



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 09:19 pm GMT

PDB ID : 3RC8
Title : Human Mitochondrial Helicase Suv3 in Complex with Short RNA Fragment
Authors : Dauter, Z.; Jedrzejczak, R.; Dauter, M.; Wang, J.; Szczesny, R.; Stepień, P.
Deposited on : 2011-03-30
Resolution : 2.90 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

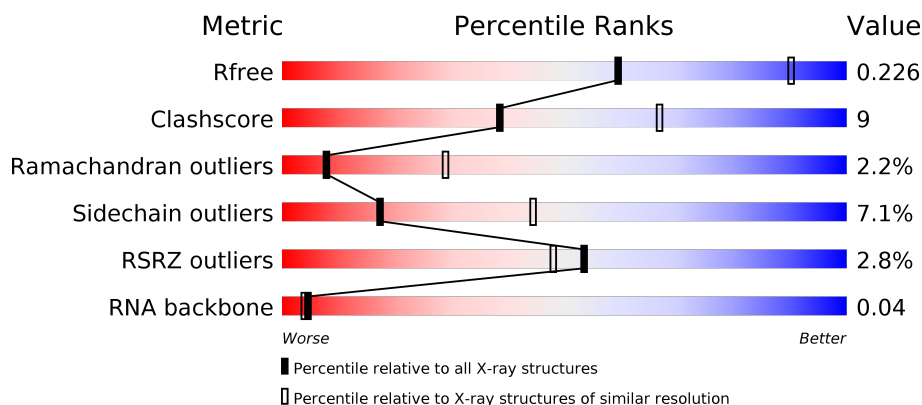
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)
RNA backbone	2435	1004 (3.20-2.60)

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	677	
2	E	6	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4975 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 SUPV3L1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	610	Total	C	N	O	S	0	0	0
			4868	3126	830	884	28			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	GLY	-	EXPRESSION TAG	UNP Q8IYB8

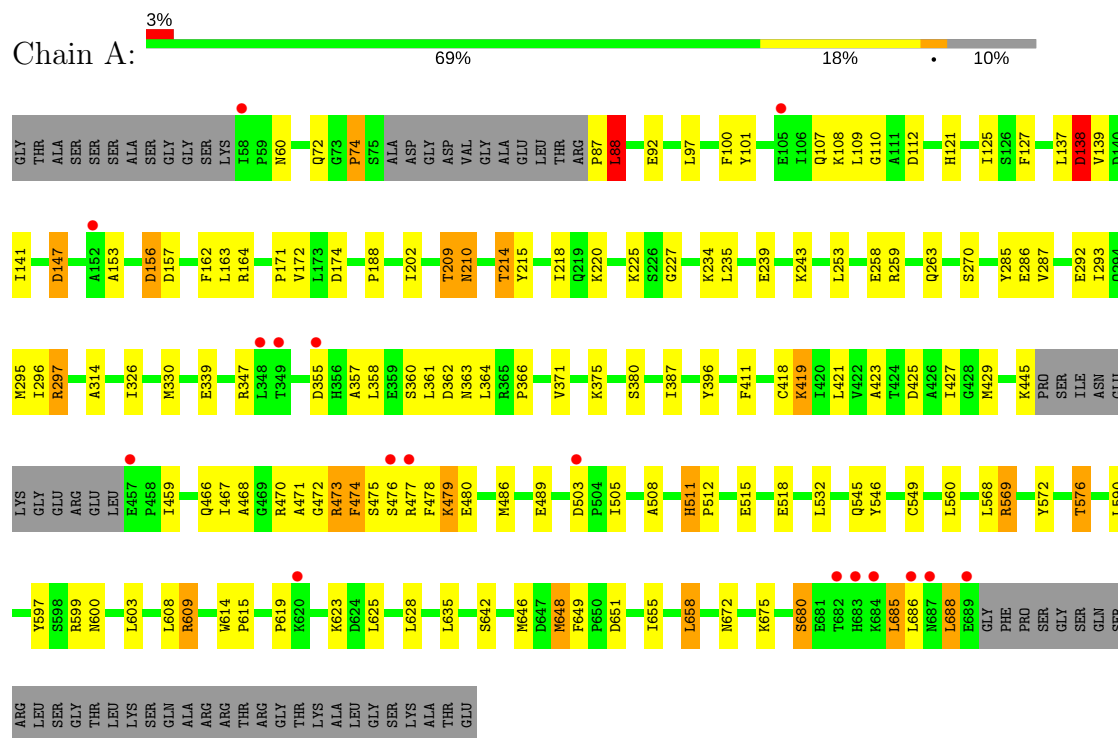
- Molecule 2 is a RNA chain called RNA fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	6	Total	C	N	O	P	0	0	0
			107	46	17	38	6			

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: ATP-dependent RNA helicase SUPV3L1, mitochondrial



- Molecule 2: RNA fragment



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	94.43Å 94.43Å 88.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.90 29.96 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-2.90) 100.0 (29.96-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.85 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.177 , 0.238 0.172 , 0.226	Depositor DCC
R_{free} test set	991 reflections (5.39%)	DCC
Wilson B-factor (Å ²)	61.8	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l 0.056 for h,-h-k,-l 0.033 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4975	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% 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

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	0.77	3/4980 (0.1%)	0.80	3/6747 (0.0%)
2	E	1.99	4/117 (3.4%)	2.65	16/180 (8.9%)
All	All	0.82	7/5097 (0.1%)	0.90	19/6927 (0.3%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	9	C	P-O5'	-10.34	1.49	1.59
2	E	9	C	P-OP1	6.74	1.60	1.49
1	A	515	GLU	CG-CD	5.77	1.60	1.51
1	A	339	GLU	CG-CD	5.65	1.60	1.51
1	A	549	CYS	CB-SG	5.51	1.91	1.82
2	E	5	C	C1'-N1	5.50	1.57	1.48
2	E	4	C	C1'-N1	5.23	1.56	1.48

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	5	C	O4'-C1'-N1	10.44	116.55	108.20
2	E	4	C	O4'-C1'-N1	9.15	115.52	108.20
2	E	6	G	C5'-C4'-O4'	6.93	117.42	109.10
2	E	9	C	OP1-P-OP2	-6.83	109.36	119.60
2	E	9	C	O5'-P-OP2	6.35	118.32	110.70
1	A	648	MET	CG-SD-CE	6.05	109.89	100.20
2	E	8	C	N3-C2-O2	-5.98	117.72	121.90
1	A	74	PRO	N-CA-CB	5.96	110.45	103.30
2	E	8	C	C5-C4-N4	5.89	124.33	120.20
2	E	6	G	O4'-C1'-N9	5.89	112.91	108.20
2	E	5	C	O4'-C4'-C3'	-5.71	98.29	104.00
2	E	4	C	N1-C2-O2	5.69	122.31	118.90
2	E	6	G	O4'-C4'-C3'	-5.65	98.35	104.00
1	A	88	LEU	CA-CB-CG	5.35	127.61	115.30
2	E	5	C	C6-N1-C2	-5.34	118.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	8	C	N3-C4-N4	-5.23	114.34	118.00
2	E	5	C	C5-C6-N1	5.22	123.61	121.00
2	E	7	C	O4'-C1'-N1	5.10	112.28	108.20
2	E	8	C	P-O5'-C5'	5.08	129.03	120.90

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	4868	0	4897	84	1
2	E	107	0	55	4	0
All	All	4975	0	4952	85	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 9.

All (85) 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:473:ARG:O	1:A:474:PHE:HB2	1.60	0.99
1:A:209:THR:HG21	1:A:466:GLN:HA	1.73	0.71
1:A:608:LEU:HD23	1:A:655:ILE:HD12	1.73	0.71
1:A:473:ARG:O	1:A:474:PHE:CB	2.40	0.68
1:A:87:PRO:O	1:A:88:LEU:HG	1.94	0.67
1:A:285:TYR:O	1:A:314:ALA:HA	1.99	0.63
1:A:380:SER:HB2	1:A:688:LEU:CB	2.30	0.62
1:A:188:PRO:HG2	1:A:546:TYR:CZ	2.35	0.61
1:A:225:LYS:HB2	1:A:286:GLU:OE1	2.01	0.61
1:A:572:TYR:O	1:A:576:THR:HG23	2.00	0.61
1:A:293:ILE:O	1:A:293:ILE:HG13	1.99	0.61
1:A:227:GLY:HA2	1:A:287:VAL:O	2.00	0.61
1:A:361:LEU:C	1:A:363:ASN:H	2.06	0.60
1:A:672:ASN:HB3	1:A:675:LYS:HD2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:ILE:O	1:A:470:ARG:HG2	2.02	0.59
1:A:609:ARG:HG2	1:A:614:TRP:HB3	1.83	0.58
1:A:121:HIS:CE1	1:A:125:ILE:HD11	2.38	0.58
1:A:380:SER:HB2	1:A:688:LEU:HB3	1.86	0.57
1:A:445:LYS:HE2	2:E:5:C:H6	1.68	0.56
1:A:418:CYS:O	1:A:419:LYS:HD2	2.04	0.56
1:A:614:TRP:CG	1:A:615:PRO:HA	2.40	0.55
1:A:658:LEU:HD12	1:A:658:LEU:O	2.06	0.55
1:A:479:LYS:O	1:A:480:GLU:HB2	2.10	0.51
1:A:380:SER:HB2	1:A:688:LEU:HB2	1.92	0.51
1:A:425:ASP:N	1:A:425:ASP:OD1	2.39	0.50
1:A:635:LEU:HD22	1:A:655:ILE:HG23	1.92	0.50
1:A:608:LEU:CD2	1:A:655:ILE:HD12	2.42	0.50
1:A:101:TYR:O	1:A:107:GLN:NE2	2.46	0.49
1:A:164:ARG:HH11	1:A:164:ARG:CB	2.26	0.48
1:A:97:LEU:O	1:A:100:PHE:HB3	2.13	0.48
2:E:5:C:H2'	2:E:6:G:H5'	1.95	0.48
1:A:371:VAL:HA	1:A:423:ALA:O	2.12	0.48
1:A:188:PRO:HG2	1:A:546:TYR:CE1	2.49	0.48
1:A:326:ILE:O	1:A:330:MET:HG2	2.14	0.48
1:A:375:LYS:HE3	1:A:396:TYR:CD1	2.49	0.47
1:A:347:ARG:NH2	1:A:471:ALA:O	2.47	0.47
1:A:511:HIS:HB2	1:A:512:PRO:HD2	1.96	0.47
1:A:164:ARG:HH11	1:A:164:ARG:HB3	1.80	0.47
1:A:292:GLU:HG3	1:A:429:MET:CE	2.43	0.47
1:A:202:ILE:HD12	1:A:202:ILE:N	2.31	0.46
1:A:259:ARG:HB2	1:A:259:ARG:HE	1.60	0.46
1:A:518:GLU:HA	1:A:568:LEU:HD22	1.96	0.46
1:A:599:ARG:O	1:A:600:ASN:C	2.52	0.46
1:A:60:ASN:OD1	1:A:60:ASN:C	2.53	0.46
1:A:361:LEU:HD22	1:A:364:LEU:HD11	1.98	0.46
1:A:138:ASP:O	1:A:141:ILE:HG22	2.16	0.45
1:A:253:LEU:HD23	1:A:258:GLU:HG2	1.98	0.45
1:A:569:ARG:HA	1:A:569:ARG:HD2	1.76	0.45
1:A:375:LYS:HB2	2:E:5:C:OP1	2.17	0.45
1:A:239:GLU:HG2	1:A:243:LYS:HE3	1.98	0.45
1:A:467:ILE:O	1:A:468:ALA:C	2.55	0.44
1:A:109:LEU:O	1:A:110:GLY:C	2.55	0.44
1:A:147:ASP:HB3	1:A:153:ALA:HB2	2.00	0.44
1:A:411:PHE:CD1	1:A:421:LEU:HB2	2.53	0.44
1:A:127:PHE:CD2	1:A:162:PHE:HD1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:THR:HG23	1:A:218:ILE:HG12	1.99	0.43
1:A:608:LEU:HD21	1:A:635:LEU:CD2	2.49	0.43
1:A:476:SER:C	1:A:478:PHE:H	2.22	0.43
1:A:642:SER:HA	1:A:649:PHE:HB2	2.01	0.43
1:A:560:LEU:HD23	1:A:590:LEU:HD23	1.99	0.43
1:A:635:LEU:HA	1:A:635:LEU:HD23	1.81	0.43
1:A:518:GLU:HA	1:A:568:LEU:CD2	2.49	0.43
1:A:614:TRP:CD2	1:A:615:PRO:HA	2.54	0.43
1:A:295:MET:C	1:A:297:ARG:H	2.22	0.42
1:A:597:TYR:O	1:A:600:ASN:N	2.52	0.42
1:A:171:PRO:O	1:A:172:VAL:C	2.57	0.42
1:A:292:GLU:HG3	1:A:429:MET:HE1	2.00	0.42
1:A:532:LEU:HD23	1:A:532:LEU:HA	1.90	0.42
1:A:375:LYS:HE3	1:A:396:TYR:CG	2.55	0.42
1:A:361:LEU:C	1:A:363:ASN:N	2.72	0.42
1:A:366:PRO:HA	1:A:419:LYS:HB3	2.02	0.41
1:A:361:LEU:O	1:A:363:ASN:N	2.53	0.41
1:A:121:HIS:O	1:A:125:ILE:HG12	2.20	0.41
1:A:209:THR:O	1:A:210:ASN:CB	2.69	0.41
1:A:358:LEU:O	1:A:360:SER:N	2.48	0.41
1:A:109:LEU:O	1:A:112:ASP:N	2.53	0.41
1:A:651:ASP:O	1:A:655:ILE:HG12	2.21	0.41
1:A:296:ILE:HG12	1:A:508:ALA:HB1	2.02	0.41
1:A:427:ILE:C	1:A:429:MET:H	2.24	0.41
1:A:680:SER:O	1:A:685:LEU:N	2.54	0.41
1:A:137:LEU:O	1:A:138:ASP:C	2.59	0.41
1:A:459:ILE:HG13	1:A:459:ILE:O	2.19	0.41
1:A:445:LYS:HE2	2:E:5:C:C6	2.52	0.40
1:A:163:LEU:HD12	1:A:163:LEU:HA	1.81	0.40
1:A:619:PRO:HG3	1:A:628:LEU:HD12	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:GLU:OE2	1:A:215:TYR:OH[1_455]	2.16	0.04

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	604/677 (89%)	548 (91%)	43 (7%)	13 (2%)	8	29

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	88	LEU
1	A	362	ASP
1	A	474	PHE
1	A	475	SER
1	A	685	LEU
1	A	156	ASP
1	A	357	ALA
1	A	686	LEU
1	A	138	ASP
1	A	210	ASN
1	A	472	GLY
1	A	477	ARG
1	A	74	PRO

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	538/589 (91%)	500 (93%)	38 (7%)	17	44

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	108	LYS
1	A	138	ASP
1	A	139	VAL
1	A	147	ASP
1	A	156	ASP
1	A	157	ASP
1	A	174	ASP
1	A	209	THR
1	A	214	THR
1	A	220	LYS
1	A	234	LYS
1	A	235	LEU
1	A	263	GLN
1	A	270	SER
1	A	297	ARG
1	A	355	ASP
1	A	387	ILE
1	A	419	LYS
1	A	473	ARG
1	A	479	LYS
1	A	486	MET
1	A	489	GLU
1	A	503	ASP
1	A	505	ILE
1	A	511	HIS
1	A	545	GLN
1	A	569	ARG
1	A	576	THR
1	A	603	LEU
1	A	609	ARG
1	A	623	LYS
1	A	625	LEU
1	A	646	MET
1	A	648	MET
1	A	658	LEU
1	A	680	SER
1	A	688	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN

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Mol	Chain	Res	Type
1	A	129	ASN
1	A	133	GLN
1	A	135	HIS
1	A	268	GLN
1	A	466	GLN
1	A	545	GLN
1	A	667	GLN
1	A	671	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	E	4/6 (66%)	2 (50%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	E	5	C
2	E	8	C

There are no RNA pucker outliers to report.

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

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 ⓘ

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	610/677 (90%)	-0.22	17 (2%) 53 48	31, 61, 99, 146	0
2	E	6/6 (100%)	0.15	0 100 100	68, 79, 88, 104	0
All	All	616/683 (90%)	-0.22	17 (2%) 53 48	31, 61, 99, 146	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	689	GLU	5.6
1	A	477	ARG	3.6
1	A	684	LYS	3.3
1	A	683	HIS	3.3
1	A	457	GLU	3.1
1	A	152	ALA	2.9
1	A	355	ASP	2.7
1	A	476	SER	2.6
1	A	58	ILE	2.5
1	A	687	ASN	2.5
1	A	105	GLU	2.4
1	A	503	ASP	2.4
1	A	348	LEU	2.3
1	A	620	LYS	2.2
1	A	686	LEU	2.2
1	A	349	THR	2.1
1	A	682	THR	2.1

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.