



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 10:32 am BST

PDB ID : 6UK0
Title : HIV-1 M184V reverse transcriptase-DNA complex
Authors : Lansdon, E.B.
Deposited on : 2019-10-03
Resolution : 2.76 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
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

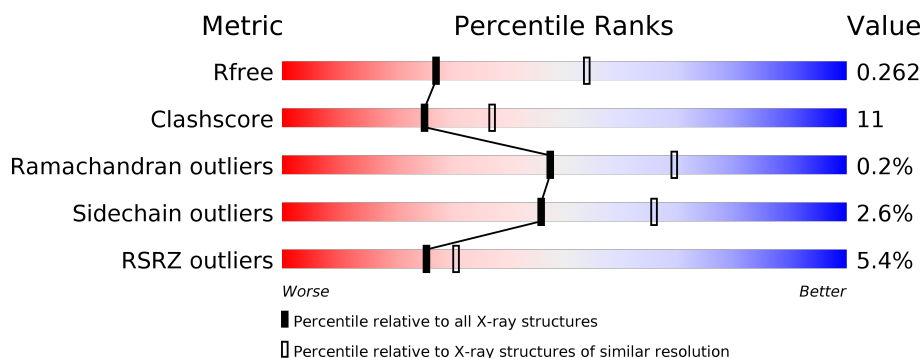
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.76 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 $\leq 5\%$. 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	572	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>20%</div> <div>• 7%</div> </div> </div>
2	B	440	<div> <div>7%</div> <div> <div></div> <div>60%</div> <div>25%</div> <div>• 14%</div> </div> </div>
3	P	21	<div> <div>24%</div> <div>62%</div> <div>14%</div> </div>
4	T	27	<div> <div>4%</div> <div> <div></div> <div>44%</div> <div>22%</div> <div>7%</div> <div>26%</div> </div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8287 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 p66 Reverse transcriptase/RNaseH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	532	Total	C	N	O	S	0	0	0
			4332	2803	722	800	7			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP P04585
A	-10	GLY	-	expression tag	UNP P04585
A	-9	SER	-	expression tag	UNP P04585
A	-8	SER	-	expression tag	UNP P04585
A	-7	HIS	-	expression tag	UNP P04585
A	-6	HIS	-	expression tag	UNP P04585
A	-5	HIS	-	expression tag	UNP P04585
A	-4	HIS	-	expression tag	UNP P04585
A	-3	HIS	-	expression tag	UNP P04585
A	-2	HIS	-	expression tag	UNP P04585
A	-1	SER	-	expression tag	UNP P04585
A	0	SER	-	expression tag	UNP P04585
A	184	VAL	MET	engineered mutation	UNP P04585
A	258	CYS	GLN	engineered mutation	UNP P04585
A	280	SER	CYS	engineered mutation	UNP P04585

- Molecule 2 is a protein called p51 Reverse transcriptase/RNaseH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	380	Total	C	N	O	S	0	0	0
			3140	2042	520	574	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	184	VAL	MET	engineered mutation	UNP P04585

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Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P04585

- Molecule 3 is a DNA chain called Primer DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	18	Total	C	N	O	P	0	0	0
			360	172	62	109	17			

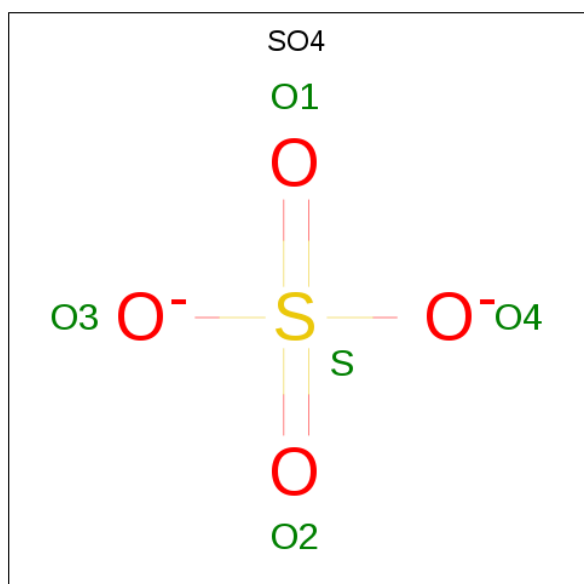
- Molecule 4 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	T	20	Total	C	N	O	P	0	0	0
			418	194	88	116	20			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	P	1	Total	O	S	0	0
			5	4	1		
6	T	1	Total	O	S	0	0
			5	4	1		

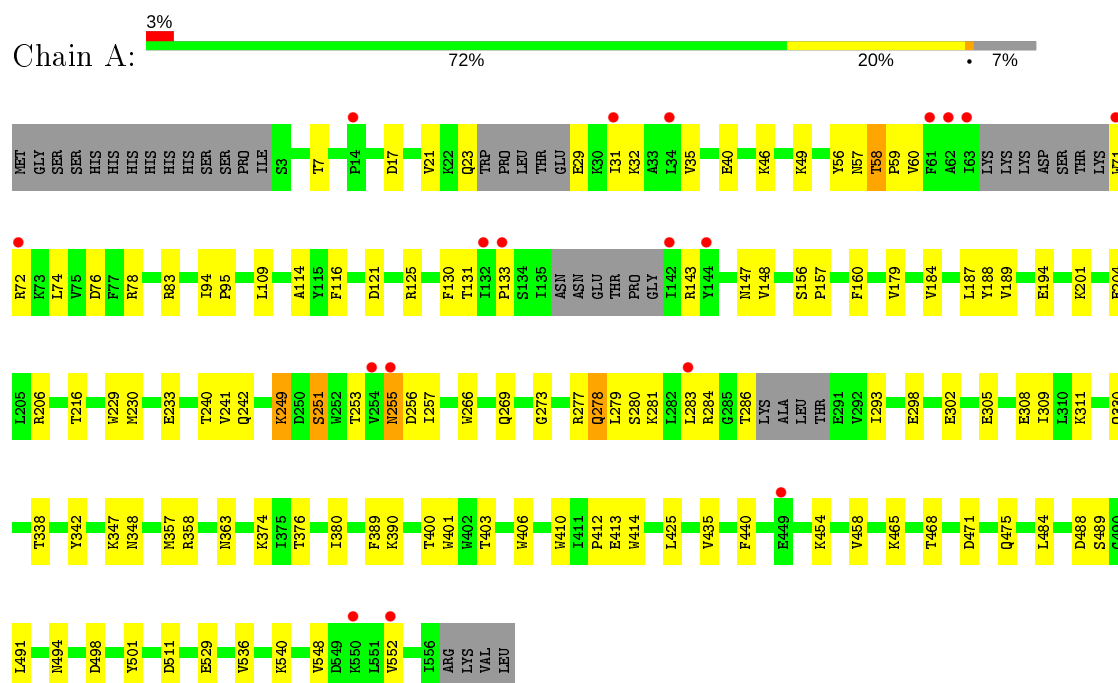
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	12	Total	O	0	0
			12	12		
7	B	6	Total	O	0	0
			6	6		
7	P	1	Total	O	0	0
			1	1		
7	T	2	Total	O	0	0
			2	2		

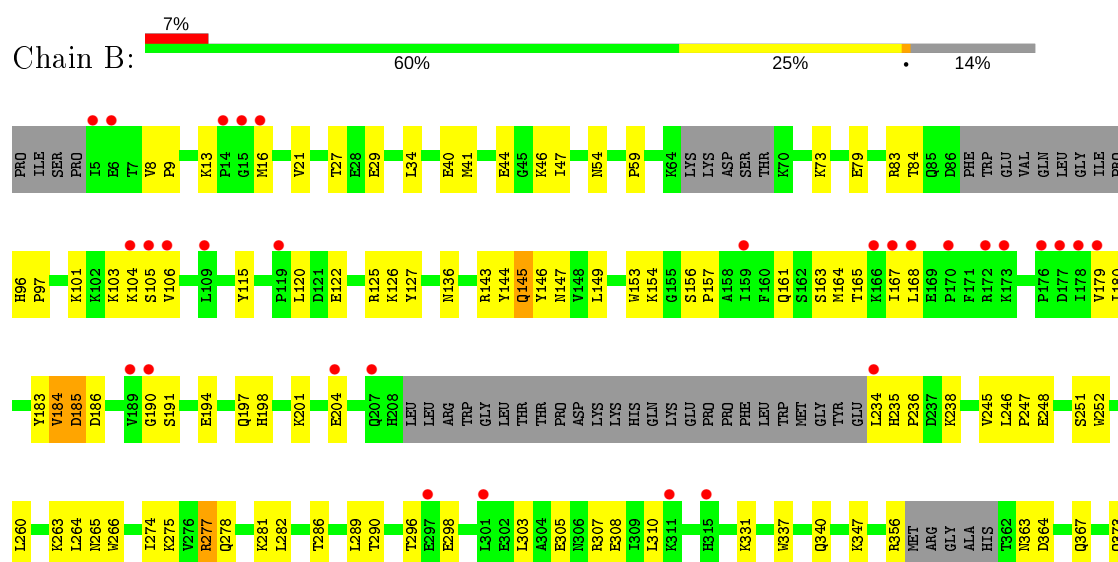
3 Residue-property plots

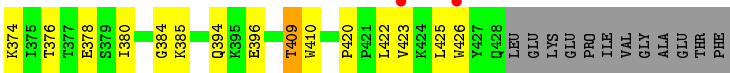
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: p66 Reverse transcriptase/RNaseH

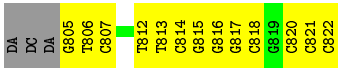
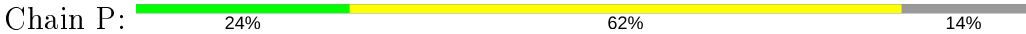


- Molecule 2: p51 Reverse transcriptase/RNaseH

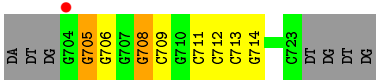




● Molecule 3: Primer DNA



● Molecule 4: Template DNA



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	167.98Å 169.68Å 97.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.68 – 2.76 48.68 – 2.76	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.68-2.76) 93.9 (48.68-2.76)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.16 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.9_1692, PHENIX 1.9_1692	Depositor
R, R_{free}	0.205 , 0.260 0.209 , 0.262	Depositor DCC
R_{free} test set	1992 reflections (5.54%)	wwPDB-VP
Wilson B-factor (Å ²)	47.5	Xtriage
Anisotropy	0.829	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8287	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DOC, MG, SO4

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	0.51	0/4440	0.62	0/6028
2	B	0.44	0/3224	0.59	0/4378
3	P	1.22	3/381 (0.8%)	1.13	1/586 (0.2%)
4	T	1.18	4/471 (0.8%)	0.90	3/726 (0.4%)
All	All	0.59	7/8516 (0.1%)	0.66	4/11718 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	814	DC	C3'-O3'	-8.53	1.32	1.44
4	T	706	DG	C3'-O3'	-8.15	1.33	1.44
4	T	708	DG	C3'-O3'	-7.02	1.34	1.44
4	T	705	DG	O3'-P	6.31	1.68	1.61
3	P	818	DC	C3'-O3'	-5.60	1.36	1.44
4	T	705	DG	C6-N1	5.08	1.43	1.39
3	P	820	DC	C3'-O3'	-5.03	1.37	1.44

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	820	DC	O4'-C4'-C3'	-6.00	102.10	104.50
4	T	705	DG	O4'-C4'-C3'	-5.73	102.21	104.50
4	T	705	DG	C4'-C3'-C2'	-5.21	98.41	103.10
4	T	706	DG	O4'-C4'-C3'	-5.09	102.47	104.50

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	4332	0	4369	77	0
2	B	3140	0	3171	91	0
3	P	360	0	203	13	0
4	T	418	0	221	10	0
5	A	1	0	0	0	0
6	A	5	0	0	0	0
6	P	5	0	0	0	0
6	T	5	0	0	0	0
7	A	12	0	0	1	0
7	B	6	0	0	0	0
7	P	1	0	0	0	0
7	T	2	0	0	0	0
All	All	8287	0	7964	174	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (174) 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)
2:B:84:THR:HG21	2:B:153:TRP:HE1	1.28	0.98
3:P:815:DG:O6	4:T:713:DC:N4	2.06	0.88
2:B:274:ILE:HD11	2:B:310:LEU:HD21	1.60	0.84
2:B:423:VAL:HA	2:B:426:TRP:CD1	2.13	0.82
1:A:7:THR:HG21	1:A:121:ASP:HA	1.66	0.77
2:B:120:LEU:HD23	2:B:125:ARG:HG2	1.69	0.74
1:A:286:THR:HG21	1:A:293:ILE:HD11	1.70	0.74
2:B:168:LEU:HD13	2:B:180:ILE:HD12	1.70	0.72
1:A:131:THR:HG23	1:A:143:ARG:HG2	1.71	0.71
1:A:435:VAL:HB	2:B:290:THR:HG21	1.72	0.70
2:B:235:HIS:H	2:B:238:LYS:NZ	1.89	0.69
1:A:21:VAL:O	1:A:57:ASN:ND2	2.25	0.67
2:B:73:LYS:NZ	2:B:146:TYR:OH	2.28	0.66
2:B:194:GLU:HB3	2:B:197:GLN:OE1	1.96	0.64
1:A:374:LYS:NZ	4:T:711:DC:OP1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ILE:HD13	1:A:133:PRO:O	1.99	0.62
1:A:363:ASN:HA	1:A:511:ASP:OD1	1.98	0.62
2:B:104:LYS:O	2:B:235:HIS:ND1	2.31	0.61
2:B:16:MET:HE3	2:B:83:ARG:HG2	1.82	0.61
2:B:260:LEU:HD21	2:B:303:LEU:HD13	1.83	0.60
2:B:246:LEU:HD11	2:B:264:LEU:HD21	1.81	0.60
1:A:74:LEU:HD13	4:T:705:DG:C4	2.36	0.60
3:P:815:DG:N1	4:T:713:DC:N3	2.33	0.60
1:A:94:ILE:HD13	4:T:709:DC:H1'	1.82	0.60
1:A:281:LYS:HG3	1:A:284:ARG:HH21	1.67	0.60
2:B:84:THR:HG21	2:B:153:TRP:NE1	2.09	0.59
1:A:206:ARG:NH2	1:A:216:THR:O	2.35	0.59
1:A:60:VAL:HG21	1:A:130:PHE:CD2	2.37	0.59
2:B:201:LYS:HA	2:B:204:GLU:OE1	2.03	0.59
2:B:235:HIS:O	2:B:238:LYS:HG2	2.03	0.58
1:A:241:VAL:HG12	1:A:242:GLN:O	2.03	0.58
1:A:230:MET:HE1	3:P:821:DC:H2''	1.86	0.57
1:A:201:LYS:NZ	1:A:204:GLU:OE2	2.33	0.57
4:T:713:DC:H2'	4:T:714:DG:C8	2.38	0.57
1:A:230:MET:HE3	3:P:822:DOC:H5''	1.87	0.57
4:T:712:DC:H2'	4:T:713:DC:C6	2.39	0.57
1:A:78:ARG:NH1	4:T:705:DG:OP1	2.38	0.56
1:A:23:GLN:OE1	1:A:133:PRO:HG3	2.04	0.56
2:B:266:TRP:CZ3	2:B:426:TRP:HB3	2.41	0.56
2:B:84:THR:O	2:B:154:LYS:NZ	2.39	0.55
2:B:79:GLU:OE1	2:B:83:ARG:NH2	2.35	0.55
1:A:253:THR:HG22	1:A:255:ASN:H	1.70	0.55
1:A:56:TYR:O	1:A:143:ARG:NH2	2.40	0.55
1:A:17:ASP:O	1:A:83:ARG:HD3	2.07	0.54
2:B:248:GLU:HA	2:B:307:ARG:HH22	1.72	0.54
2:B:122:GLU:HA	2:B:125:ARG:HE	1.73	0.54
1:A:266:TRP:O	1:A:269:GLN:HG2	2.08	0.54
1:A:46:LYS:HE2	1:A:116:PHE:O	2.07	0.54
4:T:708:DG:H2'	4:T:709:DC:C6	2.43	0.54
1:A:253:THR:HB	1:A:256:ASP:OD2	2.08	0.53
1:A:308:GLU:OE1	1:A:311:LYS:NZ	2.38	0.53
2:B:115:TYR:CD1	2:B:156:SER:HB3	2.43	0.53
2:B:54:ASN:O	2:B:143:ARG:NH2	2.41	0.53
1:A:233:GLU:HB2	1:A:240:THR:HG22	1.91	0.53
2:B:184:VAL:HG23	2:B:185:ASP:H	1.74	0.53
2:B:235:HIS:H	2:B:238:LYS:HZ2	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:VAL:O	1:A:552:VAL:HB	2.08	0.53
2:B:305:GLU:O	2:B:308:GLU:HB3	2.09	0.53
1:A:230:MET:CE	3:P:822:DOC:H5"	2.39	0.52
1:A:279:LEU:N	1:A:302:GLU:OE2	2.33	0.52
2:B:245:VAL:O	2:B:263:LYS:NZ	2.31	0.52
2:B:282:LEU:HD21	2:B:296:THR:HG23	1.90	0.52
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.91	0.52
2:B:235:HIS:HB2	2:B:238:LYS:HD3	1.91	0.52
1:A:413:GLU:HA	7:A:711:HOH:O	2.08	0.52
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.92	0.51
2:B:122:GLU:HA	2:B:125:ARG:HG3	1.91	0.51
1:A:257:ILE:HG22	1:A:283:LEU:HD21	1.93	0.51
2:B:380:ILE:O	2:B:384:GLY:N	2.42	0.51
2:B:103:LYS:O	2:B:236:PRO:HD2	2.11	0.51
2:B:184:VAL:HG23	2:B:185:ASP:N	2.25	0.51
2:B:41:MET:HA	2:B:46:LYS:HE3	1.91	0.51
2:B:154:LYS:O	2:B:157:PRO:HD2	2.11	0.51
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.92	0.50
2:B:125:ARG:HD3	2:B:147:ASN:HA	1.93	0.50
1:A:358:ARG:NH1	2:B:396:GLU:OE1	2.32	0.50
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.46	0.50
1:A:249:LYS:HB3	1:A:251:SER:O	2.12	0.50
2:B:331:LYS:HB2	2:B:337:TRP:CZ3	2.46	0.50
2:B:374:LYS:NZ	2:B:378:GLU:OE1	2.25	0.50
2:B:106:VAL:O	2:B:234:LEU:HB3	2.12	0.49
2:B:298:GLU:N	2:B:298:GLU:OE1	2.42	0.49
2:B:420:PRO:C	2:B:422:LEU:H	2.15	0.49
2:B:161:GLN:O	2:B:165:THR:HG23	2.12	0.49
1:A:540:LYS:HE2	2:B:265:ASN:OD1	2.13	0.48
1:A:465:LYS:NZ	1:A:488:ASP:OD2	2.42	0.48
3:P:806:DT:H2'	3:P:807:DC:C6	2.48	0.48
1:A:23:GLN:NE2	1:A:131:THR:O	2.47	0.48
1:A:277:ARG:NH2	1:A:357:MET:HB2	2.27	0.48
1:A:116:PHE:O	1:A:148:VAL:HG11	2.14	0.48
2:B:275:LYS:HE2	2:B:277:ARG:CB	2.44	0.48
2:B:183:TYR:O	2:B:186:ASP:HB2	2.14	0.48
1:A:412:PRO:O	1:A:414:TRP:HD1	1.97	0.47
2:B:247:PRO:O	2:B:307:ARG:NH2	2.47	0.47
2:B:331:LYS:NZ	2:B:364:ASP:OD2	2.25	0.47
2:B:164:MET:HA	2:B:167:ILE:HD12	1.97	0.47
2:B:103:LYS:HD2	2:B:179:VAL:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:TRP:CE2	2:B:363:ASN:ND2	2.83	0.47
1:A:74:LEU:HD23	1:A:74:LEU:HA	1.73	0.47
2:B:235:HIS:CD2	2:B:238:LYS:HD3	2.49	0.47
3:P:806:DT:C4	3:P:807:DC:N4	2.83	0.47
2:B:122:GLU:HA	2:B:125:ARG:NE	2.30	0.46
2:B:163:SER:O	2:B:167:ILE:HG13	2.15	0.46
2:B:27:THR:HG22	2:B:29:GLU:HG2	1.97	0.46
2:B:47:ILE:HD12	2:B:144:TYR:CD1	2.51	0.46
2:B:13:LYS:HE3	2:B:84:THR:O	2.14	0.46
2:B:266:TRP:CE3	2:B:426:TRP:HB3	2.50	0.46
2:B:278:GLN:HA	2:B:281:LYS:HE3	1.96	0.46
1:A:401:TRP:HB2	1:A:425:LEU:HD11	1.97	0.46
1:A:305:GLU:O	1:A:309:ILE:HG13	2.16	0.46
2:B:252:TRP:CZ3	2:B:260:LEU:HD22	2.51	0.46
2:B:106:VAL:HA	2:B:190:GLY:HA2	1.97	0.46
1:A:376:THR:O	1:A:380:ILE:HG13	2.15	0.45
2:B:277:ARG:O	2:B:281:LYS:HG3	2.15	0.45
2:B:422:LEU:O	2:B:425:LEU:N	2.45	0.45
2:B:115:TYR:O	2:B:149:LEU:HB2	2.16	0.45
1:A:280:SER:O	1:A:283:LEU:HD12	2.17	0.45
1:A:71:TRP:N	1:A:71:TRP:CD1	2.83	0.45
2:B:105:SER:HA	2:B:235:HIS:HD1	1.82	0.45
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.52	0.45
1:A:484:LEU:HA	1:A:484:LEU:HD23	1.66	0.45
1:A:29:GLU:O	1:A:29:GLU:HG3	2.17	0.45
2:B:286:THR:OG1	2:B:286:THR:O	2.32	0.45
2:B:34:LEU:HD21	2:B:73:LYS:HG3	1.99	0.45
2:B:197:GLN:N	2:B:197:GLN:OE1	2.42	0.44
2:B:373:GLN:HA	2:B:410:TRP:HH2	1.82	0.44
3:P:816:DG:H2'	3:P:817:DG:C8	2.52	0.44
3:P:812:DT:H2'	3:P:813:DT:H72	1.99	0.44
1:A:358:ARG:HD2	2:B:394:GLN:OE1	2.16	0.44
2:B:191:SER:OG	2:B:198:HIS:ND1	2.27	0.44
1:A:58:THR:HG22	1:A:76:ASP:O	2.16	0.44
2:B:101:LYS:HE2	2:B:101:LYS:HB3	1.72	0.44
1:A:273:GLY:H	1:A:338:THR:HG21	1.83	0.44
2:B:126:LYS:HA	2:B:145:GLN:OE1	2.18	0.44
3:P:805:DG:H2'	3:P:806:DT:C6	2.53	0.44
1:A:57:ASN:OD1	1:A:131:THR:OG1	2.23	0.43
1:A:406:TRP:O	2:B:331:LYS:HB3	2.19	0.43
3:P:805:DG:C8	3:P:806:DT:H72	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:376:THR:HB	2:B:410:TRP:CH2	2.54	0.43
4:T:712:DC:H2'	4:T:713:DC:H6	1.82	0.43
1:A:125:ARG:HD3	1:A:147:ASN:HA	2.01	0.43
1:A:32:LYS:HA	1:A:35:VAL:HG22	2.01	0.42
1:A:454:LYS:HE2	1:A:468:THR:HG22	2.01	0.42
2:B:347:LYS:HD3	2:B:347:LYS:HA	1.78	0.42
2:B:8:VAL:HA	2:B:9:PRO:HD2	1.84	0.42
3:P:815:DG:H2''	3:P:816:DG:C8	2.54	0.42
1:A:229:TRP:CE2	1:A:230:MET:HG3	2.53	0.42
1:A:342:TYR:HB3	1:A:348:ASN:HA	2.02	0.42
1:A:94:ILE:HG22	1:A:95:PRO:O	2.20	0.42
1:A:389:PHE:O	1:A:390:LYS:HD3	2.20	0.42
2:B:96:HIS:ND1	2:B:97:PRO:HD2	2.35	0.42
1:A:94:ILE:N	1:A:94:ILE:HD12	2.34	0.41
2:B:40:GLU:OE2	2:B:40:GLU:N	2.53	0.41
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.55	0.41
2:B:278:GLN:NE2	2:B:298:GLU:HG3	2.36	0.41
1:A:498:ASP:HA	1:A:536:VAL:O	2.21	0.41
1:A:109:LEU:N	1:A:187:LEU:O	2.50	0.41
1:A:491:LEU:HB3	1:A:529:GLU:HG3	2.01	0.41
3:P:812:DT:H2''	3:P:813:DT:O5'	2.20	0.41
1:A:109:LEU:HD12	1:A:109:LEU:HA	1.63	0.41
2:B:27:THR:CG2	2:B:29:GLU:HG2	2.51	0.41
1:A:179:VAL:O	1:A:189:VAL:HA	2.21	0.41
1:A:440:PHE:CE1	1:A:489:SER:HB3	2.56	0.41
2:B:235:HIS:HD2	2:B:238:LYS:HD3	1.85	0.41
1:A:494:ASN:HB3	2:B:289:LEU:HD12	2.02	0.41
1:A:400:THR:O	1:A:403:THR:HB	2.21	0.41
2:B:185:ASP:HB2	2:B:409:THR:HG21	2.03	0.41
2:B:44:GLU:HB2	2:B:46:LYS:HE2	2.02	0.41
2:B:278:GLN:HG3	2:B:298:GLU:HB2	2.02	0.40
1:A:278:GLN:HG2	1:A:298:GLU:HB3	2.04	0.40
1:A:95:PRO:HA	2:B:136:ASN:O	2.20	0.40
2:B:126:LYS:HE3	2:B:127:TYR:CZ	2.56	0.40
2:B:16:MET:HE1	2:B:83:ARG:HA	2.03	0.40
2:B:356:ARG:HD3	2:B:367:GLN:OE1	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	522/572 (91%)	492 (94%)	29 (6%)	1 (0%)	47	69
2	B	370/440 (84%)	353 (95%)	16 (4%)	1 (0%)	41	60
All	All	892/1012 (88%)	845 (95%)	45 (5%)	2 (0%)	47	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	VAL
2	B	184	VAL

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	474/511 (93%)	460 (97%)	14 (3%)	41	61
2	B	347/400 (87%)	340 (98%)	7 (2%)	55	72
All	All	821/911 (90%)	800 (97%)	21 (3%)	46	66

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	GLU
1	A	49	LYS
1	A	58	THR
1	A	72	ARG

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Mol	Chain	Res	Type
1	A	188	TYR
1	A	194	GLU
1	A	249	LYS
1	A	251	SER
1	A	255	ASN
1	A	278	GLN
1	A	330	GLN
1	A	347	LYS
1	A	458	VAL
1	A	471	ASP
2	B	145	GLN
2	B	185	ASP
2	B	251	SER
2	B	277	ARG
2	B	340	GLN
2	B	385	LYS
2	B	409	THR

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

Mol	Chain	Res	Type
2	B	330	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	DOC	P	822	3,4	14,19,20	2.22	7 (50%)	13,26,29	4.06	6 (46%)

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	822	3,4	-	1/4/18/19	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	822	DOC	C4-N3	4.32	1.42	1.35
3	P	822	DOC	C5-C4	-3.12	1.33	1.41
3	P	822	DOC	O5'-C5'	-2.93	1.37	1.44
3	P	822	DOC	C3'-C2'	-2.45	1.47	1.54
3	P	822	DOC	O4'-C1'	2.29	1.47	1.42
3	P	822	DOC	C4-N4	2.27	1.41	1.35
3	P	822	DOC	C1'-N1	-2.24	1.42	1.49

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	822	DOC	C2'-C1'-N1	11.75	134.60	112.48
3	P	822	DOC	O4'-C4'-C5'	5.44	118.47	109.52
3	P	822	DOC	C4'-O4'-C1'	-4.51	105.55	109.81
3	P	822	DOC	C2-N3-C4	2.91	119.29	116.34
3	P	822	DOC	O4'-C1'-C2'	-2.80	103.64	106.67
3	P	822	DOC	C3'-C2'-C1'	-2.05	100.40	102.78

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	P	822	DOC	O4'-C1'-N1-C6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	822	DOC	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	SO4	P	901	-	4,4,4	0.28	0	6,6,6	0.42	0
6	SO4	A	602	-	4,4,4	0.29	0	6,6,6	0.55	0
6	SO4	T	801	-	4,4,4	0.17	0	6,6,6	0.24	0

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.

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, 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	532/572 (93%)	0.17	18 (3%) 45 53	22, 38, 74, 102	0
2	B	380/440 (86%)	0.46	32 (8%) 11 13	26, 54, 98, 108	0
3	P	17/21 (80%)	-0.46	0 100 100	23, 43, 58, 61	0
4	T	20/27 (74%)	-0.29	1 (5%) 28 35	25, 48, 62, 106	0
All	All	949/1060 (89%)	0.27	51 (5%) 25 31	22, 44, 85, 108	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	133	PRO	5.0
2	B	178	ILE	5.0
2	B	168	LEU	4.6
2	B	177	ASP	3.8
1	A	550	LYS	3.7
2	B	15	GLY	3.7
2	B	109	LEU	3.7
1	A	71	TRP	3.6
2	B	426	TRP	3.6
2	B	207	GLN	3.6
2	B	16	MET	3.5
2	B	301	LEU	3.3
2	B	167	ILE	3.3
2	B	172	ARG	3.2
1	A	34	LEU	3.2
1	A	62	ALA	3.1
2	B	189	VAL	2.9
1	A	283	LEU	2.9
1	A	552	VAL	2.9
1	A	254	VAL	2.7
4	T	704	DG	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	14	PRO	2.6
2	B	204	GLU	2.6
2	B	176	PRO	2.6
1	A	132	ILE	2.6
2	B	179	VAL	2.6
1	A	72	ARG	2.6
1	A	144	TYR	2.5
2	B	311	LYS	2.5
2	B	170	PRO	2.5
1	A	31	ILE	2.5
2	B	190	GLY	2.4
2	B	5	ILE	2.4
2	B	297	GLU	2.4
1	A	255	ASN	2.4
2	B	6	GLU	2.4
1	A	61	PHE	2.3
2	B	14	PRO	2.3
2	B	105	SER	2.3
1	A	63	ILE	2.3
2	B	104	LYS	2.2
2	B	234	LEU	2.2
2	B	119	PRO	2.2
2	B	315	HIS	2.2
1	A	142	ILE	2.1
2	B	166	LYS	2.1
2	B	173	LYS	2.1
2	B	423	VAL	2.1
2	B	106	VAL	2.0
1	A	449	GLU	2.0
2	B	159	ILE	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	DOC	P	822	18/19	0.98	0.13	16,22,29,29	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	SO4	P	901	5/5	0.84	0.28	47,52,73,83	0
6	SO4	T	801	5/5	0.84	0.30	59,63,85,92	0
5	MG	A	601	1/1	0.90	0.24	50,50,50,50	0
6	SO4	A	602	5/5	0.98	0.13	27,29,33,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.