W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:58 PM GMT

PDB ID	:	4B3P
Title	:	Structures of HIV-1 RT and RNA-DNA Complex Reveal a Unique RT Conformation and Substrate Interface
Authors	:	Lapkouski, M.; Tian, L.; Miller, J.T.; Le Grice, S.F.J.; Yang, W.
Deposited on	:	2012-07-25
Resolution	:	4.84 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
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)	:	trunk26865
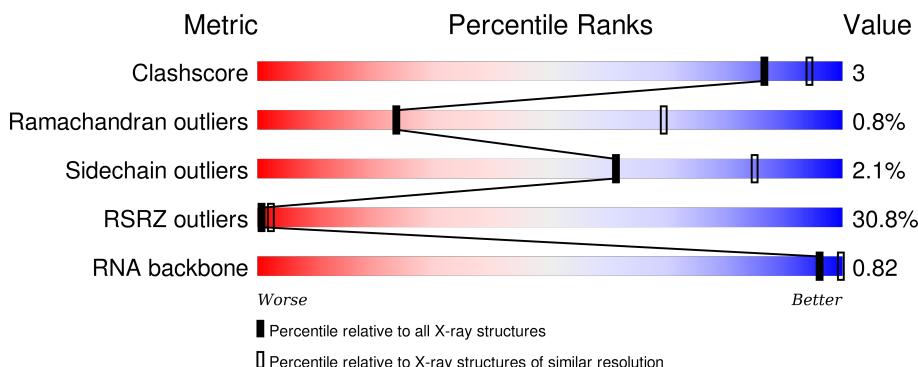
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
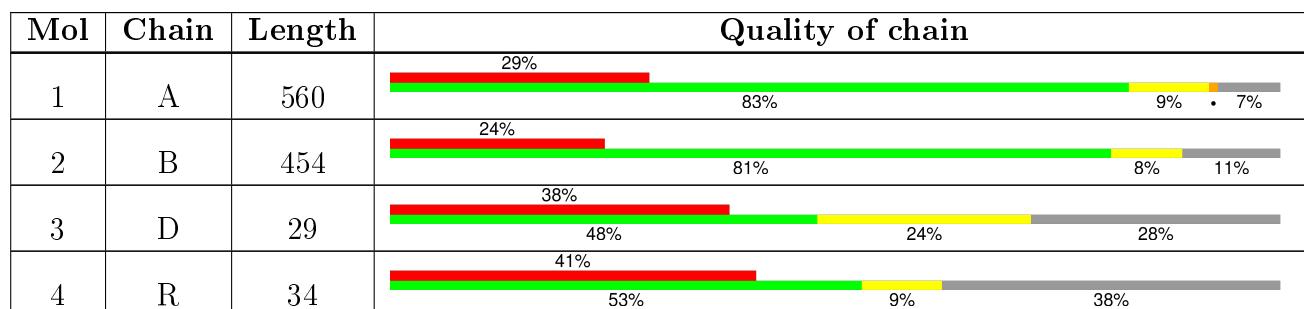
The reported resolution of this entry is 4.84 Å.

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	Percentile Ranks	Value
Clashscore		3
Ramachandran outliers		0.8%
Sidechain outliers		2.1%
RSRZ outliers		30.8%
RNA backbone		0.82

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1017 (6.00-3.66)
Ramachandran outliers	100387	1156 (6.00-3.60)
Sidechain outliers	100360	1134 (6.00-3.60)
RSRZ outliers	91569	1120 (6.00-3.60)
RNA backbone	2183	1094 (6.76-2.80)

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 <=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	560	29% / 83% 9% · 7%
2	B	454	24% / 81% 8% 11%
3	D	29	38% / 48% 24% 28%
4	R	34	41% / 53% 9% 38%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8162 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 REVERSE TRANSCRIPTASE/RIBONUCLEASE H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	0	0
			4054	2612	669	766	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	68	GLY	SER	ENGINEERED MUTATION	UNP P04585
A	83	LYS	ARG	ENGINEERED MUTATION	UNP P04585
A	411	VAL	ILE	ENGINEERED MUTATION	UNP P04585
A	447	SER	ASN	ENGINEERED MUTATION	UNP P04585
A	461	LYS	ARG	ENGINEERED MUTATION	UNP P04585
A	483	HIS	TYR	ENGINEERED MUTATION	UNP P04585
A	498	ALA	ASP	ENGINEERED MUTATION	UNP P04585
A	559	ILE	VAL	ENGINEERED MUTATION	UNP P04585

- Molecule 2 is a protein called P51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	404	Total	C	N	O	S	0	0	0
			3230	2102	524	597	7			

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	MET	-	EXPRESSION TAG	UNP P04585
B	-12	ARG	-	EXPRESSION TAG	UNP P04585
B	-11	GLY	-	EXPRESSION TAG	UNP P04585
B	-10	SER	-	EXPRESSION TAG	UNP P04585
B	-9	HIS	-	EXPRESSION TAG	UNP P04585
B	-8	HIS	-	EXPRESSION TAG	UNP P04585
B	-7	HIS	-	EXPRESSION TAG	UNP P04585
B	-6	HIS	-	EXPRESSION TAG	UNP P04585

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	EXPRESSION TAG	UNP P04585
B	-4	HIS	-	EXPRESSION TAG	UNP P04585
B	-3	GLY	-	EXPRESSION TAG	UNP P04585
B	-2	SER	-	EXPRESSION TAG	UNP P04585
B	-1	GLN	-	EXPRESSION TAG	UNP P04585
B	0	LEU	-	EXPRESSION TAG	UNP P04585
B	68	GLY	SER	ENGINEERED MUTATION	UNP P04585
B	83	LYS	ARG	ENGINEERED MUTATION	UNP P04585
B	411	VAL	ILE	ENGINEERED MUTATION	UNP P04585

- Molecule 3 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	D	21	433	207	75	130	21	0	0	0
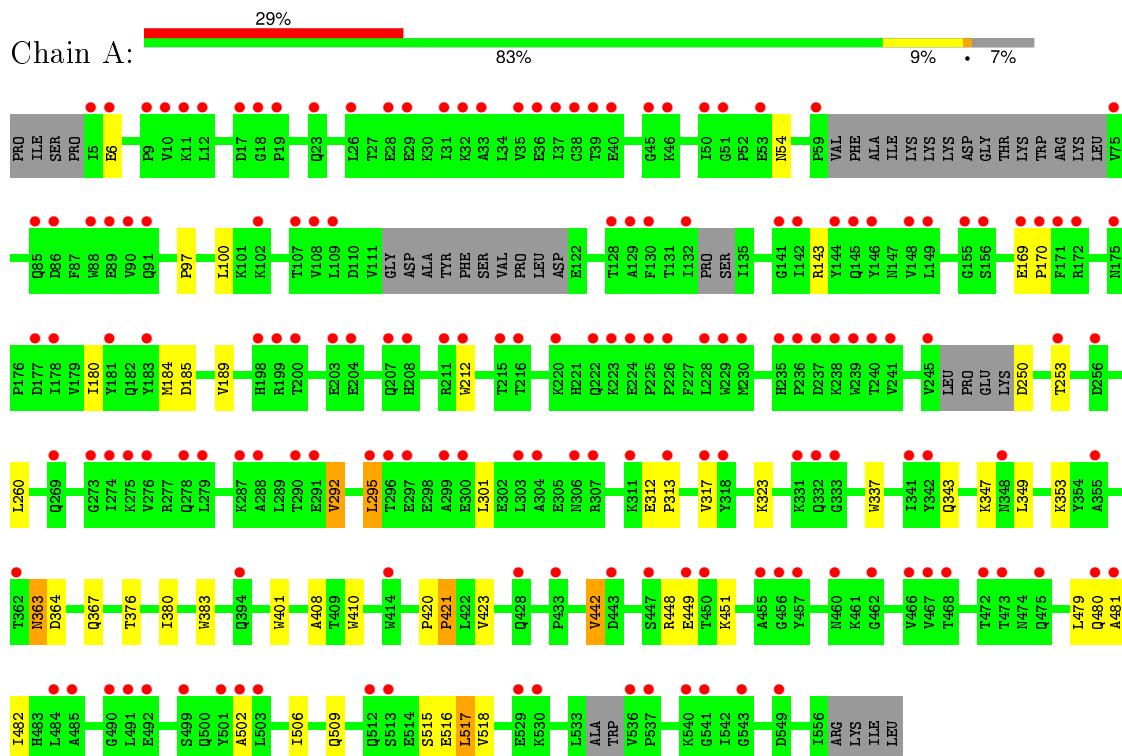
- Molecule 4 is a RNA chain called RNA.

| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	R	21	445	200	81	143	21	0	0	0
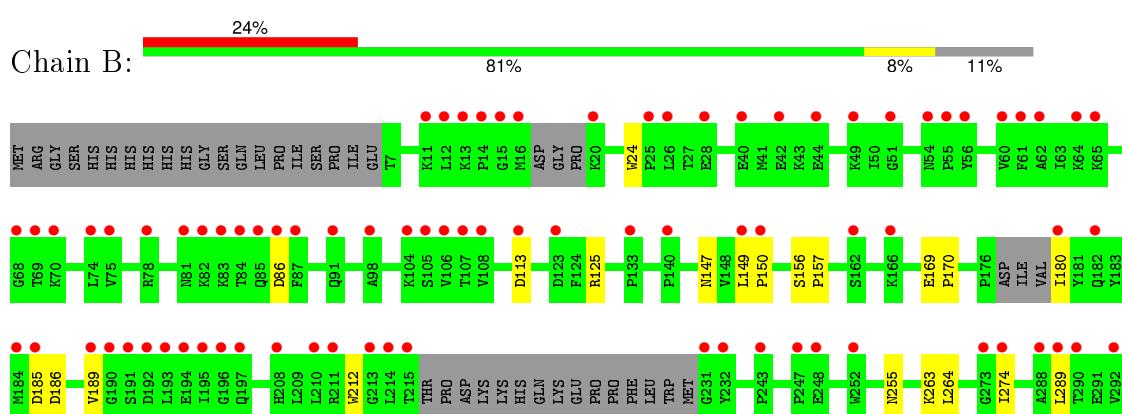
3 Residue-property plots ⓘ
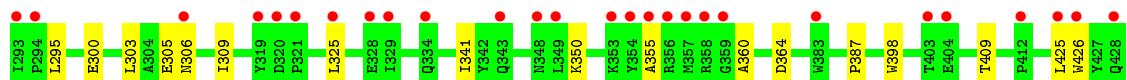
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: REVERSE TRANSCRIPTASE/RIBONUCLEASE H
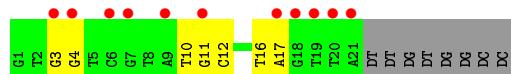
- Molecule 2: P51 RT

• Molecule 3: DNA

Chain D:

• Molecule 4: RNA

Chain R:
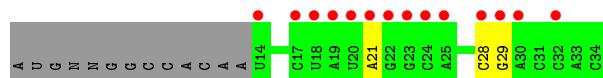
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	163.00Å 163.00Å 229.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.10 – 4.84 48.38 – 4.84	Depositor EDS
% Data completeness (in resolution range)	99.2 (46.10-4.84) 99.4 (48.38-4.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	1.25 (at 4.85Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.364 , 0.404 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å^2)	112.9	Xtriage
Anisotropy	0.683	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 139.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.26, < L^2 > = 0.10$	Xtriage
Outliers	5 of 18091 reflections (0.028%)	Xtriage
F_o,F_c correlation	0.60	EDS
Total number of atoms	8162	wwPDB-VP
Average B, all atoms (Å^2)	189.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.49	4/4146 (0.1%)	0.47	0/5648
2	B	0.53	4/3315 (0.1%)	0.47	0/4513
3	D	0.30	0/484	0.70	0/746
4	R	0.29	1/497 (0.2%)	0.65	0/771
All	All	0.49	9/8442 (0.1%)	0.50	0/11678

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	410	TRP	CD2-CE2	5.06	1.47	1.41
1	A	383	TRP	CD2-CE2	5.05	1.47	1.41
2	B	426	TRP	CD2-CE2	5.03	1.47	1.41
2	B	24	TRP	CD2-CE2	5.03	1.47	1.41
2	B	212	TRP	CD2-CE2	5.03	1.47	1.41
4	R	21	A	C3'-C2'	5.03	1.58	1.52
1	A	212	TRP	CD2-CE2	5.01	1.47	1.41
1	A	401	TRP	CD2-CE2	5.01	1.47	1.41
2	B	398	TRP	CD2-CE2	5.01	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4054	0	3965	23	0
2	B	3230	0	3186	14	0
3	D	433	0	240	5	0
4	R	445	0	228	2	0
All	All	8162	0	7619	43	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 3.

All (43) 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)
1:A:480:GLN:HG2	1:A:517:LEU:HD11	1.69	0.74
1:A:337:TRP:HE1	1:A:367:GLN:HE21	1.45	0.63
3:D:3:DG:H2'	3:D:4:DG:H8	1.69	0.58
1:A:482:ILE:HD13	1:A:506:ILE:HD11	1.85	0.57
3:D:16:DT:H2'	3:D:17:DA:C8	2.40	0.56
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.89	0.55
3:D:3:DG:H2'	3:D:4:DG:C8	2.42	0.54
1:A:482:ILE:HD11	1:A:502:ALA:HB1	1.90	0.53
2:B:263:LYS:HE2	2:B:425:LEU:HB3	1.90	0.52
2:B:185:ASP:HB2	2:B:409:THR:HG21	1.90	0.52
4:R:28:C:H2'	4:R:29:G:H8	1.75	0.51
1:A:317:VAL:HG21	1:A:347:LYS:HB3	1.94	0.50
1:A:420:PRO:HB2	1:A:421:PRO:HD3	1.93	0.50
1:A:442:VAL:HG22	1:A:481:ALA:HB1	1.92	0.50
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.94	0.48
1:A:363:ASN:HD22	1:A:509:GLN:HB2	1.79	0.48
1:A:295:LEU:H	1:A:295:LEU:HD13	1.79	0.47
1:A:479:LEU:HD21	1:A:518:VAL:HG23	1.97	0.46
2:B:156:SER:HB2	2:B:157:PRO:HD3	1.98	0.46
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.97	0.46
2:B:255:ASN:HB2	2:B:289:LEU:HB3	1.99	0.45
2:B:149:LEU:HA	2:B:150:PRO:HD3	1.85	0.45
4:R:28:C:H2'	4:R:29:G:C8	2.51	0.45
2:B:169:GLU:N	2:B:170:PRO:HD2	2.32	0.45
1:A:253:THR:HA	1:A:292:VAL:HA	1.99	0.44
2:B:306:ASN:HA	2:B:309:ILE:HD12	1.99	0.44
1:A:449:GLU:C	1:A:451:LYS:H	2.21	0.43
1:A:364:ASP:HB3	1:A:423:VAL:HG13	2.00	0.43
1:A:312:GLU:HA	1:A:313:PRO:HD3	1.87	0.43
1:A:515:SER:C	1:A:517:LEU:N	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:325:LEU:HD23	2:B:387:PRO:HB3	2.02	0.42
2:B:295:LEU:HB3	2:B:300:GLU:HG2	2.02	0.42
1:A:54:ASN:HB3	1:A:143:ARG:HH21	1.85	0.41
1:A:180:ILE:HG23	1:A:189:VAL:HG22	2.01	0.41
2:B:264:LEU:HD12	2:B:274:ILE:HG12	2.01	0.41
3:D:11:DG:H2"	3:D:12:DC:H5'	2.03	0.41
1:A:376:THR:O	1:A:380:ILE:HG12	2.21	0.41
3:D:10:DT:H2'	3:D:11:DG:C8	2.56	0.40
2:B:180:ILE:HG22	2:B:189:VAL:HG22	2.03	0.40
2:B:125:ARG:HE	2:B:147:ASN:HA	1.86	0.40
1:A:515:SER:C	1:A:517:LEU:H	2.25	0.40
2:B:341:ILE:HD12	2:B:350:LYS:HB3	2.03	0.40
1:A:97:PRO:HA	1:A:100:LEU:HD12	2.03	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	507/560 (90%)	473 (93%)	29 (6%)	5 (1%)	19	65
2	B	396/454 (87%)	383 (97%)	11 (3%)	2 (0%)	34	77
All	All	903/1014 (89%)	856 (95%)	40 (4%)	7 (1%)	24	69

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	360	ALA
1	A	6	GLU
1	A	363	ASN
2	B	355	ALA
1	A	184	MET

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Mol	Chain	Res	Type
1	A	421	PRO
1	A	292	VAL

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	426/498 (86%)	415 (97%)	11 (3%)	54	81
2	B	344/411 (84%)	339 (98%)	5 (2%)	72	89
All	All	770/909 (85%)	754 (98%)	16 (2%)	61	85

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185	ASP
1	A	250	ASP
1	A	260	LEU
1	A	295	LEU
1	A	301	LEU
1	A	323	LYS
1	A	353	LYS
1	A	442	VAL
1	A	448	ARG
1	A	516	GLU
1	A	517	LEU
2	B	86	ASP
2	B	113	ASP
2	B	186	ASP
2	B	303	LEU
2	B	305	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	GLN
1	A	367	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	R	20/34 (58%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	519/560 (92%)	1.61	163 (31%)	1	2	167, 189, 198, 207	0
2	B	404/454 (88%)	1.31	109 (26%)	1	2	172, 189, 196, 201	0
3	D	21/29 (72%)	2.71	11 (52%)	0	2	187, 193, 197, 201	0
4	R	21/34 (61%)	2.69	14 (66%)	0	1	187, 192, 195, 198	0
All	All	965/1077 (89%)	1.53	297 (30%)	1	2	167, 189, 197, 207	0

All (297) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	20	DT	9.6
1	A	307	ARG	8.6
1	A	276	VAL	8.4
2	B	358	ARG	8.1
1	A	295	LEU	8.1
1	A	332	GLN	8.1
1	A	11	LYS	8.0
2	B	359	GLY	7.9
1	A	132	ILE	7.8
1	A	491	LEU	7.8
1	A	529	GLU	7.3
1	A	38	CYS	7.3
2	B	13	LYS	7.2
1	A	17	ASP	7.1
3	D	19	DT	7.1
1	A	492	GLU	7.0
2	B	56	TYR	6.9
2	B	105	SER	6.7
2	B	190	GLY	6.4
1	A	274	ILE	6.4
2	B	12	LEU	6.3

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Mol	Chain	Res	Type	RSRZ
1	A	472	THR	6.1
2	B	293	ILE	6.1
1	A	28	GLU	6.1
2	B	150	PRO	6.0
1	A	530	LYS	5.9
2	B	319	TYR	5.8
1	A	36	GLU	5.8
2	B	62	ALA	5.7
2	B	107	THR	5.7
1	A	177	ASP	5.6
1	A	456	GLY	5.5
1	A	296	THR	5.4
4	R	24	C	5.4
1	A	18	GLY	5.4
2	B	20	LYS	5.4
1	A	142	ILE	5.3
1	A	39	THR	5.2
1	A	229	TRP	5.2
1	A	128	THR	5.2
2	B	64	LYS	5.1
1	A	107	THR	5.0
1	A	6	GLU	5.0
1	A	485	ALA	4.9
1	A	155	GLY	4.8
1	A	502	ALA	4.7
1	A	85	GLN	4.6
1	A	224	GLU	4.6
1	A	225	PRO	4.6
1	A	211	ARG	4.6
2	B	69	THR	4.6
1	A	490	GLY	4.5
2	B	14	PRO	4.4
1	A	156	SER	4.4
1	A	45	GLY	4.4
2	B	44	GLU	4.4
1	A	275	LYS	4.4
1	A	303	LEU	4.3
2	B	294	PRO	4.3
4	R	14	U	4.3
1	A	540	LYS	4.3
1	A	290	THR	4.2
2	B	106	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	129	ALA	4.2
1	A	75	VAL	4.1
2	B	191	SER	4.1
1	A	37	ILE	4.1
1	A	455	ALA	4.0
2	B	192	ASP	4.0
1	A	240	THR	4.0
1	A	35	VAL	4.0
1	A	241	VAL	4.0
1	A	306	ASN	4.0
1	A	40	GLU	4.0
2	B	68	GLY	3.9
2	B	87	PHE	3.9
1	A	297	GLU	3.9
3	D	21	DA	3.9
1	A	333	GLY	3.8
2	B	91	GLN	3.8
4	R	25	A	3.8
1	A	484	LEU	3.8
1	A	88	TRP	3.8
3	D	3	DG	3.8
2	B	349	LEU	3.8
1	A	46	LYS	3.8
1	A	33	ALA	3.8
2	B	320	ASP	3.8
2	B	61	PHE	3.8
2	B	83	LYS	3.7
1	A	428	GLN	3.7
1	A	331	LYS	3.7
2	B	162	SER	3.7
1	A	318	TYR	3.7
1	A	245	VAL	3.7
1	A	537	PRO	3.7
2	B	383	TRP	3.7
1	A	29	GLU	3.7
2	B	248	GLU	3.7
2	B	184	MET	3.6
1	A	541	GLY	3.6
1	A	291	GLU	3.6
2	B	85	GLN	3.6
4	R	21	A	3.6
1	A	109	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
3	D	6	DC	3.6
1	A	348	ASN	3.5
1	A	53	GLU	3.5
2	B	84	THR	3.5
1	A	86	ASP	3.5
3	D	18	DG	3.4
1	A	222	GLN	3.4
2	B	104	LYS	3.4
2	B	65	LYS	3.4
4	R	19	A	3.4
1	A	512	GLN	3.4
1	A	145	GLN	3.4
2	B	328	GLU	3.4
1	A	212	TRP	3.4
2	B	243	PRO	3.4
2	B	412	PRO	3.3
1	A	130	PHE	3.3
2	B	213	GLY	3.3
4	R	22	G	3.3
2	B	51	GLY	3.3
1	A	235	HIS	3.3
3	D	17	DA	3.3
2	B	231	GLY	3.3
1	A	32	LYS	3.3
1	A	102	LYS	3.3
1	A	12	LEU	3.3
2	B	149	LEU	3.3
1	A	313	PRO	3.3
1	A	19	PRO	3.3
1	A	183	TYR	3.3
4	R	28	C	3.3
2	B	55	PRO	3.2
1	A	238	LYS	3.2
4	R	17	C	3.2
1	A	543	GLY	3.2
1	A	256	ASP	3.2
1	A	549	ASP	3.2
2	B	189	VAL	3.2
1	A	10	VAL	3.1
2	B	232	TYR	3.1
4	R	23	G	3.1
2	B	70	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	169	GLU	3.1
1	A	237	ASP	3.1
1	A	443	ASP	3.1
1	A	288	ALA	3.1
2	B	166	LYS	3.0
2	B	334	GLN	3.0
1	A	466	VAL	3.0
1	A	467	VAL	3.0
2	B	355	ALA	3.0
1	A	536	VAL	3.0
2	B	325	LEU	3.0
1	A	433	PRO	3.0
2	B	321	PRO	3.0
2	B	215	THR	3.0
1	A	170	PRO	3.0
1	A	287	LYS	3.0
2	B	292	VAL	2.9
1	A	239	TRP	2.9
1	A	215	THR	2.9
2	B	273	GLY	2.9
1	A	468	THR	2.9
1	A	141	GLY	2.9
2	B	208	HIS	2.9
1	A	23	GLN	2.9
2	B	193	LEU	2.9
2	B	288	ALA	2.8
1	A	50	ILE	2.8
2	B	274	ILE	2.8
2	B	86	ASP	2.8
2	B	78	ARG	2.8
1	A	178	ILE	2.8
2	B	425	LEU	2.8
1	A	203	GLU	2.8
2	B	289	LEU	2.8
1	A	198	HIS	2.8
1	A	513	SER	2.8
1	A	253	THR	2.7
3	D	7	DG	2.7
2	B	343	GLN	2.7
1	A	199	ARG	2.7
2	B	211	ARG	2.7
2	B	348	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	317	VAL	2.7
2	B	329	ILE	2.7
1	A	273	GLY	2.7
1	A	89	GLU	2.7
1	A	223	LYS	2.7
1	A	503	LEU	2.7
1	A	460	ASN	2.7
1	A	481	ALA	2.7
1	A	447	SER	2.7
2	B	25	PRO	2.6
1	A	355	ALA	2.6
1	A	230	MET	2.6
2	B	356	ARG	2.6
2	B	214	LEU	2.6
1	A	204	GLU	2.6
2	B	353	LYS	2.6
2	B	252	TRP	2.6
2	B	195	ILE	2.6
2	B	28	GLU	2.6
1	A	207	GLN	2.6
1	A	226	PRO	2.5
1	A	108	VAL	2.5
1	A	208	HIS	2.5
2	B	113	ASP	2.5
1	A	300	GLU	2.5
1	A	394	GLN	2.5
1	A	304	ALA	2.5
2	B	74	LEU	2.5
2	B	16	MET	2.5
2	B	75	VAL	2.4
2	B	123	ASP	2.4
1	A	200	THR	2.4
1	A	475	GLN	2.4
4	R	18	U	2.4
1	A	414	TRP	2.4
3	D	4	DG	2.4
4	R	32	C	2.4
4	R	30	A	2.4
1	A	59	PRO	2.4
4	R	29	G	2.4
1	A	91	GLN	2.4
1	A	148	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	40	GLU	2.4
2	B	354	TYR	2.4
3	D	9	DA	2.4
4	R	20	U	2.4
1	A	9	PRO	2.4
1	A	299	ALA	2.4
1	A	216	THR	2.4
1	A	171	PHE	2.3
1	A	172	ARG	2.3
1	A	342	TYR	2.3
2	B	196	GLY	2.3
1	A	269	GLN	2.3
2	B	403	THR	2.3
1	A	144	TYR	2.3
1	A	499	SER	2.3
2	B	247	PRO	2.3
2	B	11	LYS	2.3
2	B	182	GLN	2.3
1	A	279	LEU	2.3
1	A	311	LYS	2.3
1	A	462	GLY	2.3
1	A	473	THR	2.3
2	B	81	ASN	2.3
1	A	501	TYR	2.3
1	A	51	GLY	2.2
2	B	197	GLN	2.2
1	A	236	PRO	2.2
1	A	90	VAL	2.2
1	A	5	ILE	2.2
2	B	42	GLU	2.2
2	B	15	GLY	2.2
2	B	290	THR	2.2
1	A	480	GLN	2.2
2	B	194	GLU	2.2
2	B	26	LEU	2.2
2	B	404	GLU	2.2
1	A	341	ILE	2.2
1	A	149	LEU	2.2
2	B	185	ASP	2.2
2	B	306	ASN	2.1
1	A	362	THR	2.1
1	A	26	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	220	LYS	2.1
1	A	449	GLU	2.1
2	B	140	PRO	2.1
2	B	54	ASN	2.1
3	D	11	DG	2.1
1	A	278	GLN	2.1
2	B	428	GLN	2.1
2	B	98	ALA	2.1
1	A	31	ILE	2.1
1	A	181	TYR	2.1
2	B	49	LYS	2.1
2	B	60	VAL	2.1
1	A	450	THR	2.1
1	A	175	ASN	2.1
2	B	133	PRO	2.1
2	B	426	TRP	2.1
1	A	457	TYR	2.0
2	B	82	LYS	2.0
1	A	228	LEU	2.0
2	B	357	MET	2.0
2	B	108	VAL	2.0
1	A	146	TYR	2.0
2	B	210	LEU	2.0
2	B	180	ILE	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.