Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2023 – 07:00 PM EDT

PDB ID	:	3H40
Title	:	Binary complex of human DNA polymerase iota with template U/T
Authors	:	Jain, R.; Nair, D.T.; Johnson, R.E.; Prakash, L.; Prakash, S.; Aggarwal, A.K.
Deposited on	:	2009-04-17
Resolution	:	2.30 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:

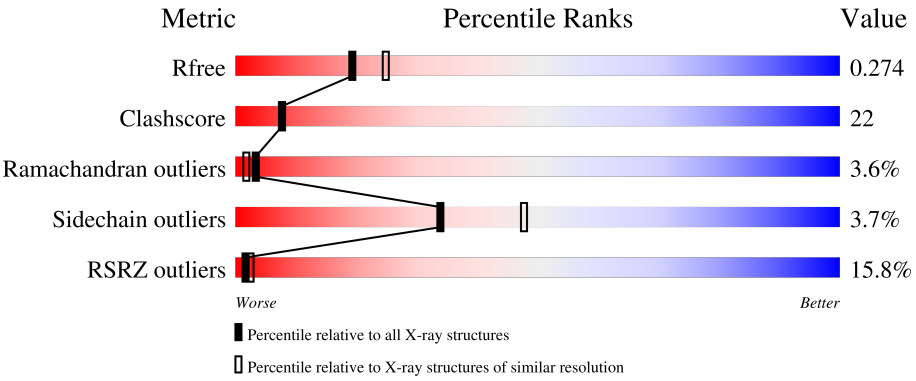
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 <=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	389	16%, 62%, 30%, . .
2	P	7	100%
3	T	9	67%, 33%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3391 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 iota.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	372	2808	1765	488	535	20	0	3	0

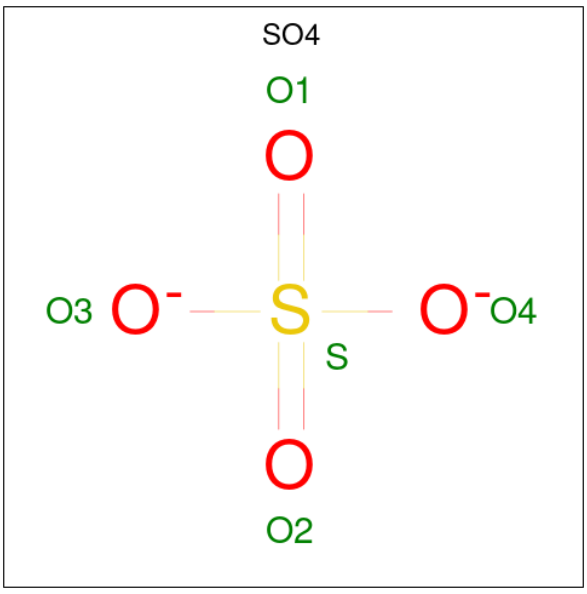
- Molecule 2 is a DNA chain called 5'-D(*TP*(BRU)P*GP*GP*GP*TP*CP*CP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	P	7	139	67	29	37	6	0	0	0

- Molecule 3 is a DNA chain called 5'-D(*AP*GP*GP*AP*CP*CP*(DOC))-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	Br	C	N	O	P			
3	T	9	201	2	96	31	63	9	0	1	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

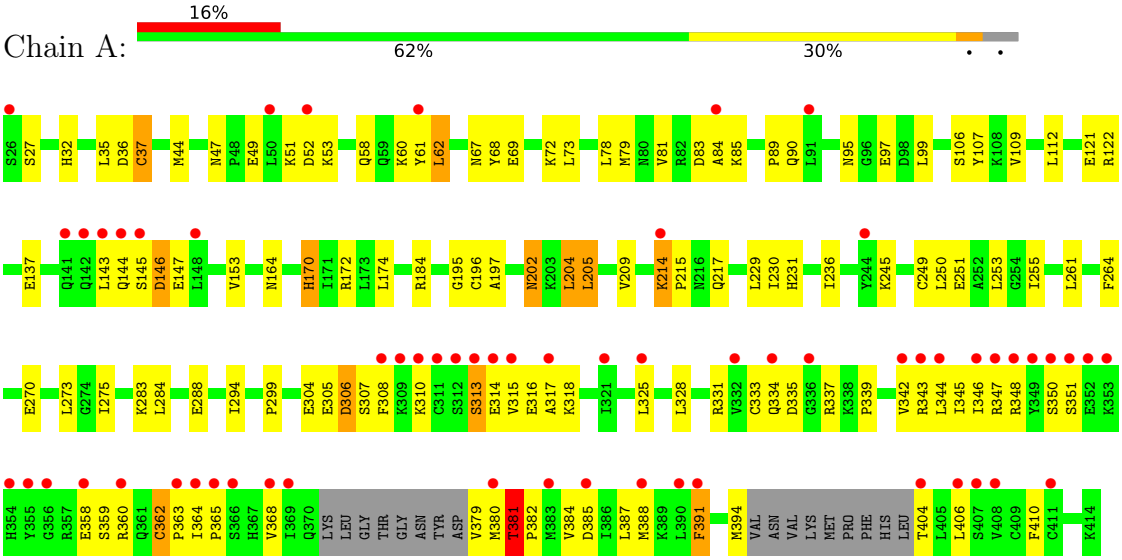
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	215	Total O 215 215	0	0
5	P	8	Total O 8 8	0	0
5	T	14	Total O 15 15	0	1

3 Residue-property plots (i)

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.

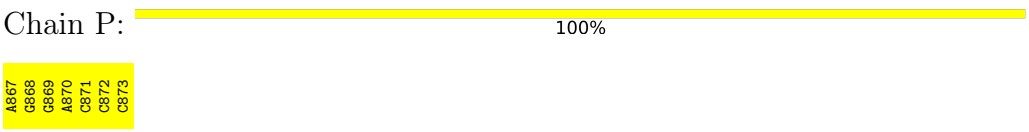
• Molecule 1: DNA polymerase iota

Chain A:



• Molecule 2: 5'-D(*TP*(BRU)P*GP*GP*GP*TP*CP*CP*T)-3'

Chain P:



• Molecule 3: 5'-D(*AP*GP*GP*AP*CP*CP*(DOC))-3'

Chain T:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	98.24Å 98.24Å 203.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.67 – 2.30 43.67 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.8 (43.67-2.30) 95.9 (43.67-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	5.13 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.253 , 0.277 0.245 , 0.274	Depositor DCC
R_{free} test set	2013 reflections (7.58%)	wwPDB-VP
Wilson B-factor (Å^2)	34.0	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 61.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	3391	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.29% 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: SO4, BRU, 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	0.34	0/2863	0.61	1/3880 (0.0%)
2	P	0.39	0/136	0.77	0/208
3	T	0.42	0/178	0.85	0/271
All	All	0.35	0/3177	0.64	1/4359 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	T	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	214	LYS	N-CA-C	5.99	127.18	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	T	842	DG	Sidechain
3	T	843	DG	Sidechain
3	T	844	DT	Sidechain

5.2 Too-close contacts (i)

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	2808	0	2729	106	0
2	P	139	0	79	9	0
3	T	201	0	111	21	0
4	A	5	0	0	0	0
5	A	215	0	0	4	1
5	P	8	0	0	2	0
5	T	15	0	0	0	0
All	All	3391	0	2919	133	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 22.

All (133) 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)
3:T:841:DG:H2”	3:T:842:DG:H5”	1.49	0.94
3:T:842:DG:H2”	3:T:843:DG:H5”	1.52	0.91
1:A:344:LEU:HD11	1:A:387:LEU:HD22	1.53	0.88
1:A:344:LEU:HD21	1:A:387:LEU:HB3	1.55	0.88
1:A:44:MET:HE2	1:A:51:LYS:HA	1.55	0.87
3:T:839:DT:H2”	3:T:840[A]:BRU:O5’	1.75	0.85
3:T:842:DG:H2”	3:T:843:DG:C5’	2.05	0.85
1:A:164:ASN:H	1:A:170:HIS:HD2	1.25	0.85
3:T:839:DT:H2”	3:T:840[B]:BRU:O5’	1.76	0.84
1:A:27:SER:HB2	5:A:553:HOH:O	1.81	0.80
3:T:841:DG:C2’	3:T:842:DG:H5”	2.12	0.80
1:A:347:ARG:HD2	1:A:404:THR:OG1	1.84	0.78
2:P:867:DA:H1’	2:P:868:DG:H5’	1.66	0.77
2:P:868:DG:N7	5:P:155:HOH:O	2.18	0.75
1:A:44:MET:CE	1:A:67:ASN:HD22	1.99	0.75
1:A:388:MET:O	1:A:391:PHE:HB3	1.88	0.74
1:A:365:PRO:O	1:A:368:VAL:HG22	1.90	0.72
1:A:44:MET:HE1	1:A:67:ASN:HD22	1.54	0.72
1:A:331:ARG:HD2	5:A:454:HOH:O	1.90	0.70
1:A:79:MET:HE3	1:A:84:ALA:HA	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:VAL:O	1:A:388:MET:HG2	1.94	0.67
1:A:335:ASP:OD2	1:A:337:ARG:HD3	1.95	0.67
1:A:215:PRO:O	1:A:217:GLN:HG3	1.95	0.66
1:A:385:ASP:HA	1:A:388:MET:HB2	1.79	0.65
1:A:342:VAL:HG21	1:A:387:LEU:HD21	1.78	0.64
1:A:51:LYS:O	1:A:53:LYS:N	2.27	0.63
1:A:214:LYS:HB3	1:A:215:PRO:HD3	1.80	0.63
1:A:381:THR:OG1	1:A:382:PRO:HD3	1.98	0.63
1:A:137:GLU:OE2	1:A:172:ARG:NH2	2.33	0.62
1:A:343:ARG:C	1:A:344:LEU:HD12	2.21	0.61
1:A:345:ILE:HG12	1:A:359:SER:HB3	1.82	0.61
1:A:379:VAL:O	1:A:382:PRO:HD2	2.00	0.61
1:A:236:ILE:HD12	1:A:250:LEU:CD1	2.30	0.60
3:T:841:DG:H2"	3:T:842:DG:C5'	2.26	0.60
1:A:164:ASN:H	1:A:170:HIS:CD2	2.15	0.60
1:A:202:ASN:ND2	1:A:205:LEU:H	2.00	0.59
1:A:68:TYR:O	1:A:72:LYS:HG3	2.03	0.59
3:T:847:DT:H6	3:T:847:DT:H5'	1.68	0.59
1:A:325:LEU:HD23	1:A:325:LEU:O	2.01	0.59
1:A:112:LEU:C	1:A:112:LEU:HD23	2.23	0.58
1:A:325:LEU:HD22	1:A:380:MET:HG2	1.86	0.58
1:A:236:ILE:HD12	1:A:250:LEU:HD12	1.85	0.57
1:A:202:ASN:HD21	1:A:205:LEU:H	1.53	0.57
1:A:106:SER:OG	1:A:122:ARG:NH2	2.39	0.56
1:A:283[A]:LYS:HE3	1:A:288:GLU:HB3	1.87	0.56
1:A:137:GLU:HG3	5:A:549:HOH:O	2.04	0.56
1:A:315:VAL:C	1:A:317:ALA:H	2.08	0.56
1:A:143:LEU:HA	1:A:147:GLU:OE2	2.06	0.55
3:T:841:DG:H1'	3:T:842:DG:H5"	1.88	0.55
1:A:202:ASN:HD22	1:A:202:ASN:C	2.09	0.55
2:P:872:DC:H2"	2:P:873:DOC:OP2	2.07	0.54
3:T:842:DG:H2"	3:T:843:DG:H5'	1.90	0.54
1:A:61:TYR:CE1	1:A:62:LEU:HD12	2.43	0.54
1:A:107:TYR:OH	1:A:299:PRO:HG3	2.07	0.53
1:A:196:CYS:HA	1:A:217:GLN:O	2.09	0.53
1:A:313:SER:O	1:A:314:GLU:HB2	2.08	0.53
1:A:51:LYS:C	1:A:53:LYS:H	2.11	0.52
1:A:339:PRO:HG3	1:A:410:PHE:HD2	1.74	0.52
1:A:347:ARG:HG2	1:A:348:ARG:N	2.24	0.52
3:T:839:DT:H2'	3:T:840[A]:BRU:BR	2.65	0.52
1:A:36:ASP:O	1:A:37:CYS:C	2.47	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:LEU:HD12	1:A:344:LEU:N	2.25	0.51
1:A:344:LEU:HD11	1:A:387:LEU:CD2	2.34	0.51
1:A:270:GLU:HG3	1:A:275:ILE:HA	1.93	0.51
1:A:62:LEU:HD23	1:A:78:LEU:HA	1.93	0.50
1:A:85:LYS:O	1:A:89:PRO:HG3	2.12	0.50
1:A:44:MET:HE1	1:A:67:ASN:ND2	2.25	0.50
1:A:385:ASP:HA	1:A:388:MET:CG	2.41	0.50
2:P:871:DC:H2"	2:P:872:DC:OP2	2.11	0.49
1:A:325:LEU:HD23	1:A:325:LEU:C	2.33	0.49
1:A:304:GLU:HG3	1:A:328:LEU:HD21	1.94	0.49
1:A:35:LEU:HD11	1:A:109:VAL:HG21	1.94	0.49
1:A:345:ILE:HA	1:A:358:GLU:O	2.13	0.48
1:A:137:GLU:CG	5:A:549:HOH:O	2.60	0.48
1:A:365:PRO:HB2	1:A:368:VAL:HG22	1.94	0.48
3:T:841:DG:C1'	3:T:842:DG:H5"	2.43	0.48
1:A:79:MET:CE	1:A:84:ALA:HA	2.43	0.48
3:T:840[B]:BRU:H2'	3:T:840[B]:BRU:O2	2.13	0.48
1:A:99:LEU:HD12	3:T:842:DG:H4'	1.96	0.48
1:A:304:GLU:HG3	1:A:328:LEU:CD2	2.44	0.48
1:A:60:LYS:HE2	1:A:307:SER:O	2.14	0.48
1:A:62:LEU:HD11	3:T:839:DT:O2	2.14	0.47
1:A:344:LEU:O	1:A:359:SER:HA	2.14	0.47
3:T:847:DT:H5'	3:T:847:DT:C6	2.49	0.47
1:A:121:GLU:HB2	1:A:294:ILE:O	2.15	0.47
3:T:843:DG:C8	3:T:844:DT:H72	2.50	0.47
1:A:44:MET:HE3	1:A:67:ASN:HD22	1.78	0.47
1:A:308:PHE:C	1:A:310:LYS:H	2.18	0.47
1:A:261:LEU:HD12	1:A:261:LEU:O	2.16	0.46
1:A:385:ASP:HA	1:A:388:MET:CB	2.44	0.46
1:A:365:PRO:HB2	1:A:368:VAL:HG13	1.96	0.46
1:A:196:CYS:SG	1:A:214:LYS:O	2.74	0.46
3:T:842:DG:C2'	3:T:843:DG:H5"	2.36	0.46
2:P:869:DG:H2"	2:P:870:DA:OP2	2.16	0.46
1:A:343:ARG:HG2	1:A:344:LEU:N	2.31	0.46
2:P:868:DG:H2"	2:P:869:DG:OP2	2.15	0.46
1:A:342:VAL:HG22	1:A:343:ARG:N	2.31	0.46
1:A:325:LEU:CD2	1:A:380:MET:HG2	2.46	0.46
1:A:381:THR:CB	1:A:382:PRO:HD3	2.46	0.46
1:A:230:ILE:CG2	1:A:231:HIS:N	2.80	0.45
1:A:249:CYS:SG	1:A:273:LEU:HD21	2.57	0.45
1:A:112:LEU:HD23	1:A:112:LEU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:GLN:H	1:A:147:GLU:CG	2.29	0.45
1:A:153:VAL:HB	1:A:174:LEU:HD22	1.98	0.45
1:A:347:ARG:HG2	1:A:348:ARG:H	1.82	0.45
1:A:79:MET:HE3	1:A:84:ALA:CA	2.46	0.45
1:A:62:LEU:HD11	3:T:839:DT:C2	2.53	0.44
1:A:144:GLN:O	1:A:146:ASP:N	2.49	0.44
1:A:47:ASN:OD1	1:A:49:GLU:HB2	2.18	0.44
2:P:871:DC:H2"	5:P:129:HOH:O	2.17	0.43
1:A:69:GLU:O	1:A:73:LEU:HD13	2.18	0.43
1:A:95:ASN:HD21	1:A:97:GLU:CD	2.21	0.43
3:T:845:DC:H2"	3:T:846:DC:OP2	2.18	0.42
1:A:58:GLN:NE2	1:A:81:VAL:HG21	2.35	0.42
1:A:305:GLU:O	1:A:306:ASP:HB2	2.20	0.42
1:A:346:ILE:HG22	1:A:406:LEU:CD2	2.50	0.42
1:A:380:MET:O	1:A:381:THR:C	2.58	0.42
1:A:251:GLU:C	1:A:253:LEU:N	2.74	0.42
2:P:870:DA:H1'	2:P:871:DC:H5'	2.01	0.42
1:A:313:SER:C	1:A:315:VAL:H	2.22	0.41
3:T:846:DC:H2"	3:T:847:DT:H5'	2.02	0.41
1:A:184:ARG:HD2	1:A:195:GLY:O	2.21	0.41
1:A:32:HIS:O	1:A:197:ALA:HA	2.20	0.41
1:A:360:ARG:HG2	1:A:394:MET:CG	2.51	0.41
1:A:81:VAL:O	1:A:84:ALA:HB3	2.20	0.41
1:A:342:VAL:HG22	1:A:343:ARG:H	1.86	0.41
1:A:255:ILE:HD11	1:A:264:PHE:CG	2.56	0.40
1:A:316:GLU:C	1:A:318:LYS:H	2.23	0.40
1:A:342:VAL:HB	1:A:364:ILE:HD11	2.02	0.40
1:A:44:MET:CE	1:A:51:LYS:HA	2.39	0.40
1:A:204:LEU:HG	1:A:284:LEU:HD22	2.03	0.40
1:A:362:CYS:HA	1:A:363:PRO:HD3	1.94	0.40
2:P:872:DC:C2'	2:P:873:DOC:OP2	2.69	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)
5:A:464:HOH:O	5:A:500:HOH:O[5_555]	2.18	0.02

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	369/389 (95%)	321 (87%)	35 (10%)	13 (4%)	3 2

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	350	SER
1	A	52	ASP
1	A	146	ASP
1	A	37	CYS
1	A	306	ASP
1	A	313	SER
1	A	381	THR
1	A	90	GLN
1	A	145	SER
1	A	245	LYS
1	A	334	GLN
1	A	333	CYS
1	A	351	SER

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	302/354 (85%)	291 (96%)	11 (4%)	35 49

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	LEU
1	A	83	ASP
1	A	170	HIS
1	A	202	ASN
1	A	204	LEU
1	A	205	LEU
1	A	209	VAL
1	A	229	LEU
1	A	362	CYS
1	A	381	THR
1	A	391	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	67	ASN
1	A	95	ASN
1	A	170	HIS
1	A	202	ASN
1	A	235	HIS
1	A	262	GLN
1	A	334	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are 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	BRU	T	840[B]	3	18,21,22	0.48	0	26,30,33	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	BRU	T	840[A]	3	18,21,22	0.31	0	26,30,33	0.52	0
2	DOC	P	873	2,3	16,19,20	0.36	0	20,26,29	0.59	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	BRU	T	840[B]	3	-	5/7/21/22	0/2/2/2
3	BRU	T	840[A]	3	-	4/7/21/22	0/2/2/2
2	DOC	P	873	2,3	-	0/7/18/19	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	T	840[B]	BRU	C2'-C1'-N1-C2
3	T	840[B]	BRU	O4'-C1'-N1-C6
3	T	840[B]	BRU	C2'-C1'-N1-C6
3	T	840[B]	BRU	O4'-C1'-N1-C2
3	T	840[A]	BRU	C2'-C1'-N1-C6
3	T	840[A]	BRU	O4'-C1'-N1-C6
3	T	840[B]	BRU	O4'-C4'-C5'-O5'
3	T	840[A]	BRU	O4'-C1'-N1-C2
3	T	840[A]	BRU	C2'-C1'-N1-C2

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	T	840[B]	BRU	2	0
3	T	840[A]	BRU	2	0
2	P	873	DOC	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand 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	SO4	A	1	-	4,4,4	1.00	0	6,6,6	1.67	1 (16%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1	SO4	O4-S-O3	3.84	125.47	109.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	372/389 (95%)	0.75	61 (16%) 1 2	18, 46, 101, 117	0
2	P	6/7 (85%)	0.97	0 100 100	49, 60, 64, 66	0
3	T	8/9 (88%)	0.37	0 100 100	37, 40, 57, 88	0
All	All	386/405 (95%)	0.74	61 (15%) 2 2	18, 46, 100, 117	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	349	TYR	11.5
1	A	355	TYR	10.9
1	A	354	HIS	7.8
1	A	350	SER	7.2
1	A	353	LYS	7.0
1	A	313	SER	6.3
1	A	388	MET	6.2
1	A	308	PHE	6.0
1	A	348	ARG	5.7
1	A	312	SER	5.1
1	A	315	VAL	4.5
1	A	347	ARG	4.4
1	A	406	LEU	4.1
1	A	311	CYS	4.1
1	A	368	VAL	4.0
1	A	148	LEU	3.8
1	A	366	SER	3.7
1	A	336	GLY	3.7
1	A	309	LYS	3.7
1	A	390	LEU	3.6
1	A	408	VAL	3.6
1	A	351	SER	3.6
1	A	244	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	404	THR	3.4
1	A	385	ASP	3.4
1	A	358	GLU	3.3
1	A	380	MET	3.2
1	A	346	ILE	3.2
1	A	352	GLU	3.2
1	A	91	LEU	3.2
1	A	145	SER	3.0
1	A	344	LEU	3.0
1	A	26	SER	3.0
1	A	364	ILE	2.9
1	A	360	ARG	2.8
1	A	391	PHE	2.7
1	A	84	ALA	2.6
1	A	214	LYS	2.6
1	A	141	GLN	2.5
1	A	369	ILE	2.5
1	A	317	ALA	2.5
1	A	314	GLU	2.5
1	A	142	GLN	2.5
1	A	144	GLN	2.4
1	A	310	LYS	2.3
1	A	356	GLY	2.3
1	A	332	VAL	2.3
1	A	365	PRO	2.3
1	A	50	LEU	2.3
1	A	383	MET	2.3
1	A	325	LEU	2.2
1	A	52	ASP	2.2
1	A	363	PRO	2.2
1	A	343	ARG	2.2
1	A	61	TYR	2.2
1	A	321	ILE	2.1
1	A	342	VAL	2.1
1	A	143	LEU	2.1
1	A	334	GLN	2.1
1	A	411	CYS	2.0
1	A	407	SER	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	BRU	T	840[A]	20/21	0.82	0.20	62,75,80,80	20
3	BRU	T	840[B]	20/21	0.82	0.20	60,64,78,78	20
2	DOC	P	873	18/19	0.97	0.14	34,38,44,45	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{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
4	SO4	A	1	5/5	0.89	0.17	86,87,88,88	0

6.5 Other polymers (i)

There are no such residues in this entry.