Full wwPDB X-ray Structure Validation Report

May 15, 2020 – 11:08 am BST

PDB ID	:	5C51
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.; Amiralaei, S.; Schinazi, R.F.; Anderson, K.S.; Whitney, Y.Y.
Deposited on	:	2015-06-19
Resolution	:	3.43 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

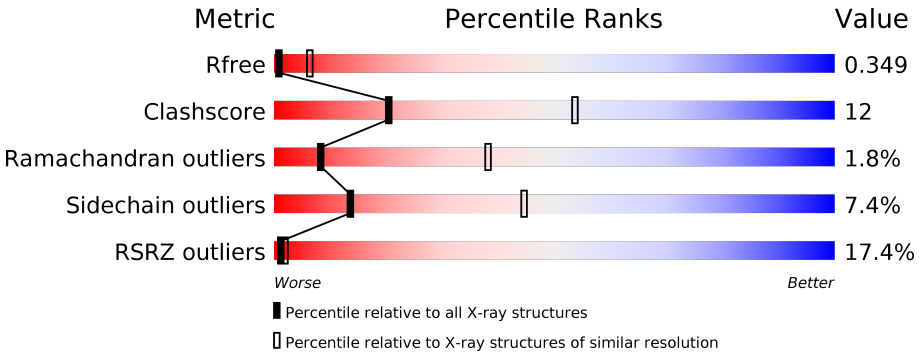
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.43 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	1486 (3.50-3.34)
Clashscore	141614	1572 (3.50-3.34)
Ramachandran outliers	138981	1534 (3.50-3.34)
Sidechain outliers	138945	1535 (3.50-3.34)
RSRZ outliers	127900	1395 (3.50-3.34)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	16% 55% 23% • 18%
2	B	485	7% 56% 17% • 25%
2	C	485	13% 55% 17% • 26%
3	P	22	41% 41% 59%
4	T	25	28% 32% 64% •

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
3	DOC	P	24	-	-	X	-
6	1RY	A	4003	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14620 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
			7802	4966	1374	1413	49			

There are 11 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
A	948	ARG	ILE	conflict	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
			2888	1852	506	514	16			

- Molecule 3 is a DNA chain called DNA (5'-D(*(AD)P*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
3	P	22	Total	C	N	O	P	0	0	0
			451	214	92	124	21			

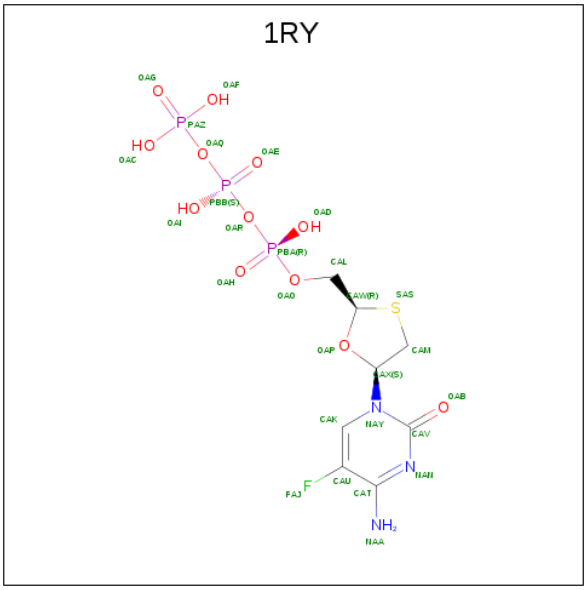
- Molecule 4 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	T	25	Total	C	N	O	P	0	0	0
			506	241	87	154	24			

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 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: $C_8H_{13}FN_3O_{12}P_3S$).



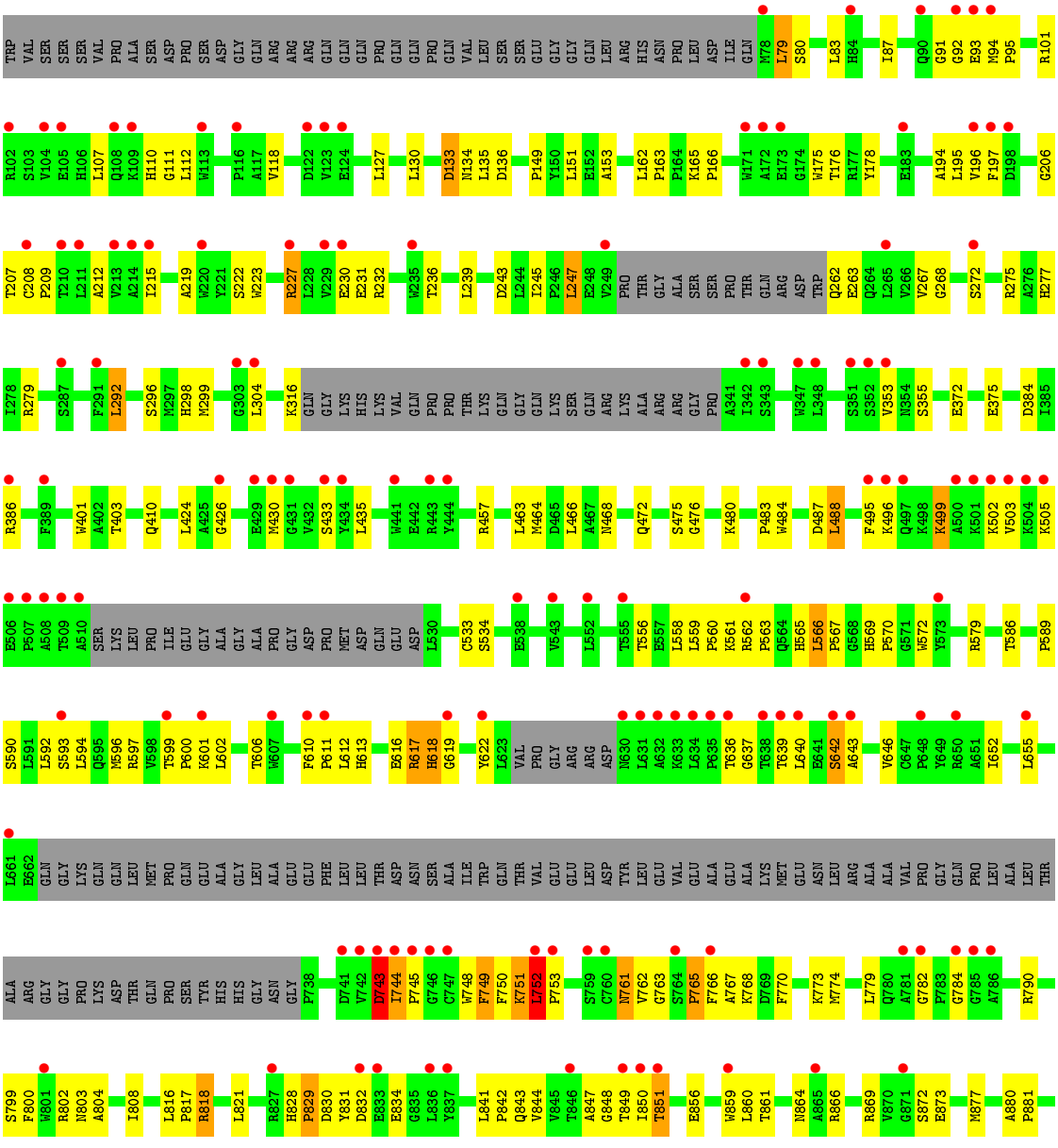
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
6	A	1	Total	C	F	N	O	P	S	0	0
			28	8	1	3	12	3	1		

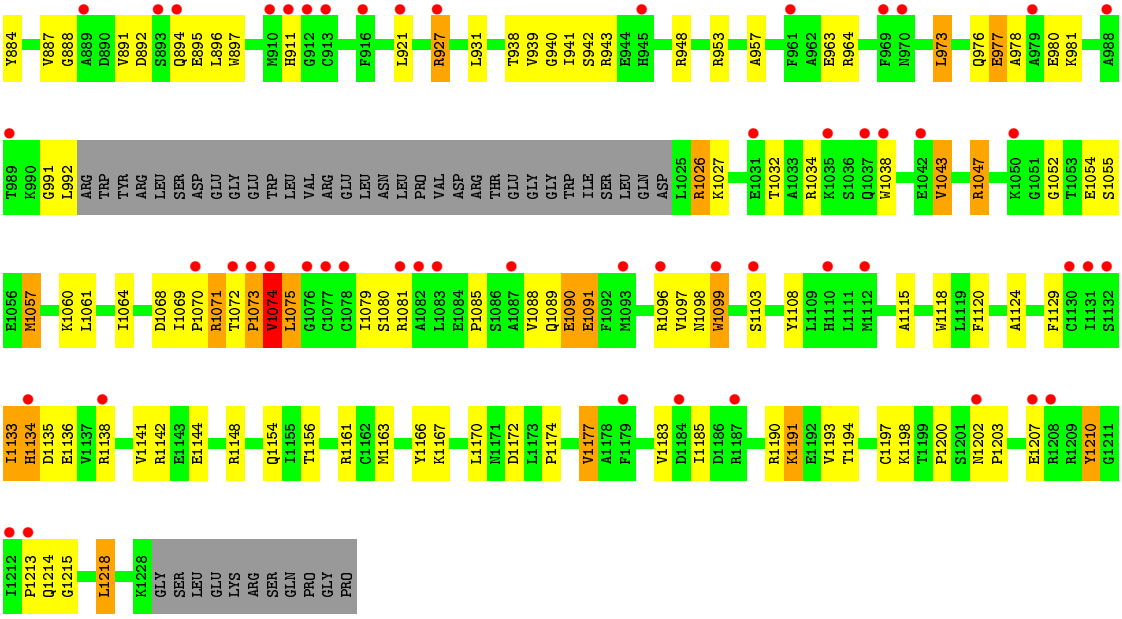
3 Residue-property plots (i)

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: DNA polymerase subunit gamma-1

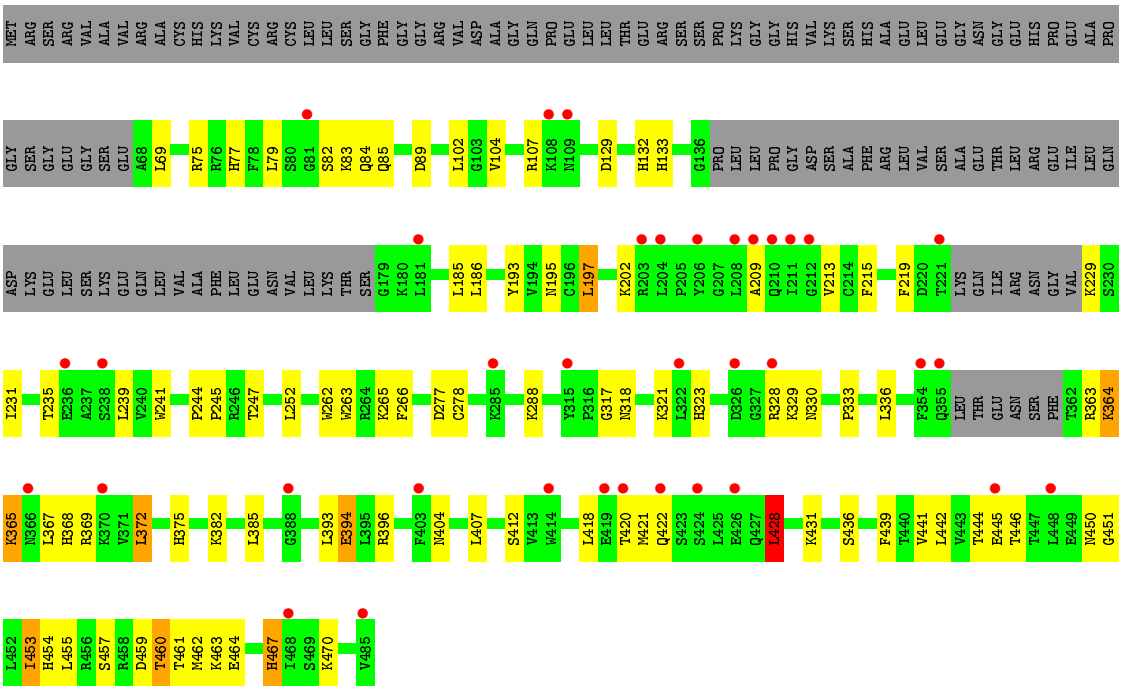
Chain A:





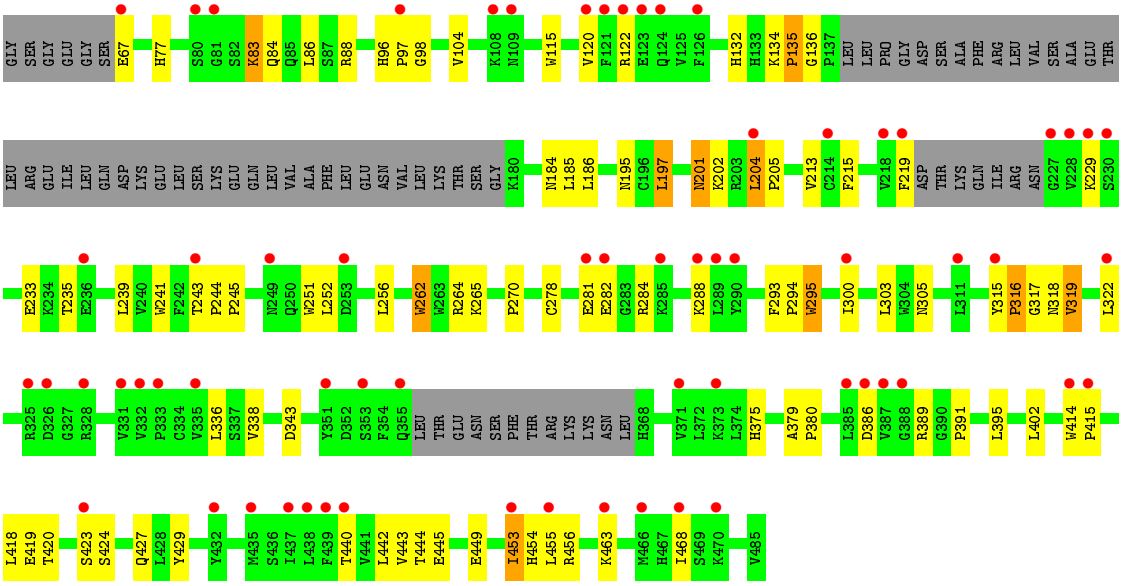
- Molecule 2: DNA polymerase subunit gamma-2, mitochondrial

Chain B:

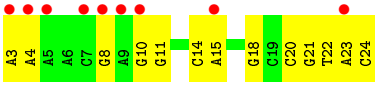


- Molecule 2: DNA polymerase subunit gamma-2, mitochondrial

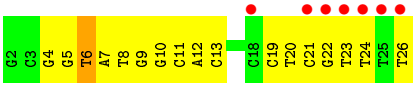
Chain C:



• Molecule 3: DNA (5'-D(*(AD)P*AP*AP*AP*CP*GP*AP*GP*GP*GP*CP*CP*AP*GP*TP*GP*CP*CP*GP*TP*AP*C)-3')



• Molecule 4: DNA



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	215.05Å 215.05Å 161.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.02 – 3.43 49.64 – 3.42	Depositor EDS
% Data completeness (in resolution range)	98.2 (47.02-3.43) 84.8 (49.64-3.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.33 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.315 , 0.345 0.340 , 0.349	Depositor DCC
R_{free} test set	2000 reflections (3.94%)	wwPDB-VP
Wilson B-factor (Å^2)	134.7	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 8.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	14620	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.05% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.22	0/8002	0.43	2/10855 (0.0%)
2	B	0.22	0/3016	0.39	1/4074 (0.0%)
2	C	0.23	0/2961	0.42	2/4002 (0.0%)
3	P	0.48	0/488	0.75	0/752
4	T	0.44	0/565	1.13	1/870 (0.1%)
All	All	0.25	0/15032	0.49	6/20553 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	135	PRO	CA-N-CD	-8.68	99.35	111.50
2	C	96	HIS	C-N-CD	-7.00	105.19	120.60
1	A	752	LEU	C-N-CD	-6.60	106.07	120.60
4	T	6	DT	N3-C4-O4	5.48	123.19	119.90
1	A	752	LEU	C-N-CA	5.08	143.34	122.00
2	B	428	LEU	CA-CB-CG	5.01	126.82	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	7802	0	7694	212	1
2	B	2943	0	2939	64	0
2	C	2888	0	2862	65	1
3	P	451	0	245	31	0
4	T	506	0	279	37	0
5	A	2	0	0	0	0
6	A	28	0	11	15	0
All	All	14620	0	14030	350	1

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 (350) 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)
6:A:4003:1RY:CAX	6:A:4003:1RY:OAP	1.63	1.38
1:A:948:ARG:NE	6:A:4003:1RY:NAA	1.86	1.23
1:A:948:ARG:NH2	3:P:24:DOC:N4	1.88	1.21
1:A:948:ARG:NH2	3:P:24:DOC:HN42	1.42	1.18
2:C:135:PRO:HD2	2:C:136:GLY:H	1.13	1.12
3:P:20:DC:O2	4:T:10:DG:N2	1.86	1.08
1:A:948:ARG:CZ	6:A:4003:1RY:NAA	2.21	1.04
1:A:948:ARG:NH2	6:A:4003:1RY:NAA	2.12	0.97
1:A:948:ARG:NH2	6:A:4003:1RY:H12	1.67	0.92
1:A:948:ARG:NE	6:A:4003:1RY:H13	1.64	0.91
2:C:419:GLU:H	2:C:420:THR:HA	1.35	0.91
3:P:20:DC:C2	4:T:10:DG:N2	2.39	0.91
1:A:948:ARG:NE	6:A:4003:1RY:H12	1.63	0.89
2:C:135:PRO:HD2	2:C:136:GLY:N	1.88	0.87
1:A:850:ILE:HG22	4:T:6:DT:H4'	1.58	0.86
1:A:948:ARG:HH22	3:P:24:DOC:HN42	0.86	0.85
3:P:10:DG:N2	4:T:19:DC:O2	2.09	0.85
1:A:948:ARG:HE	6:A:4003:1RY:H12	1.15	0.84
1:A:948:ARG:HH21	6:A:4003:1RY:H12	1.22	0.83
1:A:948:ARG:CZ	6:A:4003:1RY:H12	1.84	0.82
2:C:135:PRO:CD	2:C:136:GLY:H	1.94	0.80
3:P:10:DG:N2	4:T:20:DT:O2	2.17	0.78
2:C:442:LEU:HB3	2:C:454:HIS:HB2	1.70	0.74
2:C:67:GLU:HG3	2:C:88:ARG:NH2	2.03	0.73
2:B:77:HIS:HE1	2:B:431:LYS:HG3	1.54	0.72
1:A:464:MET:HB2	1:A:589:PRO:HG2	1.72	0.72
2:C:443:VAL:HG22	2:C:453:ILE:HD11	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:ASP:OD2	1:A:601:LYS:NZ	2.23	0.70
1:A:561:LYS:HE2	4:T:22:DG:OP2	1.92	0.70
1:A:963:GLU:HG3	1:A:981:LYS:HZ3	1.57	0.69
1:A:243:ASP:HB3	1:A:279:ARG:HE	1.57	0.68
1:A:1108:TYR:OH	1:A:1161:ARG:NH1	2.27	0.68
3:P:18:DG:C2	4:T:12:DA:C2	2.81	0.67
3:P:21:DG:N2	4:T:8:DT:H3	1.92	0.67
1:A:1068:ASP:HA	1:A:1085:PRO:HG2	1.75	0.67
3:P:10:DG:N1	4:T:19:DC:N3	2.35	0.66
1:A:884:TYR:HA	1:A:1142:ARG:HA	1.78	0.66
1:A:153:ALA:HB1	1:A:194:ALA:HB2	1.77	0.65
2:B:197:LEU:HD22	2:B:202:LYS:HA	1.78	0.65
1:A:79:LEU:H	1:A:83:LEU:HG	1.62	0.65
1:A:1161:ARG:HE	1:A:1177:VAL:HG22	1.63	0.64
1:A:463:LEU:HD21	1:A:594:LEU:HD23	1.79	0.64
1:A:856:GLU:OE1	1:A:859:TRP:N	2.28	0.64
1:A:896:LEU:HD21	1:A:931:LEU:HD23	1.78	0.64
1:A:1057:MET:N	1:A:1057:MET:SD	2.71	0.64
1:A:533:CYS:SG	1:A:534:SER:N	2.70	0.63
2:C:134:LYS:HG2	2:C:135:PRO:CD	2.27	0.63
2:C:278:CYS:SG	2:C:288:LYS:NZ	2.72	0.63
2:C:134:LYS:HG2	2:C:135:PRO:HD2	1.80	0.63
1:A:1069:ILE:O	1:A:1071:ARG:N	2.33	0.62
2:C:213:VAL:HG22	2:C:235:THR:HG22	1.81	0.62
1:A:208:CYS:SG	1:A:227:ARG:NH2	2.73	0.62
3:P:21:DG:N2	4:T:8:DT:O2	2.33	0.61
2:C:135:PRO:CD	2:C:136:GLY:N	2.56	0.61
2:C:83:LYS:HG2	2:C:84:GLN:HG2	1.81	0.61
1:A:1135:ASP:HB2	6:A:4003:1RY:H5	1.83	0.61
1:A:938:THR:N	1:A:939:VAL:HA	2.16	0.60
1:A:938:THR:H	1:A:939:VAL:HA	1.66	0.60
2:C:424:SER:HB3	2:C:427:GLN:HG2	1.84	0.60
2:B:278:CYS:SG	2:B:288:LYS:NZ	2.73	0.60
2:B:442:LEU:HB3	2:B:454:HIS:HB2	1.83	0.60
1:A:849:THR:HG22	1:A:850:ILE:HD13	1.81	0.60
1:A:134:ASN:ND2	1:A:1166:TYR:OH	2.34	0.60
1:A:502:LYS:HB3	1:A:503:VAL:HB	1.83	0.59
2:C:429:TYR:HE1	2:C:463:LYS:HZ3	1.49	0.59
1:A:861:THR:HG21	4:T:8:DT:H1'	1.84	0.59
1:A:978:ALA:HA	1:A:981:LYS:HD2	1.84	0.59
1:A:232:ARG:NH2	2:C:468:ILE:HG21	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:10:DG:C2	4:T:20:DT:O2	2.56	0.59
1:A:744:ILE:HG23	1:A:745:PRO:HD3	1.84	0.58
1:A:230:GLU:OE2	1:A:386:ARG:NH1	2.37	0.58
1:A:239:LEU:O	1:A:279:ARG:NH1	2.37	0.58
1:A:800:PHE:HB2	1:A:869:ARG:HE	1.68	0.58
4:T:9:DG:H2'	4:T:10:DG:C8	2.39	0.58
1:A:1142:ARG:NH1	1:A:1144:GLU:OE1	2.34	0.57
3:P:21:DG:H22	4:T:8:DT:H3	1.50	0.57
1:A:911:HIS:NE2	1:A:1172:ASP:O	2.36	0.57
1:A:1098:ASN:ND2	4:T:5:DG:H1'	2.20	0.57
3:P:4:DA:N3	4:T:26:DT:C1'	2.62	0.56
2:C:419:GLU:N	2:C:420:THR:HA	2.07	0.56
1:A:1061:LEU:HB3	1:A:1097:VAL:HG13	1.88	0.56
2:B:83:LYS:HG2	2:B:85:GLN:H	1.70	0.56
1:A:556:THR:OG1	2:B:450:ASN:O	2.13	0.56
2:C:197:LEU:HD12	2:C:202:LYS:HG2	1.87	0.56
1:A:488:LEU:H	1:A:488:LEU:HD13	1.70	0.56
2:B:363:ARG:HD3	2:B:364:LYS:H	1.70	0.56
1:A:831:TYR:H	1:A:832:ASP:HA	1.70	0.56
3:P:21:DG:N2	4:T:8:DT:C2	2.73	0.56
1:A:212:ALA:HB3	1:A:223:TRP:HB3	1.88	0.56
2:B:132:HIS:CD2	2:C:213:VAL:HG11	2.40	0.56
1:A:299:MET:HG2	1:A:848:GLY:HA2	1.87	0.56
2:C:184:ASN:OD1	2:C:185:LEU:N	2.39	0.55
3:P:21:DG:N2	4:T:8:DT:N3	2.52	0.55
1:A:567:PRO:HD2	2:B:464:GLU:OE1	2.07	0.55
2:B:428:LEU:HD13	2:B:428:LEU:H	1.71	0.55
1:A:484:TRP:HZ3	2:B:364:LYS:HZ1	1.51	0.55
1:A:353:VAL:HG13	1:A:355:SER:H	1.71	0.55
1:A:743:ASP:OD1	1:A:743:ASP:N	2.40	0.55
1:A:466:LEU:HB3	1:A:602:LEU:HD21	1.89	0.54
1:A:752:LEU:HB2	1:A:753:PRO:HA	1.88	0.54
1:A:869:ARG:HB2	1:A:872:SER:HB2	1.90	0.54
1:A:94:MET:HG3	1:A:1170:LEU:HD11	1.88	0.54
1:A:977:GLU:HB3	1:A:981:LYS:HZ2	1.72	0.54
2:C:235:THR:OG1	2:C:343:ASP:OD1	2.24	0.54
1:A:372:GLU:HG3	1:A:375:GLU:H	1.72	0.54
1:A:991:GLY:HA2	1:A:1052:GLY:HA2	1.90	0.54
1:A:1079:ILE:HG12	1:A:1099:TRP:CZ3	2.43	0.54
1:A:761:ASN:N	1:A:761:ASN:OD1	2.42	0.53
2:B:185:LEU:H	2:B:185:LEU:HD23	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1089:GLN:N	1:A:1090:GLU:HA	2.24	0.53
1:A:921:LEU:HD22	1:A:1174:PRO:HG2	1.91	0.53
2:B:219:PHE:HA	2:B:229:LYS:N	2.24	0.53
1:A:1073:PRO:HA	1:A:1074:VAL:HG13	1.90	0.53
1:A:296:SER:HB2	1:A:847:ALA:HB3	1.91	0.53
2:B:365:LYS:H	2:B:365:LYS:HD2	1.72	0.53
2:B:77:HIS:CE1	2:B:431:LYS:HG3	2.41	0.52
1:A:472:GLN:OE1	2:B:369:ARG:HD3	2.09	0.52
1:A:606:THR:HB	1:A:612:LEU:HD13	1.90	0.52
1:A:948:ARG:CZ	6:A:4003:1RY:H13	2.07	0.52
1:A:866:ARG:HH21	1:A:869:ARG:HD2	1.74	0.52
1:A:107:LEU:O	1:A:112:LEU:N	2.42	0.52
1:A:495:PHE:HB3	1:A:496:LYS:HB2	1.92	0.52
2:B:404:ASN:HA	2:B:407:LEU:HG	1.91	0.52
2:C:219:PHE:HD1	2:C:229:LYS:HG2	1.74	0.52
1:A:196:VAL:HG22	1:A:215:ILE:HG12	1.92	0.52
2:C:444:THR:OG1	2:C:445:GLU:N	2.43	0.52
1:A:468:ASN:HB3	2:B:459:ASP:O	2.10	0.52
1:A:803:ASN:HA	4:T:10:DG:H4'	1.90	0.52
2:B:129:ASP:HB2	2:C:104:VAL:HG22	1.92	0.52
1:A:887:VAL:HG22	1:A:1185:ILE:HG23	1.91	0.52
3:P:4:DA:C6	4:T:26:DT:N3	2.72	0.52
2:B:213:VAL:HG11	2:C:132:HIS:CE1	2.46	0.51
2:B:215:PHE:HE1	2:C:132:HIS:HB2	1.75	0.51
1:A:597:ARG:NH1	4:T:13:DC:H4'	2.26	0.51
1:A:1115:ALA:HB3	1:A:1156:THR:HG23	1.92	0.51
1:A:93:GLU:HA	1:A:94:MET:HB2	1.92	0.51
2:B:195:ASN:O	2:C:77:HIS:NE2	2.44	0.51
1:A:457:ARG:NH1	2:B:265:LYS:HA	2.25	0.50
2:B:457:SER:OG	2:B:460:THR:O	2.28	0.50
1:A:1183:VAL:HB	1:A:1214:GLN:HB3	1.93	0.50
1:A:750:PHE:HD1	1:A:751:LYS:HG2	1.75	0.50
3:P:14:DC:H2'	3:P:15:DA:C8	2.46	0.50
1:A:1096:ARG:HA	1:A:1099:TRP:HB3	1.93	0.50
1:A:384:ASP:OD1	1:A:384:ASP:N	2.36	0.50
1:A:162:LEU:HG	1:A:401:TRP:CZ3	2.46	0.50
2:B:241:TRP:HB3	2:B:336:LEU:HB3	1.93	0.50
1:A:1074:VAL:HB	1:A:1167:LYS:HB3	1.94	0.50
1:A:484:TRP:CZ3	2:B:364:LYS:NZ	2.76	0.49
2:C:205:PRO:HB3	2:C:243:THR:HA	1.94	0.49
1:A:566:LEU:HD13	1:A:566:LEU:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:209:ALA:HB2	2:B:239:LEU:HD13	1.95	0.49
1:A:562:ARG:HH11	1:A:563:PRO:HD2	1.77	0.49
1:A:866:ARG:HE	1:A:869:ARG:HD2	1.78	0.48
1:A:856:GLU:H	1:A:860:LEU:HD12	1.78	0.48
1:A:178:TYR:O	1:A:219:ALA:HB1	2.14	0.48
1:A:818:ARG:H	1:A:818:ARG:HE	1.61	0.48
1:A:1154:GLN:HG3	1:A:1218:LEU:HD21	1.95	0.48
1:A:262:GLN:HB2	1:A:263:GLU:HG2	1.95	0.48
2:B:215:PHE:CE1	2:C:132:HIS:HB2	2.49	0.48
3:P:23:DA:H2'	3:P:24:DOC:H6	1.96	0.48
2:C:67:GLU:HG3	2:C:88:ARG:HH22	1.76	0.48
1:A:1088:VAL:HG12	1:A:1090:GLU:HA	1.94	0.48
2:B:104:VAL:HG23	2:B:107:ARG:HH21	1.79	0.47
2:B:372:LEU:HD13	2:B:436:SER:HB2	1.96	0.47
3:P:20:DC:O2	4:T:10:DG:C2	2.61	0.47
1:A:1133:ILE:HG12	1:A:1136:GLU:HB3	1.95	0.47
1:A:1214:GLN:HA	1:A:1215:GLY:HA3	1.61	0.47
2:B:428:LEU:HA	2:B:431:LYS:HB3	1.95	0.47
1:A:586:THR:HG1	1:A:590:SER:HG	1.60	0.47
2:B:82:SER:OG	2:C:195:ASN:OD1	2.20	0.47
2:C:262:TRP:HA	2:C:265:LYS:HE2	1.97	0.47
1:A:135:LEU:H	1:A:135:LEU:HD23	1.78	0.47
6:A:4003:1RY:CAK	6:A:4003:1RY:OAP	2.63	0.47
1:A:782:GLY:HA2	1:A:784:GLY:HA2	1.97	0.47
1:A:817:PRO:HB2	1:A:818:ARG:HH21	1.79	0.47
1:A:864:ASN:O	1:A:872:SER:OG	2.26	0.47
1:A:579:ARG:HH12	3:P:11:DG:H5"	1.80	0.47
1:A:175:TRP:CD2	1:A:223:TRP:HB2	2.50	0.47
2:B:393:LEU:HD12	2:B:394:GLU:HG2	1.97	0.47
2:C:241:TRP:HD1	2:C:336:LEU:HD22	1.79	0.47
2:C:389:ARG:HD3	2:C:395:LEU:HD11	1.97	0.47
1:A:642:SER:HA	1:A:643:ALA:HA	1.59	0.47
3:P:8:DG:H1	4:T:21:DC:H42	1.63	0.47
1:A:1060:LYS:HE2	1:A:1064:ILE:HD11	1.96	0.47
1:A:484:TRP:HZ3	2:B:364:LYS:NZ	2.10	0.46
1:A:617:ARG:HB2	1:A:763:GLY:HA3	1.97	0.46
1:A:977:GLU:HB3	1:A:981:LYS:NZ	2.30	0.46
2:C:252:LEU:HD22	2:C:305:ASN:HB2	1.98	0.46
1:A:586:THR:OG1	1:A:590:SER:OG	2.27	0.46
1:A:869:ARG:NH1	3:P:22:DT:OP1	2.48	0.46
2:B:441:VAL:HG23	2:B:453:ILE:HG13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:ARG:NH1	2:B:84:GLN:OE1	2.49	0.46
1:A:593:SER:O	1:A:599:THR:OG1	2.21	0.46
1:A:91:GLY:HA2	1:A:92:GLY:HA3	1.60	0.46
1:A:953:ARG:HG3	1:A:957:ALA:HB2	1.97	0.46
1:A:275:ARG:NH2	1:A:433:SER:O	2.42	0.46
1:A:475:SER:HA	1:A:476:GLY:HA2	1.50	0.46
2:B:323:HIS:HB3	2:B:330:ASN:HB2	1.97	0.46
2:B:213:VAL:HA	2:B:235:THR:HA	1.97	0.46
1:A:1098:ASN:CG	4:T:5:DG:H2"	2.36	0.46
1:A:268:GLY:HA2	1:A:403:THR:HG21	1.97	0.46
1:A:611:PRO:HG3	1:A:652:ILE:HD13	1.98	0.46
2:C:134:LYS:CG	2:C:135:PRO:CD	2.92	0.46
2:B:262:TRP:HA	2:B:265:LYS:HE2	1.97	0.46
1:A:435:LEU:HG	1:A:842:PRO:HG3	1.98	0.45
1:A:804:ALA:O	1:A:808:ILE:HG12	2.16	0.45
1:A:556:THR:HA	1:A:559:LEU:HD13	1.98	0.45
1:A:272:SER:HB3	1:A:843:GLN:HA	1.98	0.45
1:A:897:TRP:CD1	1:A:1177:VAL:HG21	2.51	0.45
2:B:266:PHE:HA	2:B:375:HIS:CD2	2.52	0.45
1:A:505:LYS:HD3	1:A:505:LYS:HA	1.81	0.45
4:T:4:DG:H2'	4:T:5:DG:H8	1.82	0.45
1:A:1200:PRO:O	1:A:1202:ASN:N	2.46	0.45
1:A:206:GLY:HA3	1:A:207:THR:HA	1.79	0.45
1:A:267:VAL:HG12	1:A:292:LEU:HB3	1.98	0.45
1:A:942:SER:HA	1:A:943:ARG:HA	1.59	0.45
1:A:616:GLU:HB2	1:A:617:ARG:HD3	1.99	0.45
1:A:887:VAL:HG13	1:A:1185:ILE:HG12	1.99	0.45
2:B:79:LEU:HG	2:B:102:LEU:HB2	1.98	0.45
2:C:201:ASN:ND2	2:C:201:ASN:O	2.46	0.45
1:A:851:THR:HG21	1:A:1103:SER:HB2	1.99	0.45
1:A:851:THR:O	1:A:851:THR:OG1	2.29	0.44
1:A:864:ASN:HB3	1:A:1191:LYS:HD3	1.98	0.44
1:A:953:ARG:HA	1:A:957:ALA:HB2	1.98	0.44
2:C:303:LEU:HD22	2:C:338:VAL:HG22	1.99	0.44
1:A:849:THR:O	4:T:7:DA:O5'	2.35	0.44
1:A:799:SER:HA	1:A:802:ARG:HH12	1.82	0.44
1:A:298:HIS:HB2	1:A:410:GLN:HE22	1.83	0.44
2:C:444:THR:OG1	2:C:445:GLU:OE2	2.36	0.44
2:C:67:GLU:N	2:C:88:ARG:HH21	2.14	0.44
1:A:939:VAL:HA	1:A:940:GLY:HA3	1.71	0.44
1:A:948:ARG:NH2	3:P:24:DOC:HN41	2.02	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:252:LEU:HD13	2:B:336:LEU:HD11	1.99	0.44
3:P:3:DA:C6	4:T:26:DT:O4	2.70	0.44
2:B:133:HIS:ND1	2:C:233:GLU:OE2	2.48	0.44
1:A:888:GLY:HA3	1:A:1138:ARG:HD2	1.99	0.44
1:A:894:GLN:HG3	1:A:895:GLU:N	2.32	0.44
1:A:243:ASP:N	1:A:243:ASP:OD1	2.44	0.44
1:A:800:PHE:HB2	1:A:869:ARG:HH21	1.82	0.44
2:B:421:MET:HA	2:B:422:GLN:HB3	1.99	0.44
1:A:272:SER:OG	1:A:844:VAL:O	2.29	0.44
1:A:110:HIS:HB3	1:A:111:GLY:HA2	1.99	0.43
1:A:569:HIS:HA	2:B:462:MET:HG2	2.00	0.43
1:A:1183:VAL:N	1:A:1214:GLN:O	2.50	0.43
2:C:317:GLY:HA3	2:C:318:ASN:HA	1.60	0.43
2:C:414:TRP:HA	2:C:415:PRO:HD3	1.85	0.43
1:A:765:PRO:HA	1:A:766:PHE:HA	1.58	0.43
1:A:622:TYR:HB2	1:A:770:PHE:HE2	1.83	0.43
1:A:828:HIS:O	1:A:830:ASP:N	2.43	0.43
1:A:1134:HIS:HD2	3:P:24:DOC:H1'	1.82	0.43
2:C:244:PRO:HA	2:C:245:PRO:HD3	1.82	0.43
1:A:483:PRO:HG2	1:A:484:TRP:CE3	2.52	0.43
1:A:849:THR:HA	1:A:850:ILE:HA	1.80	0.43
2:C:389:ARG:HB3	2:C:395:LEU:HD11	2.00	0.43
1:A:1032:THR:O	1:A:1034:ARG:NH2	2.51	0.43
1:A:831:TYR:N	1:A:832:ASP:HA	2.29	0.43
1:A:231:GLU:HA	2:C:449:GLU:O	2.19	0.43
2:C:440:THR:OG1	2:C:456:ARG:HB3	2.19	0.43
6:A:4003:1RY:H8	3:P:24:DOC:H2'	2.00	0.43
1:A:149:PRO:HB3	1:A:262:GLN:N	2.34	0.43
1:A:299:MET:SD	1:A:849:THR:HG23	2.59	0.43
2:B:193:TYR:OH	2:B:333:PRO:HG3	2.18	0.43
1:A:299:MET:HG3	1:A:849:THR:HG23	2.01	0.42
2:C:315:TYR:N	2:C:316:PRO:HD3	2.34	0.42
2:C:319:VAL:HA	2:C:322:LEU:HD13	2.01	0.42
4:T:11:DC:H6	4:T:11:DC:H2'	1.64	0.42
1:A:1026:ARG:HD2	1:A:1026:ARG:O	2.19	0.42
1:A:976:GLN:O	1:A:980:GLU:HG2	2.19	0.42
2:C:293:PHE:H	2:C:294:PRO:HA	1.83	0.42
4:T:23:DT:H2"	4:T:24:DT:C6	2.54	0.42
3:P:21:DG:H1	4:T:8:DT:H3	1.67	0.42
1:A:1090:GLU:O	1:A:1091:GLU:HG2	2.19	0.42
1:A:463:LEU:HB3	1:A:592:LEU:HD12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:HIS:CD2	1:A:619:GLY:H	2.37	0.42
1:A:850:ILE:HD12	1:A:850:ILE:HA	1.93	0.42
1:A:973:LEU:HD21	1:A:976:GLN:HG3	2.02	0.42
2:B:407:LEU:HD13	2:C:120:VAL:HG12	2.01	0.42
2:C:264:ARG:HG3	2:C:270:PRO:HB3	2.00	0.42
2:C:293:PHE:HB3	2:C:295:TRP:H	1.84	0.42
2:C:239:LEU:HB3	2:C:338:VAL:HB	2.00	0.42
1:A:262:GLN:HA	1:A:263:GLU:HA	1.53	0.42
3:P:8:DG:H1	4:T:21:DC:N4	2.18	0.42
1:A:612:LEU:HA	1:A:612:LEU:HD12	1.76	0.42
1:A:79:LEU:HD13	1:A:80:SER:H	1.85	0.42
2:B:439:PHE:HB3	2:B:455:LEU:HD11	2.02	0.42
1:A:891:VAL:HG13	1:A:1161:ARG:HH12	1.84	0.42
1:A:599:THR:N	1:A:600:PRO:HD2	2.35	0.42
2:C:83:LYS:HE2	2:C:83:LYS:HB3	1.95	0.42
1:A:1124:ALA:O	1:A:1148:ARG:NH2	2.45	0.42
1:A:834:GLU:HG3	2:B:328:ARG:HH21	1.85	0.42
1:A:880:ALA:HA	1:A:881:PRO:HD3	1.94	0.42
1:A:232:ARG:HH21	2:C:468:ILE:HG21	1.84	0.42
6:A:4003:1RY:CAT	4:T:4:DG:H1	2.31	0.42
1:A:1047:ARG:HG3	1:A:1047:ARG:H	1.62	0.41
1:A:1054:GLU:HB3	1:A:1055:SER:H	1.46	0.41
1:A:1163:MET:SD	1:A:1167:LYS:HE2	2.60	0.41
1:A:247:LEU:H	1:A:247:LEU:HD13	1.84	0.41
1:A:499:LYS:H	1:A:499:LYS:HG3	1.62	0.41
1:A:1075:LEU:HD23	1:A:1075:LEU:H	1.86	0.41
1:A:176:THR:OG1	1:A:222:SER:OG	2.32	0.41
2:B:197:LEU:HD23	2:B:197:LEU:HA	1.81	0.41
2:B:382:LYS:H	2:B:412:SER:HB2	1.85	0.41
2:B:385:LEU:HA	2:B:441:VAL:HG13	2.01	0.41
1:A:828:HIS:CG	1:A:829:PRO:HD2	2.55	0.41
2:C:205:PRO:HB3	2:C:244:PRO:HD3	2.02	0.41
1:A:570:PRO:HB2	1:A:572:TRP:CD1	2.55	0.41
1:A:790:ARG:HD2	1:A:790:ARG:HA	1.90	0.41
2:B:365:LYS:HG2	2:B:367:LEU:H	1.86	0.41
2:B:393:LEU:HA	2:B:394:GLU:HA	1.66	0.41
2:C:418:LEU:N	2:C:419:GLU:HA	2.34	0.41
1:A:1193:VAL:HG21	1:A:1213:PRO:HG3	2.02	0.41
2:B:444:THR:OG1	2:B:445:GLU:N	2.54	0.41
2:C:375:HIS:O	2:C:379:ALA:N	2.49	0.41
1:A:133:ASP:N	1:A:133:ASP:OD2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:LEU:HA	1:A:151:LEU:HD23	1.96	0.41
1:A:209:PRO:HG3	1:A:277:HIS:CD2	2.56	0.41
2:B:244:PRO:HA	2:B:245:PRO:HD3	1.86	0.41
2:B:133:HIS:HE1	2:C:233:GLU:HG3	1.86	0.41
1:A:162:LEU:HD22	1:A:163:PRO:HD2	2.01	0.41
1:A:480:LYS:HD3	1:A:646:VAL:HG11	2.03	0.41
1:A:773:LYS:HD2	1:A:773:LYS:HA	1.89	0.41
2:B:420:THR:HG23	2:B:421:MET:HG2	2.03	0.41
2:B:446:THR:O	2:B:450:ASN:ND2	2.53	0.41
1:A:850:ILE:HD12	1:A:851:THR:HA	2.03	0.41
1:A:963:GLU:HG3	1:A:981:LYS:NZ	2.29	0.41
2:B:454:HIS:ND1	2:B:463:LYS:HE3	2.36	0.41
2:B:467:HIS:HB3	2:B:470:LYS:HB2	2.03	0.41
4:T:4:DG:H2'	4:T:5:DG:C8	2.56	0.41
1:A:1079:ILE:HG12	1:A:1099:TRP:CE3	2.56	0.41
1:A:1194:THR:HG22	1:A:1210:TYR:HE1	1.85	0.41
2:B:418:LEU:HD22	2:C:204:LEU:HD12	2.02	0.41
2:C:67:GLU:HG3	2:C:88:ARG:HH21	1.82	0.41
3:P:4:DA:N3	4:T:26:DT:H1'	2.36	0.41
1:A:1098:ASN:OD1	4:T:5:DG:H2"	2.21	0.41
1:A:1202:ASN:HA	1:A:1203:PRO:HD2	1.96	0.40
1:A:87:ILE:HD13	1:A:127:LEU:HD22	2.02	0.40
3:P:4:DA:C2	4:T:26:DT:O4'	2.74	0.40
1:A:1072:THR:OG1	1:A:1072:THR:O	2.36	0.40
1:A:636:THR:OG1	1:A:637:GLY:N	2.55	0.40
2:C:215:PHE:CD2	2:C:233:GLU:HG2	2.56	0.40
1:A:165:LYS:HA	1:A:166:PRO:HD3	1.93	0.40
1:A:873:GLU:O	1:A:877:MET:HG2	2.21	0.40
2:B:247:THR:O	2:B:247:THR:OG1	2.37	0.40
1:A:894:GLN:HG3	1:A:895:GLU:H	1.87	0.40
2:B:318:ASN:HB2	2:B:321:LYS:NZ	2.36	0.40
4:T:5:DG:H2'	4:T:6:DT:H6	1.86	0.40
1:A:1133:ILE:O	1:A:1135:ASP:N	2.55	0.40
1:A:426:GLY:O	1:A:430:MET:HB2	2.21	0.40
2:C:316:PRO:HA	2:C:317:GLY:HA2	1.59	0.40
2:C:455:LEU:HA	2:C:455:LEU:HD23	1.94	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ASP:OD2	2:C:318:ASN:ND2[5_545]	2.19	0.01

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%)	837 (86%)	111 (12%)	21 (2%)	6 35
2	B	355/485 (73%)	326 (92%)	27 (8%)	2 (1%)	25 61
2	C	350/485 (72%)	324 (93%)	19 (5%)	7 (2%)	7 36
All	All	1674/2175 (77%)	1487 (89%)	157 (9%)	30 (2%)	8 38

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	752	LEU
1	A	1070	PRO
2	C	97	PRO
1	A	749	PHE
1	A	767	ALA
1	A	1134	HIS
1	A	1177	VAL
2	C	423	SER
1	A	1073	PRO
1	A	1080	SER
1	A	1091	GLU
2	C	98	GLY
2	C	316	PRO
2	C	391	PRO
1	A	95	PRO
1	A	642	SER
1	A	743	ASP
1	A	927	ARG
1	A	1207	GLU

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Mol	Chain	Res	Type
2	C	319	VAL
2	C	380	PRO
1	A	610	PHE
1	A	618	HIS
1	A	765	PRO
1	A	1074	VAL
1	A	560	PRO
2	B	317	GLY
2	B	451	GLY
1	A	1043	VAL
1	A	829	PRO

5.3.2 Protein sidechains (i)

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%)	752 (91%)	71 (9%)	10	38
2	B	325/426 (76%)	306 (94%)	19 (6%)	20	53
2	C	317/426 (74%)	298 (94%)	19 (6%)	19	52
All	All	1465/1869 (78%)	1356 (93%)	109 (7%)	13	44

All (109) 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	197	PHE
1	A	227	ARG
1	A	236	THR
1	A	245	ILE
1	A	247	LEU

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Mol	Chain	Res	Type
1	A	292	LEU
1	A	304	LEU
1	A	316	LYS
1	A	424	LEU
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	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
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	1047	ARG

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Mol	Chain	Res	Type
1	A	1057	MET
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	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
2	B	364	LYS
2	B	365	LYS
2	B	368	HIS
2	B	372	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	83	LYS
2	C	86	LEU
2	C	115	TRP
2	C	122	ARG
2	C	186	LEU

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Mol	Chain	Res	Type
2	C	197	LEU
2	C	201	ASN
2	C	204	LEU
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	295	TRP
2	C	300	ILE
2	C	386	ASP
2	C	402	LEU
2	C	453	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1134	HIS

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	$\#\|Z\| > 2$
3	DOC	P	24	3,4	14,19,20	0.81	0	13,26,29	1.08	1 (7%)

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
3	DOC	P	24	3,4	-	0/4/18/19	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	P	24	DOC	C2-N3-C4	3.61	120.00	116.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	24	DOC	7	0

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	$\#\|Z\| > 2$
6	1RY	A	4003	5	22,29,29	3.56	7 (31%)	28,45,45	1.97	6 (21%)

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
6	1RY	A	4003	5	-	4/19/31/31	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	4003	1RY	OAP-CAX	9.58	1.63	1.42
6	A	4003	1RY	CAW-SAS	-7.40	1.56	1.81
6	A	4003	1RY	CAX-NAY	-7.29	1.27	1.49
6	A	4003	1RY	CAM-SAS	-5.74	1.64	1.81
6	A	4003	1RY	CAT-NAA	3.90	1.43	1.34
6	A	4003	1RY	CAL-CAW	2.75	1.60	1.51
6	A	4003	1RY	CAV-NAN	-2.32	1.33	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	4003	1RY	CAM-SAS-CAW	6.55	105.46	88.24
6	A	4003	1RY	CAV-NAN-CAT	4.13	121.01	116.02
6	A	4003	1RY	CAW-OAP-CAX	-3.03	106.18	112.59
6	A	4003	1RY	PBB-OAQ-PAZ	-2.86	123.02	132.83
6	A	4003	1RY	NAA-CAT-NAN	2.75	120.92	117.03
6	A	4003	1RY	PBA-OAR-PBB	-2.11	125.60	132.83

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	4003	1RY	OAO-CAL-CAW-OAP
6	A	4003	1RY	OAO-CAL-CAW-SAS
6	A	4003	1RY	PBA-OAR-PBB-OAE
6	A	4003	1RY	PBA-OAR-PBB-OAI

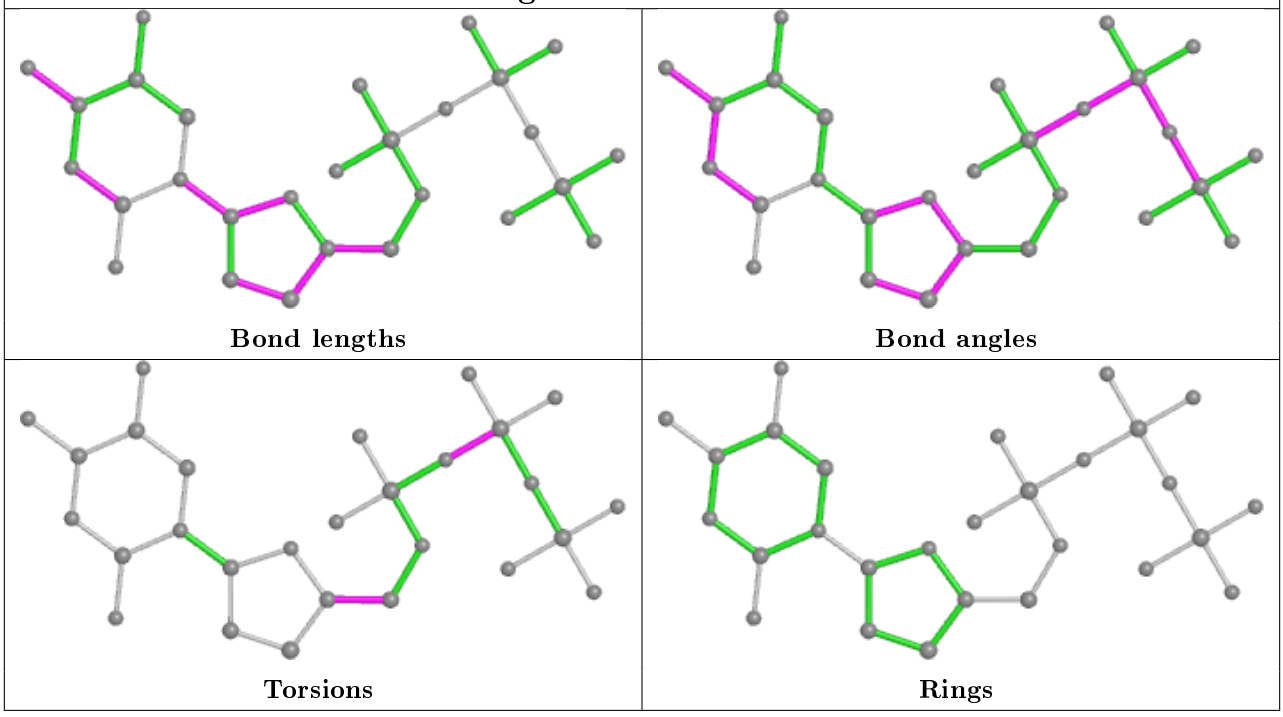
There are no ring outliers.

1 monomer is involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	4003	1RY	15	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 then 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.

Ligand 1RY A 4003



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^{th} 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%)	1.09	187 (19%) 1 2	38, 67, 106, 401	0
2	B	363/485 (74%)	0.76	36 (9%) 7 10	42, 59, 96, 263	0
2	C	358/485 (73%)	0.98	65 (18%) 1 2	41, 65, 97, 154	0
3	P	21/22 (95%)	2.08	9 (42%) 0 0	101, 105, 106, 111	0
4	T	25/25 (100%)	1.56	7 (28%) 0 0	65, 82, 104, 115	0
All	All	1750/2222 (78%)	1.02	304 (17%) 1 2	38, 66, 105, 401	0

All (304) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	746	GLY	28.6
1	A	745	PRO	19.4
1	A	747	CYS	12.3
2	C	228	VAL	11.3
1	A	510	ALA	10.7
1	A	744	ILE	10.6
1	A	304	LEU	9.6
1	A	230	GLU	8.1
1	A	509	THR	8.1
1	A	631	LEU	7.8
1	A	760	CYS	7.6
1	A	784	GLY	7.2
3	P	3	DA	7.2
1	A	630	ASN	7.1
1	A	622	TYR	6.9
2	C	121	PHE	6.8
2	C	282	GLU	6.8
4	T	25	DT	6.3
1	A	610	PHE	6.1
1	A	235	TRP	6.1

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Mol	Chain	Res	Type	RSRZ
1	A	507	PRO	6.0
1	A	1213	PRO	5.9
3	P	4	DA	5.8
2	C	219	PHE	5.8
1	A	506	GLU	5.5
2	C	388	GLY	5.4
2	B	366	ASN	5.4
1	A	640	LEU	5.4
2	C	122	ARG	5.4
2	C	328	ARG	5.4
1	A	1081	ARG	5.3
2	C	123	GLU	5.3
1	A	508	ALA	5.3
1	A	785	GLY	5.2
1	A	229	VAL	5.2
2	B	328	ARG	5.1
1	A	214	ALA	5.0
1	A	912	GLY	5.0
1	A	632	ALA	4.9
1	A	836	LEU	4.9
1	A	342	ILE	4.9
1	A	122	ASP	4.9
1	A	786	ALA	4.8
1	A	249	VAL	4.8
1	A	94	MET	4.8
1	A	764	SER	4.6
2	C	355	GLN	4.6
1	A	93	GLU	4.6
1	A	90	GLN	4.5
1	A	431	GLY	4.5
1	A	619	GLY	4.5
1	A	1050	LYS	4.4
1	A	741	ASP	4.4
1	A	910	MET	4.4
1	A	743	ASP	4.4
1	A	661	LEU	4.3
1	A	504	LYS	4.3
2	C	229	LYS	4.3
2	C	468	ILE	4.3
3	P	10	DG	4.2
2	C	120	VAL	4.2
2	B	414	TRP	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	171	TRP	4.2
2	C	414	TRP	4.1
2	C	204	LEU	4.1
2	B	422	GLN	4.1
2	C	351	TYR	4.1
1	A	555	THR	4.0
3	P	5	DA	4.0
2	B	420	THR	4.0
2	C	109	ASN	4.0
1	A	1082	ALA	3.9
1	A	611	PRO	3.9
1	A	501	LYS	3.9
1	A	573	TYR	3.9
1	A	1207	GLU	3.8
1	A	893	SER	3.8
1	A	92	GLY	3.7
1	A	1038	TRP	3.7
2	C	466	MET	3.7
1	A	348	LEU	3.7
2	C	325	ARG	3.7
1	A	109	LYS	3.6
1	A	303	GLY	3.6
1	A	1042	GLU	3.6
2	C	285	LYS	3.6
1	A	969	PHE	3.6
1	A	1130	CYS	3.6
1	A	865	ALA	3.6
2	B	388	GLY	3.5
4	T	21	DC	3.5
1	A	500	ALA	3.5
1	A	593	SER	3.5
1	A	116	PRO	3.5
1	A	753	PRO	3.5
2	C	289	LEU	3.5
1	A	1134	HIS	3.5
1	A	1110	HIS	3.4
1	A	988	ALA	3.4
1	A	1099	TRP	3.4
1	A	894	GLN	3.4
1	A	1132	SER	3.4
1	A	1035	LYS	3.4
4	T	26	DT	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	638	THR	3.3
1	A	642	SER	3.3
1	A	636	THR	3.3
1	A	846	THR	3.3
1	A	105	GLU	3.3
2	C	281	GLU	3.3
1	A	210	THR	3.3
2	C	81	GLY	3.3
2	C	124	GLN	3.3
1	A	1184	ASP	3.3
2	C	80	SER	3.3
1	A	1037	GLN	3.3
1	A	759	SER	3.3
1	A	1131	ILE	3.3
2	C	227	GLY	3.3
2	C	230	SER	3.2
1	A	849	THR	3.2
1	A	850	ILE	3.2
1	A	1076	GLY	3.2
1	A	78	MET	3.2
1	A	213	VAL	3.2
1	A	650	ARG	3.2
3	P	8	DG	3.2
1	A	353	VAL	3.2
1	A	102	ARG	3.2
2	B	448	LEU	3.1
2	C	423	SER	3.1
1	A	1077	CYS	3.1
1	A	291	PHE	3.1
3	P	7	DC	3.1
1	A	1087	ALA	3.1
1	A	1078	CYS	3.1
1	A	601	LYS	3.1
1	A	1096	ARG	3.1
1	A	782	GLY	3.0
2	C	322	LEU	3.0
2	C	326	ASP	3.0
1	A	503	VAL	3.0
1	A	108	GLN	3.0
2	C	108	LYS	2.9
2	C	455	LEU	2.9
1	A	173	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	989	THR	2.9
2	C	373	LYS	2.9
2	C	415	PRO	2.9
4	T	22	DG	2.9
1	A	927	ARG	2.9
2	C	218	VAL	2.9
1	A	123	VAL	2.9
1	A	634	LEU	2.9
2	B	81	GLY	2.9
1	A	837	TYR	2.9
1	A	183	GLU	2.9
4	T	24	DT	2.9
1	A	635	PRO	2.9
1	A	197	PHE	2.8
2	B	315	TYR	2.8
1	A	265	LEU	2.8
4	T	18	DC	2.8
2	B	221	THR	2.8
1	A	389	PHE	2.8
1	A	1208	ARG	2.8
1	A	752	LEU	2.8
1	A	502	LYS	2.8
2	C	387	VAL	2.8
1	A	172	ALA	2.8
1	A	215	ILE	2.8
1	A	1070	PRO	2.8
1	A	441	TRP	2.7
1	A	351	SER	2.7
1	A	552	LEU	2.7
2	B	108	LYS	2.7
1	A	104	VAL	2.7
1	A	742	VAL	2.7
1	A	287	SER	2.7
1	A	352	SER	2.7
1	A	220	TRP	2.7
1	A	913	CYS	2.7
2	B	354	PHE	2.7
1	A	889	ALA	2.7
2	B	285	LYS	2.6
2	C	288	LYS	2.6
2	C	439	PHE	2.6
1	A	639	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	607	TRP	2.6
1	A	916	PHE	2.6
1	A	648	PRO	2.6
1	A	84	HIS	2.6
2	B	203	ARG	2.6
1	A	599	THR	2.6
1	A	921	LEU	2.6
1	A	827	ARG	2.6
1	A	430	MET	2.6
1	A	911	HIS	2.6
2	B	211	ILE	2.6
2	C	335	VAL	2.5
1	A	1202	ASN	2.5
3	P	15	DA	2.5
1	A	945	HIS	2.5
1	A	1072	THR	2.5
2	C	331	VAL	2.5
1	A	196	VAL	2.5
2	C	290	TYR	2.5
2	C	126	PHE	2.5
1	A	343	SER	2.5
2	B	355	GLN	2.5
2	B	204	LEU	2.4
2	C	432	TYR	2.4
1	A	434	TYR	2.4
1	A	124	GLU	2.4
1	A	433	SER	2.4
1	A	505	LYS	2.4
1	A	429	GLU	2.4
2	C	214	CYS	2.4
1	A	781	ALA	2.4
1	A	871	GLY	2.4
2	B	206	TYR	2.4
1	A	1138	ARG	2.4
2	C	300	ILE	2.4
1	A	211	LEU	2.4
1	A	1031	GLU	2.4
2	C	243	THR	2.4
1	A	198	ASP	2.4
2	B	109	ASN	2.4
1	A	496	LYS	2.4
1	A	426	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
2	C	453	ILE	2.4
2	C	311	LEU	2.4
2	C	97	PRO	2.3
2	C	315	TYR	2.3
2	B	212	GLY	2.3
1	A	1212	ILE	2.3
3	P	23	DA	2.3
1	A	1083	LEU	2.3
2	B	485	VAL	2.3
2	C	437	ILE	2.3
1	A	766	PHE	2.3
1	A	1179	PHE	2.3
3	P	9	DA	2.3
2	C	67	GLU	2.3
1	A	495	PHE	2.3
2	B	326	ASP	2.3
2	C	236	GLU	2.3
1	A	562	ARG	2.3
2	B	370	LYS	2.3
1	A	444	TYR	2.3
2	C	440	THR	2.3
1	A	633	LYS	2.3
2	C	386	ASP	2.2
1	A	801	TRP	2.2
1	A	1103	SER	2.2
2	C	371	VAL	2.2
1	A	833	GLU	2.2
2	C	438	LEU	2.2
2	C	333	PRO	2.2
1	A	655	LEU	2.2
2	C	463	LYS	2.2
1	A	1093	MET	2.2
1	A	543	VAL	2.2
1	A	208	CYS	2.2
2	B	426	GLU	2.2
1	A	1112	MET	2.2
2	B	424	SER	2.2
2	B	468	ILE	2.2
1	A	1187	ARG	2.2
1	A	272	SER	2.1
1	A	113	TRP	2.1
2	B	419	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	435	MET	2.1
2	C	385	LEU	2.1
2	B	403	PHE	2.1
2	C	249	ASN	2.1
2	B	322	LEU	2.1
1	A	832	ASP	2.1
1	A	979	ALA	2.1
2	C	470	LYS	2.1
1	A	1074	VAL	2.1
1	A	497	GLN	2.1
2	B	208	LEU	2.1
1	A	538	GLU	2.1
2	B	238	SER	2.1
2	C	353	SER	2.1
2	C	253	ASP	2.1
1	A	386	ARG	2.1
2	B	210	GLN	2.1
2	C	332	VAL	2.1
4	T	23	DT	2.1
2	B	445	GLU	2.1
1	A	347	TRP	2.1
2	B	209	ALA	2.1
1	A	443	ARG	2.0
1	A	643	ALA	2.0
1	A	851	THR	2.0
1	A	1073	PRO	2.0
1	A	227	ARG	2.0
1	A	961	PHE	2.0
1	A	859	TRP	2.0
2	B	181	LEU	2.0
1	A	970	ASN	2.0
2	B	236	GLU	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^{th} 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
3	DOC	P	24	18/19	0.70	0.37	99,102,106,106	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

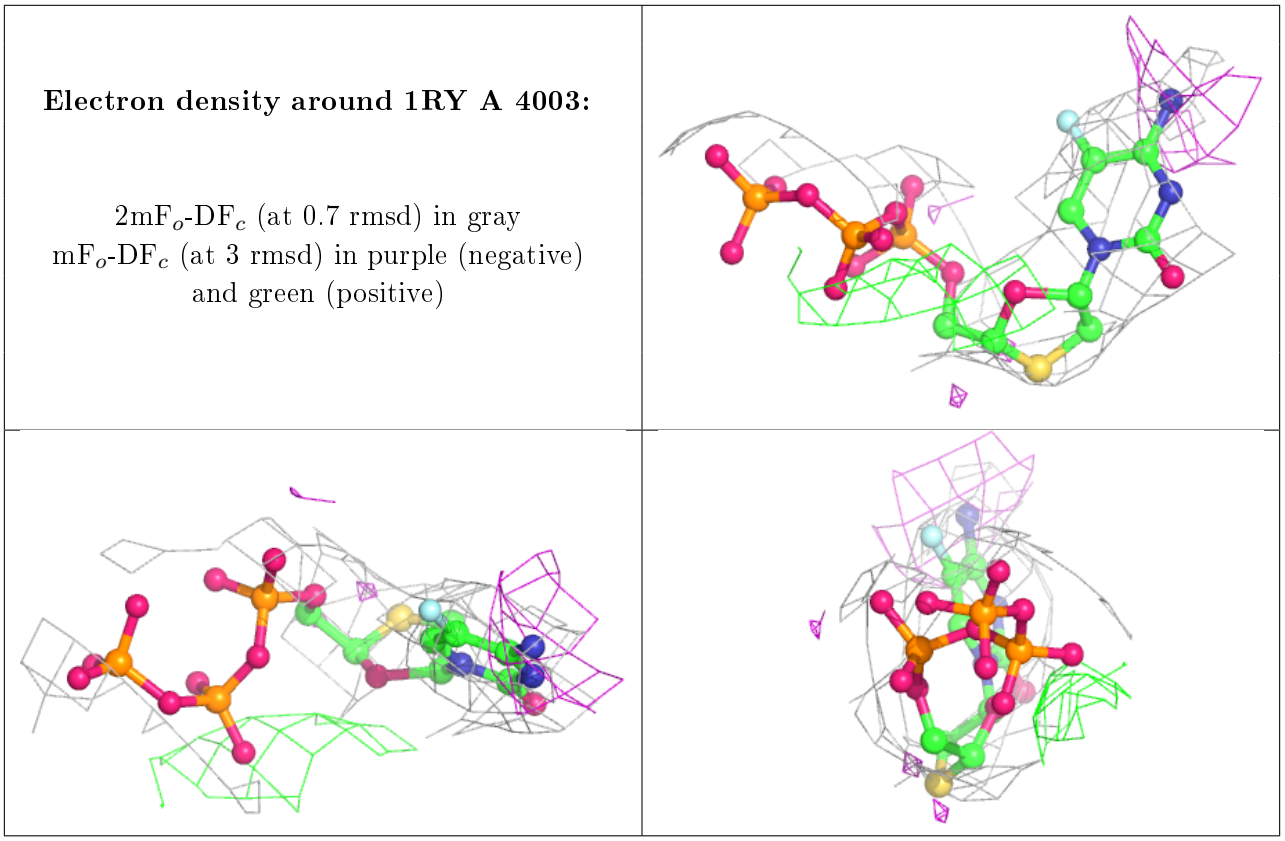
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
5	MG	A	4002	1/1	0.75	0.31	87,87,87,87	0
5	MG	A	4001	1/1	0.77	0.36	88,88,88,88	0
6	1RY	A	4003	28/28	0.78	0.33	63,66,78,79	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.

Electron density around 1RY A 4003:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.