



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:21 am GMT

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.; Amiralaie, 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

<http://wwpdb.org/validation/2016/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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

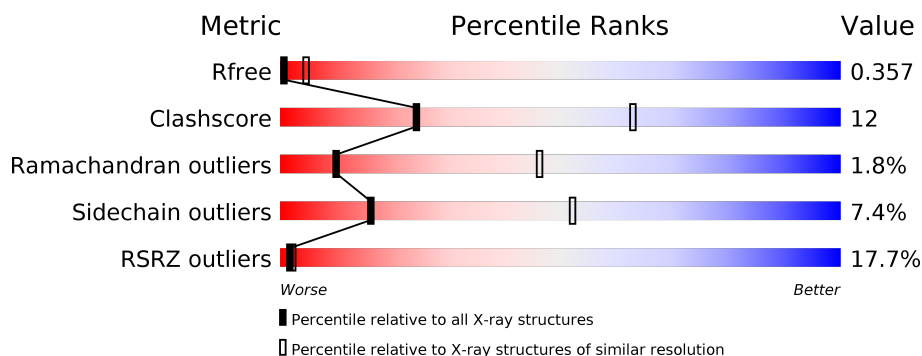
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.43 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}	100719	1074 (3.50-3.34)
Clashscore	112137	1179 (3.50-3.34)
Ramachandran outliers	110173	1147 (3.50-3.34)
Sidechain outliers	110143	1148 (3.50-3.34)
RSRZ outliers	101464	1100 (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. 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>15%</div> <div>55%</div> <div>23%</div> <div>18%</div> </div>
2	B	485	<div> <div>9%</div> <div>56%</div> <div>17%</div> <div>25%</div> </div>
2	C	485	<div> <div>13%</div> <div>55%</div> <div>17%</div> <div>26%</div> </div>
3	P	22	<div> <div>45%</div> <div>41%</div> <div>59%</div> </div>
4	T	25	<div> <div>28%</div> <div>32%</div> <div>64%</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
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			

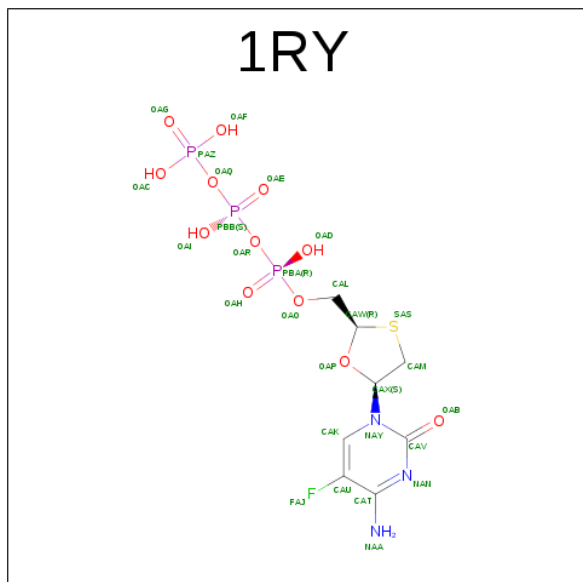
- Molecule 4 is a DNA chain called DNA.

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: C₈H₁₃FN₃O₁₂P₃S).

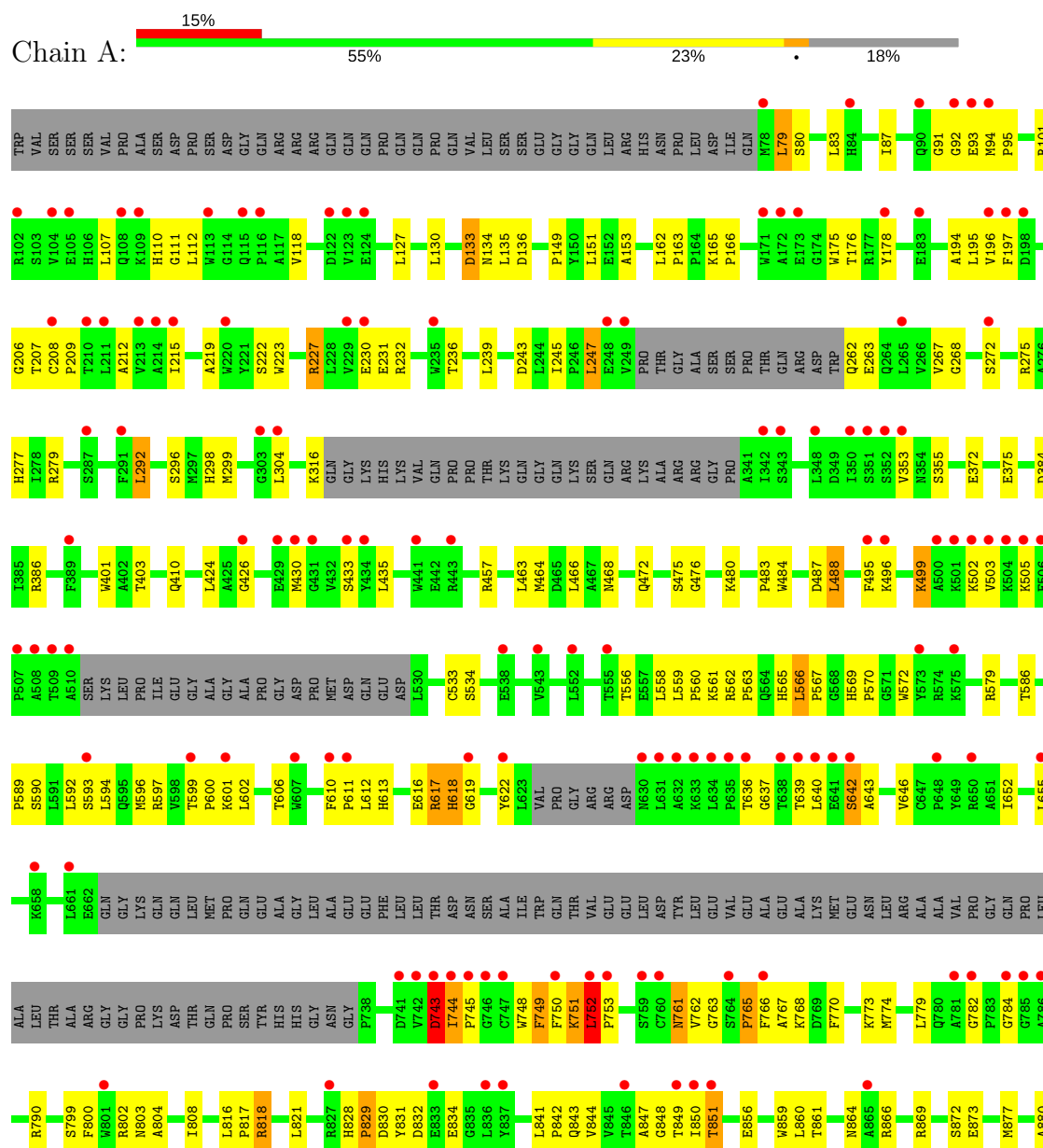


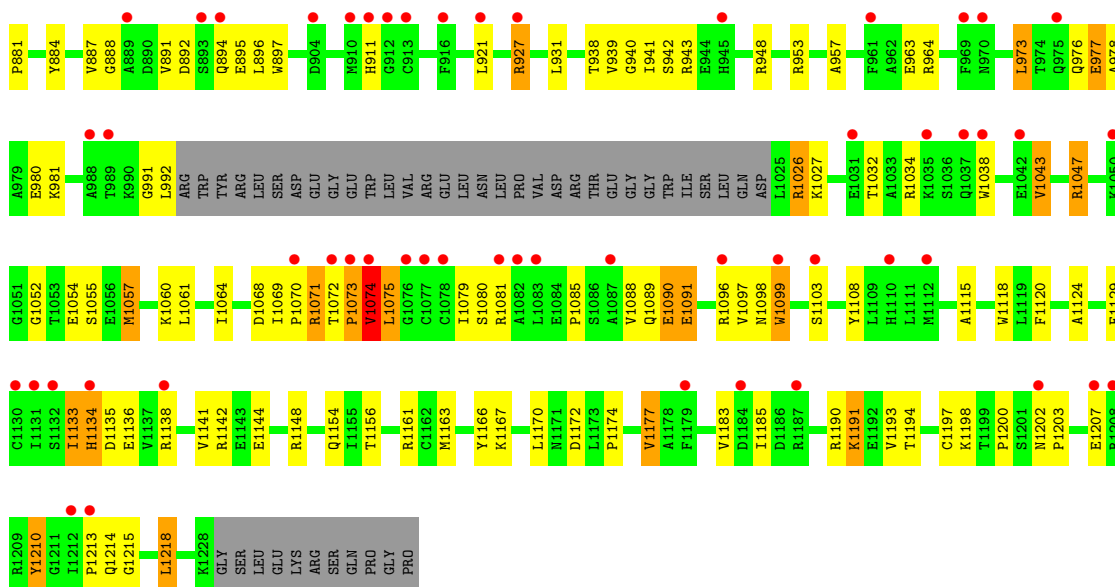
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	F	N	O	P	S	
			28	8	1	3	12	3	1	

3 Residue-property plots [i](#)

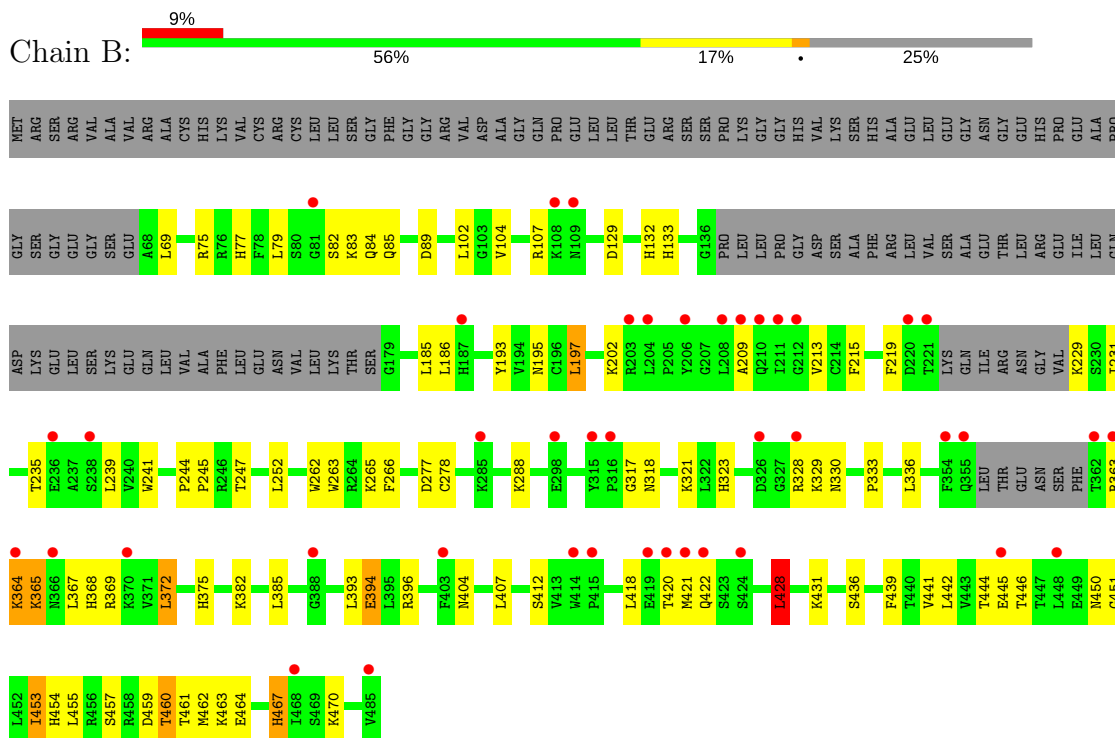
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

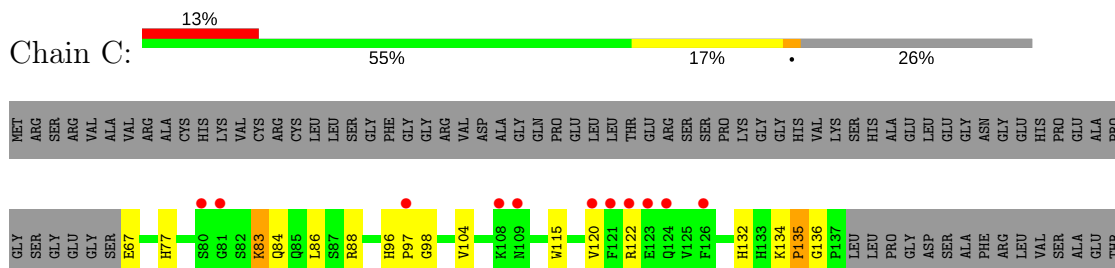


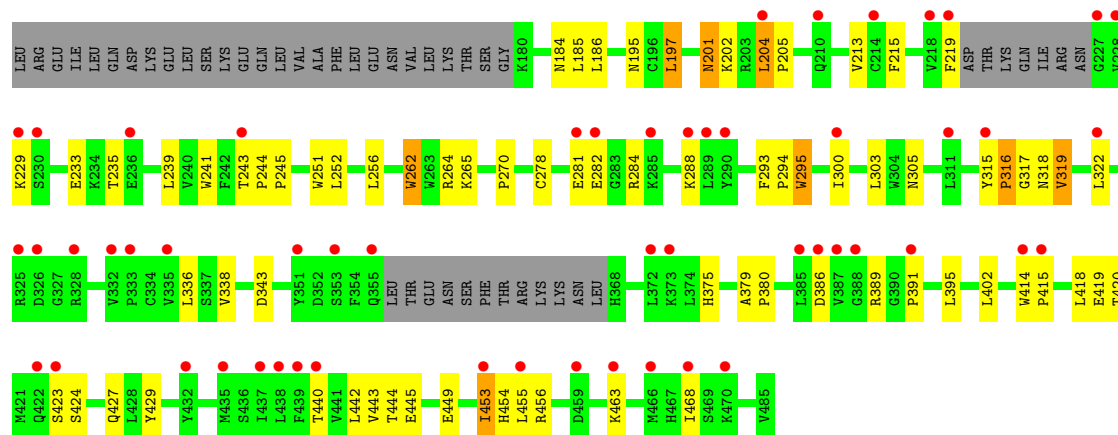


- Molecule 2: DNA polymerase subunit gamma-2, mitochondrial

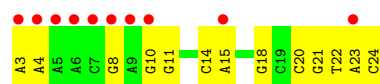


- Molecule 2: DNA polymerase subunit gamma-2, mitochondrial

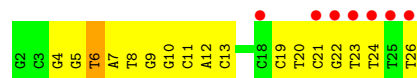




● Molecule 3: DNA (5'-D(* (AD)P*AP*AP*AP*CP*GP*AP*GP*GP*GP*CP*CP*AP*GP*TP*GP*CP*CP*GP*TP*AP*C)-3')



● Molecule 4: DNA



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.315 , 0.345 0.349 , 0.357	Depositor DCC
R_{free} test set	2000 reflections (4.77%)	DCC
Wilson B-factor (Å ²)	139.0	Xtriage
Anisotropy	0.414	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 8.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	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 2.07% 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: 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(°)	Ideal(°)
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%)	8	42
2	B	355/485 (73%)	326 (92%)	27 (8%)	2 (1%)	28	68
2	C	350/485 (72%)	324 (93%)	19 (5%)	7 (2%)	9	44
All	All	1674/2175 (77%)	1487 (89%)	157 (9%)	30 (2%)	10	46

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 ⓘ

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%)	12	45
2	B	325/426 (76%)	306 (94%)	19 (6%)	23	61
2	C	317/426 (74%)	298 (94%)	19 (6%)	22	60
All	All	1465/1869 (78%)	1356 (93%)	109 (7%)	16	52

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	13,19,20	0.90	0	12,26,29	0.44	0

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	-	0/3/18/19	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

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	21,29,29	3.32	7 (33%)	21,45,45	2.09	3 (14%)

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	-	0/18/31/31	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	CAW-SAS	-7.33	1.56	1.81
6	A	4003	1RY	CAM-SAS	-6.07	1.64	1.81
6	A	4003	1RY	CAV-NAN	-2.32	1.33	1.38
6	A	4003	1RY	PAZ-OAQ	2.63	1.64	1.60
6	A	4003	1RY	CAL-CAW	3.37	1.60	1.50
6	A	4003	1RY	CAT-NAA	3.74	1.43	1.34
6	A	4003	1RY	OAP-CAX	9.45	1.63	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	4003	1RY	CAW-OAP-CAX	-3.20	106.18	112.60
6	A	4003	1RY	NAA-CAT-NAN	2.65	120.92	117.00
6	A	4003	1RY	CAM-SAS-CAW	7.49	105.46	88.06

There are no chirality outliers.

There are no torsion outliers.

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

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%)	1.13	185 (18%) 1 2	38, 67, 106, 401	0
2	B	363/485 (74%)	0.80	42 (11%) 5 7	42, 59, 96, 263	0
2	C	358/485 (73%)	1.00	65 (18%) 1 2	41, 65, 97, 154	0
3	P	21/22 (95%)	2.16	10 (47%) 0 0	101, 105, 106, 111	0
4	T	25/25 (100%)	1.68	7 (28%) 1 1	65, 82, 104, 115	0
All	All	1750/2222 (78%)	1.06	309 (17%) 2 2	38, 66, 105, 401	0

All (309) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	746	GLY	29.8
1	A	745	PRO	19.7
1	A	747	CYS	12.6
2	C	228	VAL	12.3
1	A	510	ALA	10.9
1	A	744	ILE	10.6
1	A	304	LEU	9.7
1	A	631	LEU	8.1
1	A	760	CYS	7.9
1	A	630	ASN	7.8
1	A	230	GLU	7.8
1	A	509	THR	7.6
2	C	282	GLU	7.6
1	A	784	GLY	7.5
3	P	3	DA	7.4
1	A	622	TYR	7.0
2	C	121	PHE	6.5
1	A	235	TRP	6.5
1	A	506	GLU	6.4
4	T	25	DT	6.4

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Mol	Chain	Res	Type	RSRZ
1	A	610	PHE	6.2
1	A	507	PRO	6.1
1	A	1213	PRO	6.1
3	P	4	DA	6.0
2	B	366	ASN	5.7
2	C	388	GLY	5.6
1	A	640	LEU	5.4
2	C	219	PHE	5.4
1	A	836	LEU	5.3
1	A	1081	ARG	5.2
1	A	632	ALA	5.2
2	C	328	ARG	5.2
2	B	328	ARG	5.2
1	A	94	MET	5.2
1	A	785	GLY	5.2
2	C	123	GLU	5.1
1	A	249	VAL	5.0
2	C	122	ARG	5.0
1	A	122	ASP	4.8
1	A	508	ALA	4.8
1	A	743	ASP	4.8
1	A	912	GLY	4.7
1	A	741	ASP	4.7
2	C	229	LYS	4.7
1	A	229	VAL	4.7
1	A	661	LEU	4.6
1	A	93	GLU	4.6
1	A	786	ALA	4.6
1	A	348	LEU	4.6
1	A	504	LYS	4.6
1	A	214	ALA	4.5
1	A	90	GLN	4.5
1	A	431	GLY	4.4
1	A	342	ILE	4.4
1	A	501	LYS	4.4
2	C	355	GLN	4.3
1	A	619	GLY	4.3
1	A	1050	LYS	4.3
1	A	764	SER	4.3
1	A	1038	TRP	4.2
2	C	468	ILE	4.2
1	A	109	LYS	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	171	TRP	4.1
1	A	611	PRO	4.1
1	A	642	SER	4.1
3	P	10	DG	4.0
1	A	92	GLY	4.0
1	A	555	THR	4.0
2	B	422	GLN	3.9
2	C	466	MET	3.9
1	A	893	SER	3.9
2	C	325	ARG	3.9
2	C	120	VAL	3.9
3	P	5	DA	3.9
2	C	414	TRP	3.9
2	B	414	TRP	3.8
1	A	782	GLY	3.8
2	C	109	ASN	3.8
1	A	116	PRO	3.8
1	A	573	TYR	3.8
2	C	351	TYR	3.8
1	A	500	ALA	3.8
1	A	636	THR	3.8
2	C	204	LEU	3.8
1	A	1134	HIS	3.8
1	A	865	ALA	3.7
1	A	1035	LYS	3.7
4	T	21	DC	3.7
1	A	1042	GLU	3.7
1	A	1132	SER	3.6
2	B	81	GLY	3.6
1	A	910	MET	3.6
1	A	969	PHE	3.6
2	B	420	THR	3.6
1	A	105	GLU	3.6
1	A	1087	ALA	3.6
2	C	230	SER	3.6
2	C	326	ASP	3.6
2	B	388	GLY	3.5
2	C	285	LYS	3.5
2	C	281	GLU	3.5
1	A	988	ALA	3.5
1	A	102	ARG	3.5
2	C	289	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
4	T	26	DT	3.5
1	A	989	THR	3.5
1	A	846	THR	3.4
1	A	1130	CYS	3.4
1	A	593	SER	3.4
1	A	638	THR	3.4
1	A	1076	GLY	3.4
1	A	1082	ALA	3.4
1	A	1099	TRP	3.4
1	A	759	SER	3.4
1	A	601	LYS	3.4
3	P	8	DG	3.3
1	A	1078	CYS	3.3
1	A	894	GLN	3.3
1	A	1110	HIS	3.3
2	C	124	GLN	3.3
2	C	227	GLY	3.3
2	C	290	TYR	3.3
1	A	1202	ASN	3.3
3	P	7	DC	3.3
1	A	650	ARG	3.3
1	A	108	GLN	3.2
1	A	1037	GLN	3.2
1	A	1131	ILE	3.2
2	B	221	THR	3.2
4	T	18	DC	3.2
1	A	213	VAL	3.2
1	A	753	PRO	3.2
1	A	781	ALA	3.2
2	C	218	VAL	3.2
1	A	502	LYS	3.2
1	A	634	LEU	3.2
1	A	1207	GLU	3.2
2	C	80	SER	3.2
1	A	1077	CYS	3.2
1	A	291	PHE	3.2
1	A	441	TRP	3.1
2	C	455	LEU	3.1
1	A	183	GLU	3.1
2	C	387	VAL	3.1
1	A	850	ILE	3.1
1	A	1184	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	78	MET	3.1
1	A	389	PHE	3.1
4	T	22	DG	3.1
2	B	448	LEU	3.1
2	C	81	GLY	3.1
1	A	123	VAL	3.1
2	C	373	LYS	3.1
1	A	927	ARG	3.1
1	A	210	THR	3.0
1	A	849	THR	3.0
1	A	742	VAL	3.0
1	A	173	GLU	3.0
1	A	1096	ARG	2.9
2	C	108	LYS	2.9
1	A	827	ARG	2.9
2	B	285	LYS	2.9
1	A	351	SER	2.9
1	A	353	VAL	2.9
1	A	916	PHE	2.9
1	A	635	PRO	2.9
2	B	315	TYR	2.9
1	A	303	GLY	2.9
4	T	24	DT	2.9
1	A	503	VAL	2.9
1	A	104	VAL	2.8
2	C	236	GLU	2.8
1	A	913	CYS	2.8
1	A	1208	ARG	2.8
1	A	343	SER	2.8
2	C	423	SER	2.8
1	A	172	ALA	2.8
2	C	322	LEU	2.8
2	B	211	ILE	2.8
1	A	752	LEU	2.8
2	C	415	PRO	2.8
1	A	833	GLU	2.7
1	A	639	THR	2.7
1	A	265	LEU	2.7
1	A	1212	ILE	2.7
2	B	108	LYS	2.7
1	A	197	PHE	2.7
2	B	355	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	552	LEU	2.7
1	A	84	HIS	2.7
1	A	607	TRP	2.7
1	A	889	ALA	2.7
1	A	837	TYR	2.6
1	A	220	TRP	2.6
1	A	287	SER	2.6
1	A	1072	THR	2.6
2	C	288	LYS	2.6
1	A	648	PRO	2.6
2	C	432	TYR	2.6
3	P	9	DA	2.6
1	A	1070	PRO	2.6
2	B	212	GLY	2.6
2	C	439	PHE	2.6
1	A	505	LYS	2.6
1	A	430	MET	2.6
3	P	15	DA	2.6
1	A	1187	ARG	2.6
2	C	214	CYS	2.5
1	A	196	VAL	2.5
1	A	599	THR	2.5
2	C	243	THR	2.5
1	A	538	GLU	2.5
1	A	208	CYS	2.5
2	B	206	TYR	2.5
2	C	440	THR	2.5
1	A	429	GLU	2.5
2	C	437	ILE	2.5
1	A	426	GLY	2.5
1	A	352	SER	2.5
2	B	354	PHE	2.5
1	A	945	HIS	2.5
2	C	335	VAL	2.4
2	B	419	GLU	2.4
2	C	315	TYR	2.4
2	B	203	ARG	2.4
2	C	453	ILE	2.4
2	B	236	GLU	2.4
2	B	362	THR	2.4
2	C	126	PHE	2.4
1	A	1138	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	215	ILE	2.4
1	A	1103	SER	2.4
2	C	311	LEU	2.4
2	B	424	SER	2.4
1	A	921	LEU	2.4
1	A	543	VAL	2.3
2	C	391	PRO	2.3
2	B	220	ASP	2.3
3	P	23	DA	2.3
1	A	1179	PHE	2.3
2	C	463	LYS	2.3
2	B	363	ARG	2.3
1	A	496	LYS	2.3
1	A	911	HIS	2.3
1	A	961	PHE	2.3
1	A	1031	GLU	2.3
1	A	113	TRP	2.3
1	A	124	GLU	2.3
2	C	300	ILE	2.3
2	B	485	VAL	2.3
2	C	470	LYS	2.3
2	C	386	ASP	2.3
2	C	438	LEU	2.3
2	B	204	LEU	2.3
1	A	198	ASP	2.2
2	B	326	ASP	2.2
2	B	370	LYS	2.2
1	A	904	ASP	2.2
1	A	1074	VAL	2.2
2	C	385	LEU	2.2
1	A	115	GLN	2.2
2	B	403	PHE	2.2
1	A	434	TYR	2.2
1	A	801	TRP	2.2
2	C	353	SER	2.2
1	A	248	GLU	2.2
2	B	210	GLN	2.2
1	A	350	ILE	2.2
2	B	445	GLU	2.2
1	A	633	LYS	2.2
2	B	364	LYS	2.2
2	B	316	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	421	MET	2.2
2	B	187	HIS	2.2
1	A	495	PHE	2.2
1	A	211	LEU	2.1
1	A	655	LEU	2.1
1	A	178	TYR	2.1
1	A	766	PHE	2.1
2	B	209	ALA	2.1
1	A	641	GLU	2.1
2	B	238	SER	2.1
2	B	415	PRO	2.1
2	C	435	MET	2.1
2	B	298	GLU	2.1
1	A	1112	MET	2.1
1	A	433	SER	2.1
2	C	333	PRO	2.1
2	C	210	GLN	2.1
1	A	443	ARG	2.1
1	A	658	LYS	2.1
2	B	208	LEU	2.1
1	A	272	SER	2.1
2	C	459	ASP	2.1
3	P	6	DA	2.1
2	C	422	GLN	2.1
2	B	109	ASN	2.1
1	A	1073	PRO	2.1
1	A	1083	LEU	2.1
4	T	23	DT	2.0
2	C	97	PRO	2.0
1	A	975	GLN	2.0
1	A	575	LYS	2.0
1	A	750	PHE	2.0
2	C	332	VAL	2.0
2	B	468	ILE	2.0
1	A	970	ASN	2.0
1	A	851	THR	2.0
2	C	372	LEU	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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	DOC	P	24	18/19	0.71	0.36	-	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
6	1RY	A	4003	28/28	0.78	0.34	-0.29	63,66,78,79	0
5	MG	A	4001	1/1	0.77	0.40	-0.65	88,88,88,88	0
5	MG	A	4002	1/1	0.76	0.33	-	87,87,87,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.