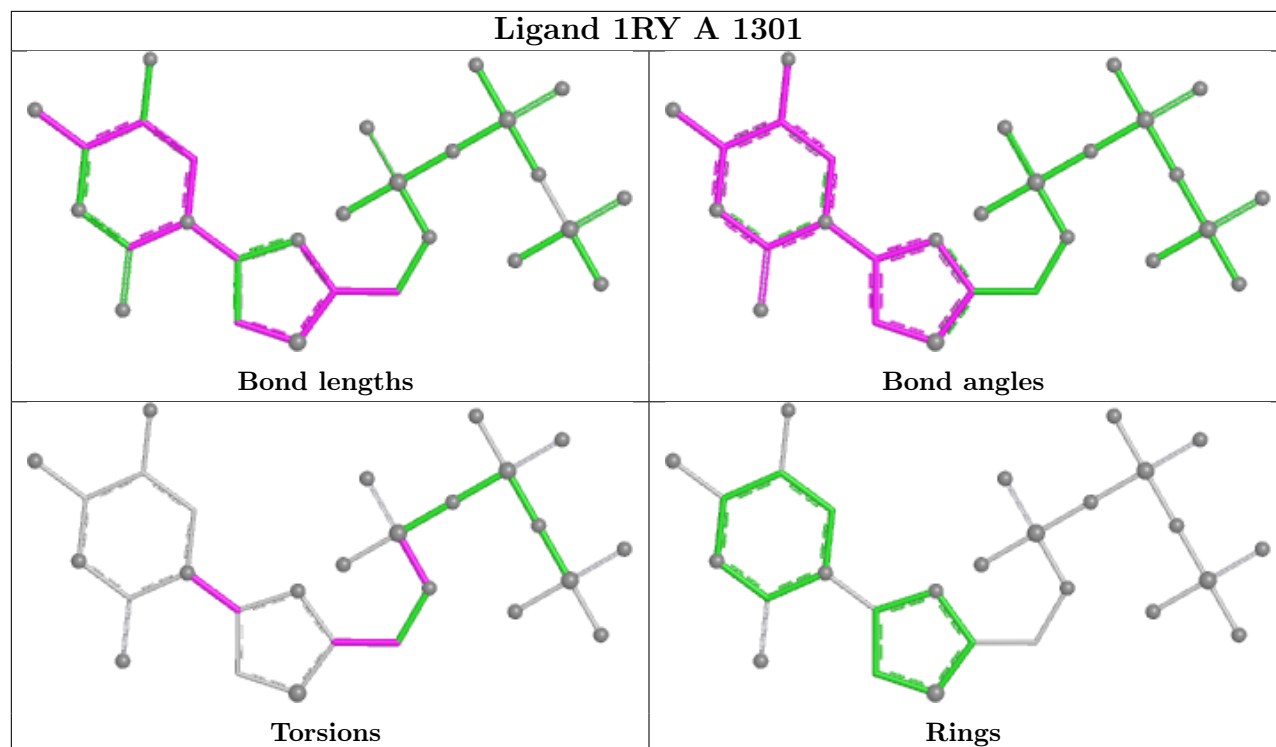
Mol	Chain	Res	Type	Atoms
5	A	1301	1RY	CAL-OAO-PBA-OAR
5	A	1301	1RY	CAL-OAO-PBA-OAH
5	A	1301	1RY	CAL-OAO-PBA-OAD
5	A	1301	1RY	OAO-CAL-CAW-OAP
5	A	1301	1RY	OAO-CAL-CAW-SAS
5	A	1301	1RY	CAM-CAX-NAY-CAK
5	A	1301	1RY	CAM-CAX-NAY-CAV
5	A	1301	1RY	OAP-CAX-NAY-CAK
5	A	1301	1RY	OAP-CAX-NAY-CAV

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, 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	983/1205 (81%)	-0.12	7 (0%) 84 62	68, 92, 132, 164	0
2	B	363/485 (74%)	-0.19	0 100 100	69, 82, 122, 162	0
2	C	358/485 (73%)	-0.26	2 (0%) 85 65	69, 87, 123, 162	0
3	T	26/26 (100%)	-0.10	0 100 100	110, 120, 129, 132	0
4	P	21/22 (95%)	-0.27	0 100 100	111, 119, 130, 132	0
All	All	1751/2223 (78%)	-0.17	9 (0%) 87 67	68, 88, 131, 164	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	850	ILE	3.4
1	A	912	GLY	2.8
1	A	865	ALA	2.7
2	C	236	GLU	2.6
2	C	121	PHE	2.6
1	A	619	GLY	2.3
1	A	738	PRO	2.3
1	A	530	LEU	2.1
1	A	1174	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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(Å ²)	Q<0.9
4	DOC	P	24	18/19	0.83	0.10	107,111,116,116	0

6.3 Carbohydrates [i](#)

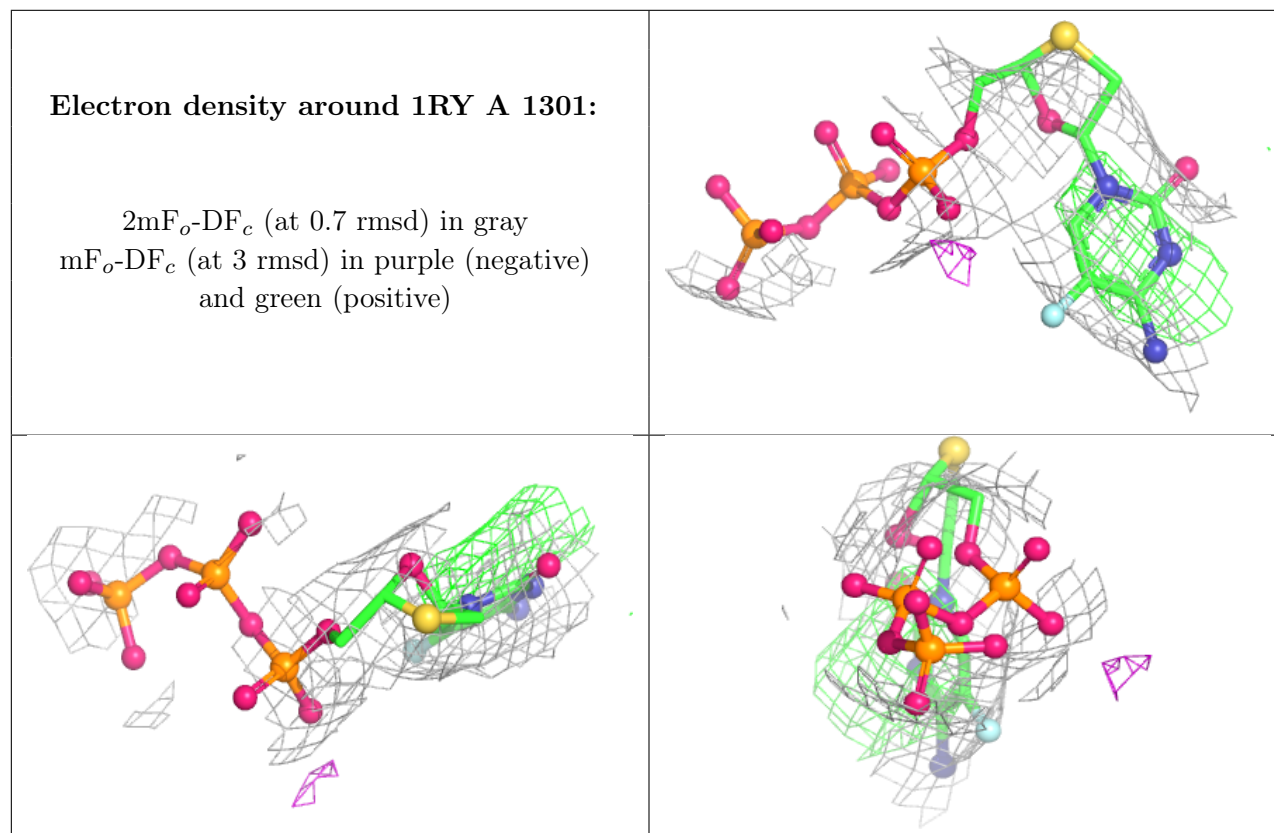
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
6	MG	A	1302	1/1	0.78	0.08	84,84,84,84	0
5	1RY	A	1301	28/28	0.88	0.12	137,137,137,137	0
6	MG	A	1303	1/1	1.00	0.09	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.