



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:53 PM GMT

PDB ID : 5E7I
Title : Crystal structure of the active catalytic core of the human DEAD-box protein DDX3
Authors : Floor, S.N.; Condon, K.J.; Doudna, J.A.
Deposited on : 2015-10-12
Resolution : 2.22 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 : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
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) : rb-20026982

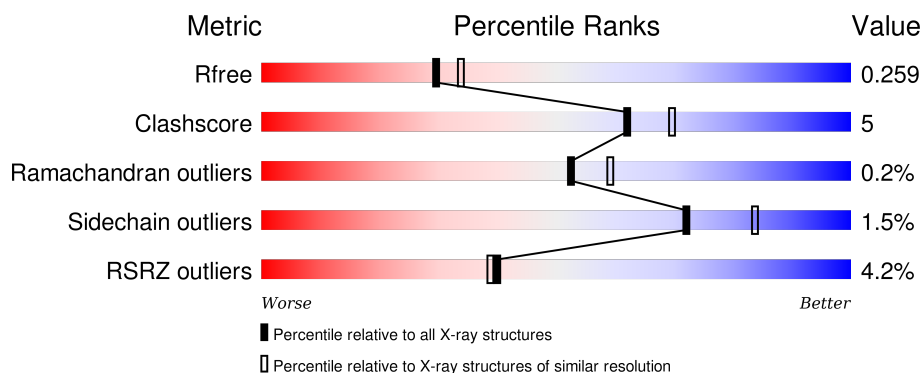
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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}	91344	4405 (2.24-2.20)
Clashscore	102246	5146 (2.24-2.20)
Ramachandran outliers	100387	5065 (2.24-2.20)
Sidechain outliers	100360	5066 (2.24-2.20)
RSRZ outliers	91569	4414 (2.24-2.20)

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	452	<div> <div>4%</div> <div>83% 12% 5%</div> </div>
1	B	452	<div> <div>3%</div> <div>81% 11% 8%</div> </div>
1	C	452	<div> <div>4%</div> <div>81% 13% 6%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 10060 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.

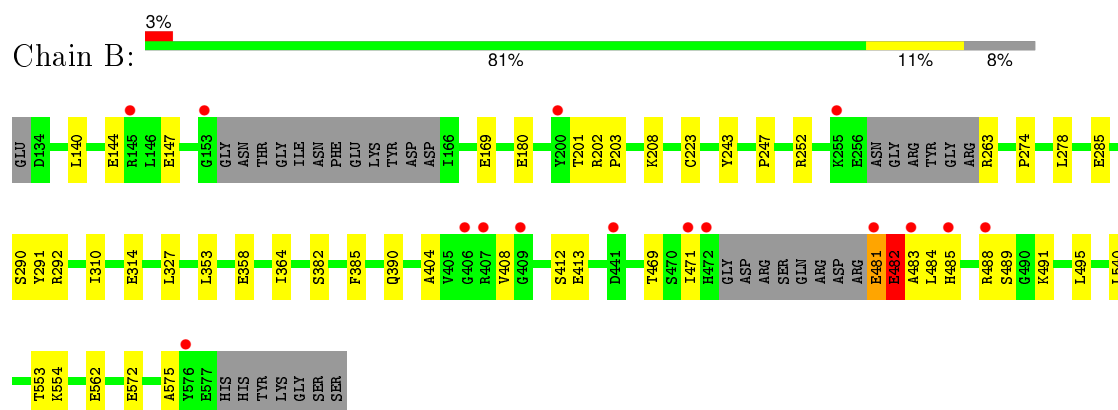
- Molecule 1 is a protein called ATP-dependent RNA helicase DDX3X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	418	Total	C	N	O	S	0	0	0
			3305	2092	570	624	19			
1	A	430	Total	C	N	O	S	0	0	0
			3404	2144	595	646	19			
1	C	424	Total	C	N	O	S	0	0	0
			3351	2113	586	633	19			

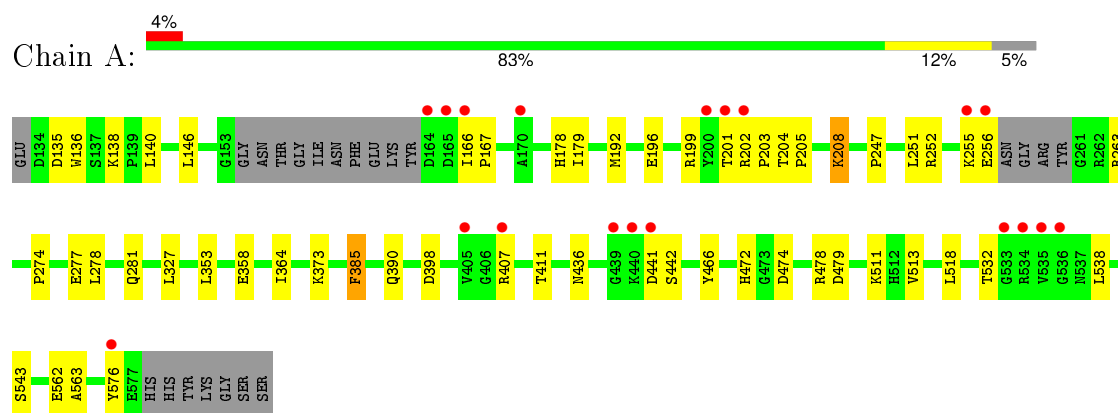
3 Residue-property plots

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.

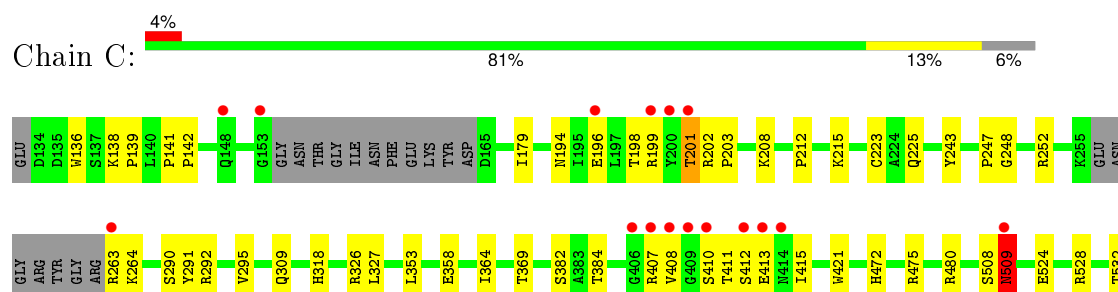
- Molecule 1: ATP-dependent RNA helicase DDX3X

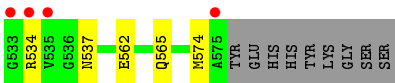


- Molecule 1: ATP-dependent RNA helicase DDX3X



- Molecule 1: ATP-dependent RNA helicase DDX3X





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.71Å 105.38Å 94.61Å 90.00° 114.54° 90.00°	Depositor
Resolution (Å)	86.06 – 2.22 86.06 – 2.22	Depositor EDS
% Data completeness (in resolution range)	97.9 (86.06-2.22) 97.9 (86.06-2.22)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 2.22Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.226 , 0.259 0.226 , 0.259	Depositor DCC
R_{free} test set	3984 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	32.8	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.6	EDS
Estimated twinning fraction	0.022 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 79703 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10060	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.27	0/3467	0.43	0/4681
1	B	0.29	1/3367 (0.0%)	0.46	0/4548
1	C	0.24	0/3413	0.42	0/4609
All	All	0.27	1/10247 (0.0%)	0.43	0/13838

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
1	B	0	1
1	C	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	482	GLU	CB-CG	-6.60	1.39	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	481	GLU	Peptide
1	C	508	SER	Peptide

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	3404	0	3394	33	0
1	B	3305	0	3306	39	0
1	C	3351	0	3353	39	0
All	All	10060	0	10053	108	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 5.

All (108) 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:436:ASN:ND2	1:A:466:TYR:OH	1.99	0.96
1:B:484:LEU:O	1:B:488:ARG:N	2.01	0.92
1:C:509:ASN:HD22	1:C:509:ASN:H	1.23	0.84
1:B:485:HIS:HA	1:B:488:ARG:HB2	1.58	0.84
1:B:481:GLU:HG3	1:B:482:GLU:N	1.97	0.80
1:C:534:ARG:HG3	1:C:537:ASN:HB3	1.65	0.76
1:A:513:VAL:HG23	1:A:532:THR:HG23	1.69	0.75
1:C:509:ASN:ND2	1:C:509:ASN:H	1.85	0.75
1:A:436:ASN:HD21	1:A:466:TYR:HH	1.33	0.74
1:A:442:SER:HA	1:A:511:LYS:HE3	1.72	0.70
1:B:572:GLU:OE2	1:C:202:ARG:NH1	2.25	0.69
1:B:223:CYS:HB3	1:B:408:VAL:HG11	1.73	0.69
1:A:251:LEU:O	1:A:255:LYS:HG2	1.93	0.68
1:B:180:GLU:O	1:B:202:ARG:NH1	2.27	0.68
1:C:179:ILE:HG23	1:C:212:PRO:HG3	1.78	0.65
1:B:489:SER:OG	1:B:491:LYS:HG2	1.97	0.64
1:B:482:GLU:C	1:B:484:LEU:H	2.00	0.62
1:B:469:THR:OG1	1:B:483:ALA:HB1	2.00	0.60
1:C:509:ASN:N	1:C:509:ASN:HD22	1.98	0.60
1:A:411:THR:HG21	1:A:563:ALA:HB2	1.83	0.59
1:C:225:GLN:HG3	1:C:407:ARG:HH21	1.67	0.59
1:A:274:PRO:HD2	1:A:278:LEU:HD23	1.84	0.59
1:A:201:THR:OG1	1:A:202:ARG:N	2.36	0.58
1:A:263:ARG:HH11	1:A:263:ARG:HG3	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:509:ASN:HA	1:C:534:ARG:HH12	1.67	0.58
1:A:353:LEU:HD22	1:A:358:GLU:HB2	1.85	0.58
1:B:482:GLU:CD	1:B:485:HIS:H	2.05	0.57
1:B:202:ARG:HH11	1:B:202:ARG:HG2	1.68	0.57
1:B:274:PRO:HD2	1:B:278:LEU:HD23	1.86	0.56
1:A:136:TRP:CZ2	1:A:247:PRO:HG3	2.41	0.56
1:C:309:GLN:OE1	1:C:326:ARG:NH1	2.39	0.55
1:B:201:THR:OG1	1:B:202:ARG:N	2.39	0.54
1:A:203:PRO:HG2	1:A:208:LYS:HG2	1.91	0.53
1:B:144:GLU:HA	1:B:147:GLU:HB2	1.91	0.52
1:A:478:ARG:NH1	1:A:479:ASP:OD1	2.43	0.52
1:A:277:GLU:O	1:A:281:GLN:HG3	2.10	0.52
1:C:421:TRP:HZ3	1:C:574:MET:HE1	1.75	0.51
1:B:327:LEU:HD23	1:B:364:ILE:HD13	1.92	0.51
1:B:353:LEU:HD22	1:B:358:GLU:HB2	1.93	0.51
1:B:169:GLU:HG2	1:B:404:ALA:HB3	1.93	0.51
1:A:327:LEU:HD23	1:A:364:ILE:HD13	1.92	0.51
1:C:415:ILE:HD12	1:C:532:THR:HG23	1.94	0.49
1:B:481:GLU:HG3	1:B:482:GLU:C	2.33	0.49
1:C:411:THR:O	1:C:413:GLU:HG3	2.12	0.48
1:C:509:ASN:HA	1:C:534:ARG:NH1	2.28	0.48
1:B:482:GLU:OE1	1:B:485:HIS:N	2.21	0.48
1:B:223:CYS:HA	1:B:382:SER:O	2.13	0.48
1:B:471:ILE:HD12	1:B:495:LEU:HD11	1.95	0.48
1:C:291:TYR:CZ	1:C:292:ARG:HG3	2.49	0.47
1:C:203:PRO:HB2	1:C:208:LYS:HG2	1.94	0.47
1:C:327:LEU:HD23	1:C:364:ILE:HD13	1.96	0.47
1:C:248:GLY:O	1:C:252:ARG:HG3	2.14	0.47
1:C:353:LEU:HD22	1:C:358:GLU:HB2	1.95	0.47
1:A:204:THR:O	1:A:208:LYS:HG3	2.14	0.47
1:A:385:PHE:CE2	1:A:390:GLN:HG2	2.49	0.47
1:B:485:HIS:CE1	1:B:488:ARG:CZ	2.98	0.47
1:C:136:TRP:CE2	1:C:247:PRO:HG3	2.50	0.47
1:B:247:PRO:HG2	1:B:252:ARG:HG3	1.96	0.46
1:A:256:GLU:OE1	1:A:256:GLU:N	2.48	0.46
1:B:243:TYR:OH	1:B:290:SER:HA	2.15	0.46
1:B:202:ARG:HG2	1:B:202:ARG:NH1	2.30	0.46
1:A:192:MET:O	1:A:196:GLU:HG2	2.15	0.46
1:C:472:HIS:CE1	1:C:475:ARG:HG2	2.51	0.46
1:B:482:GLU:OE2	1:B:484:LEU:HB2	2.16	0.46
1:B:482:GLU:CD	1:B:485:HIS:ND1	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:HIS:HD2	1:A:179:ILE:O	1.99	0.45
1:C:243:TYR:OH	1:C:290:SER:HA	2.17	0.45
1:A:441:ASP:OD1	1:A:441:ASP:N	2.49	0.45
1:A:518:LEU:HD21	1:A:543:SER:HB3	1.99	0.45
1:B:469:THR:HG21	1:B:483:ALA:O	2.17	0.45
1:C:215:LYS:HA	1:C:215:LYS:HD2	1.70	0.45
1:B:310:ILE:O	1:B:314:GLU:HG3	2.16	0.44
1:A:255:LYS:N	1:A:256:GLU:OE1	2.50	0.44
1:B:412:SER:O	1:B:413:GLU:HB3	2.17	0.44
1:B:553:THR:HG22	1:B:575:ALA:HB2	2.00	0.44
1:B:554:LYS:HG2	1:C:201:THR:HB	1.99	0.44
1:B:562:GLU:HG2	1:C:208:LYS:NZ	2.33	0.44
1:C:141:PRO:HA	1:C:142:PRO:HD3	1.82	0.44
1:C:384:THR:HG21	1:C:412:SER:HA	2.00	0.43
1:B:203:PRO:HG2	1:B:208:LYS:HG2	2.00	0.43
1:A:407:ARG:HB3	1:A:407:ARG:HE	1.64	0.43
1:B:385:PHE:CE2	1:B:390:GLN:HG2	2.54	0.43
1:A:263:ARG:HG3	1:A:263:ARG:NH1	2.33	0.43
1:A:208:LYS:HG3	1:A:208:LYS:H	1.66	0.43
1:C:201:THR:OG1	1:C:202:ARG:HG2	2.19	0.43
1:B:481:GLU:HG3	1:B:482:GLU:H	1.79	0.43
1:C:475:ARG:O	1:C:480:ARG:NH1	2.51	0.43
1:C:263:ARG:HB2	1:C:264:LYS:H	1.57	0.43
1:A:135:ASP:OD2	1:A:138:LYS:HG2	2.19	0.43
1:C:524:GLU:OE2	1:C:528:ARG:NH2	2.53	0.42
1:C:410:SER:OG	1:C:562:GLU:OE2	2.37	0.42
1:B:291:TYR:CZ	1:B:292:ARG:HG3	2.54	0.42
1:A:472:HIS:CE1	1:A:474:ASP:HB2	2.54	0.42
1:A:247:PRO:HD2	1:A:252:ARG:NH1	2.34	0.42
1:B:481:GLU:O	1:B:482:GLU:HB2	2.15	0.42
1:C:194:ASN:O	1:C:198:THR:HG23	2.19	0.42
1:A:205:PRO:HA	1:A:208:LYS:NZ	2.35	0.42
1:C:252:ARG:HB3	1:C:252:ARG:HE	1.56	0.42
1:A:166:ILE:HA	1:A:167:PRO:HD3	1.70	0.42
1:C:534:ARG:CG	1:C:537:ASN:HB3	2.42	0.41
1:C:295:VAL:HG13	1:C:318:HIS:HB2	2.03	0.41
1:C:509:ASN:N	1:C:509:ASN:ND2	2.59	0.41
1:A:411:THR:HG23	1:A:562:GLU:OE1	2.21	0.41
1:B:147:GLU:HG3	1:B:291:TYR:CZ	2.56	0.41
1:C:223:CYS:HA	1:C:382:SER:O	2.20	0.41
1:C:415:ILE:O	1:C:565:GLN:NE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:LYS:HD2	1:A:398:ASP:HB2	2.03	0.41
1:C:138:LYS:HA	1:C:139:PRO:HD3	1.86	0.40

There are no symmetry-related clashes.

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	424/452 (94%)	415 (98%)	8 (2%)	1 (0%)	52	59
1	B	410/452 (91%)	401 (98%)	8 (2%)	1 (0%)	52	59
1	C	418/452 (92%)	407 (97%)	10 (2%)	1 (0%)	52	59
All	All	1252/1356 (92%)	1223 (98%)	26 (2%)	3 (0%)	52	59

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	482	GLU
1	C	509	ASN
1	A	199	ARG

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	372/390 (95%)	366 (98%)	6 (2%)	70	82
1	B	362/390 (93%)	358 (99%)	4 (1%)	80	89
1	C	367/390 (94%)	361 (98%)	6 (2%)	70	82
All	All	1101/1170 (94%)	1085 (98%)	16 (2%)	72	84

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

Mol	Chain	Res	Type
1	B	140	LEU
1	B	263	ARG
1	B	285	GLU
1	B	540	LEU
1	A	140	LEU
1	A	146	LEU
1	A	208	LYS
1	A	385	PHE
1	A	538	LEU
1	A	576	TYR
1	C	196	GLU
1	C	199	ARG
1	C	201	THR
1	C	369	THR
1	C	408	VAL
1	C	509	ASN

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	436	ASN
1	C	509	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	430/452 (95%)	0.10	19 (4%) 38 37	18, 40, 90, 150	0
1	B	418/452 (92%)	0.04	15 (3%) 46 45	21, 38, 88, 137	0
1	C	424/452 (93%)	0.11	20 (4%) 35 34	22, 41, 90, 129	0
All	All	1272/1356 (93%)	0.09	54 (4%) 40 39	18, 40, 90, 150	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	472	HIS	6.2
1	C	153	GLY	6.0
1	A	535	VAL	6.0
1	C	407	ARG	5.6
1	A	165	ASP	5.3
1	C	200	TYR	5.3
1	A	576	TYR	5.1
1	B	153	GLY	5.0
1	C	201	THR	4.8
1	A	255	LYS	4.7
1	A	534	ARG	4.0
1	C	414	ASN	4.0
1	A	166	ILE	3.8
1	B	485	HIS	3.8
1	A	200	TYR	3.5
1	C	408	VAL	3.5
1	C	535	VAL	3.5
1	A	256	GLU	3.5
1	B	145	ARG	3.5
1	C	412	SER	3.4
1	B	200	TYR	3.3
1	A	536	GLY	3.2
1	C	413	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	441	ASP	3.2
1	B	481	GLU	3.0
1	B	576	TYR	2.9
1	C	263	ARG	2.8
1	C	509	ASN	2.8
1	B	471	ILE	2.7
1	B	488	ARG	2.6
1	C	534	ARG	2.6
1	A	439	GLY	2.6
1	C	148	GLN	2.6
1	B	409	GLY	2.6
1	A	441	ASP	2.5
1	C	406	GLY	2.5
1	A	201	THR	2.5
1	A	170	ALA	2.5
1	B	255	LYS	2.5
1	C	409	GLY	2.5
1	B	483	ALA	2.5
1	B	407	ARG	2.4
1	A	405	VAL	2.3
1	C	196	GLU	2.3
1	A	202	ARG	2.3
1	A	164	ASP	2.3
1	C	533	GLY	2.2
1	C	575	ALA	2.2
1	A	533	GLY	2.2
1	B	406	GLY	2.2
1	A	440	LYS	2.1
1	C	410	SER	2.1
1	A	407	ARG	2.1
1	C	199	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

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.