Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:21 AM GMT

PDB ID	:	3EBE
Title	:	Crystal structure of xenopus laevis replication initiation factor MCM10 internal domain
Authors	:	Warren, E.M.; Eichman, B.F.
Deposited on	:	2008-08-27
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

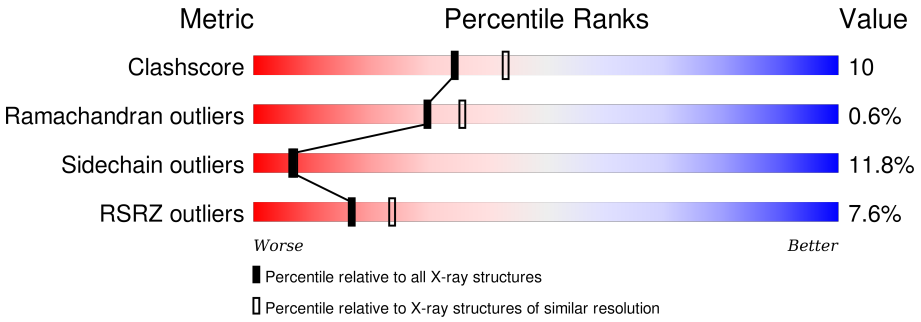
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 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))
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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 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	200	4% 69% 15% 14%
1	B	200	9% 62% 15% 6% 17%
1	C	200	7% 63% 22% 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4280 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 Protein MCM10 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	172	Total	C	N	O	S	0	1	0
			1383	876	244	253	10			
1	B	166	Total	C	N	O	S	0	0	0
			1337	844	236	247	10			
1	C	177	Total	C	N	O	S	0	2	0
			1408	890	248	260	10			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	228	GLY	-	EXPRESSION TAG	UNP Q5EAW4
A	229	PRO	-	EXPRESSION TAG	UNP Q5EAW4
B	228	GLY	-	EXPRESSION TAG	UNP Q5EAW4
B	229	PRO	-	EXPRESSION TAG	UNP Q5EAW4
C	228	GLY	-	EXPRESSION TAG	UNP Q5EAW4
C	229	PRO	-	EXPRESSION TAG	UNP Q5EAW4

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	58	Total	O	0	0
			58	58		

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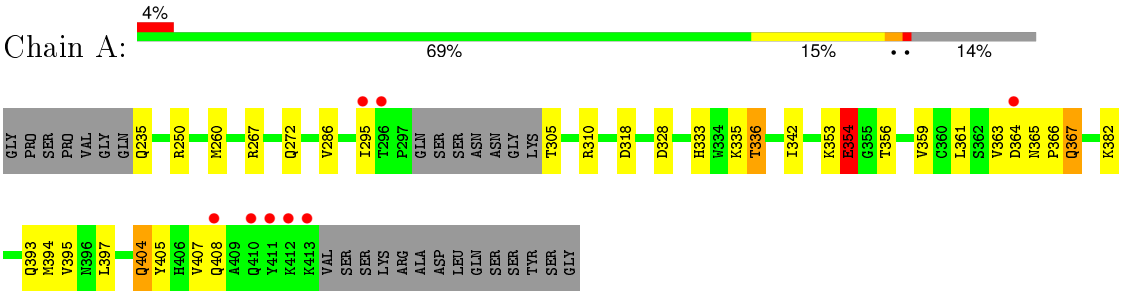
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	43	Total O 43 43	0	0
3	C	48	Total O 48 48	0	0

3 Residue-property plots (i)

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.

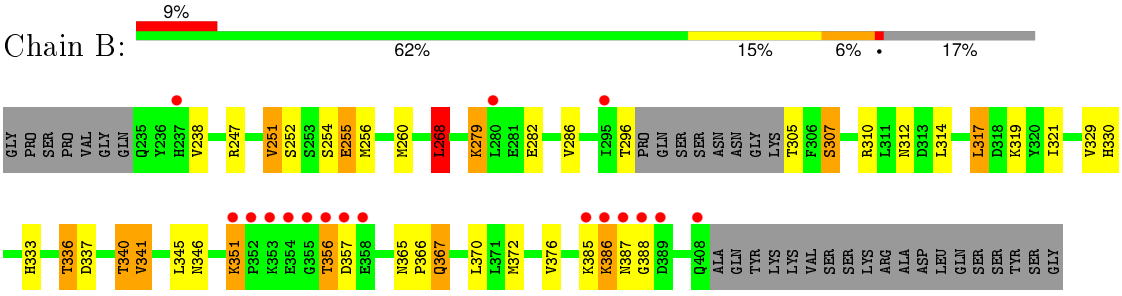
- Molecule 1: Protein MCM10 homolog

Chain A:



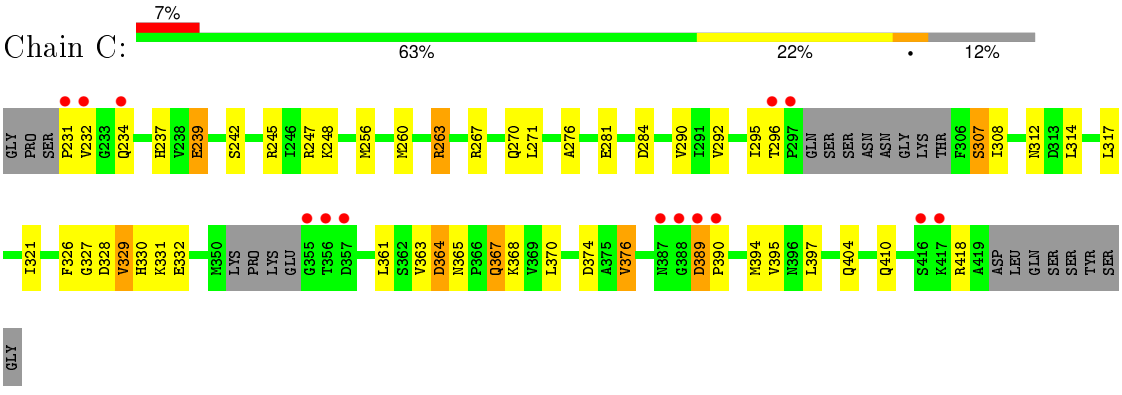
- Molecule 1: Protein MCM10 homolog

Chain B:



- Molecule 1: Protein MCM10 homolog

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	54.56Å 94.41Å 69.78Å 90.00° 112.79° 90.00°	Depositor
Resolution (Å)	44.40 – 2.30 44.40 – 2.28	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.40-2.30) 99.0 (44.40-2.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.44 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.202 , 0.247 0.206 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	41.9	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 50.2	EDS
Estimated twinning fraction	0.027 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 29404 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4280	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN

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	0.67	0/1407	0.76	0/1891
1	B	0.67	0/1359	0.81	1/1826 (0.1%)
1	C	0.64	0/1437	0.77	1/1932 (0.1%)
All	All	0.66	0/4203	0.78	2/5649 (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
1	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	268	LEU	CA-CB-CG	6.89	131.15	115.30
1	C	263	ARG	NE-CZ-NH2	-5.24	117.68	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	364	ASP	Peptide

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	1383	0	1392	23	0
1	B	1337	0	1352	32	0
1	C	1408	0	1408	33	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	58	0	0	0	0
3	B	43	0	0	0	0
3	C	48	0	0	2	0
All	All	4280	0	4152	83	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 10.

All (83) 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:B:356:THR:HB	1:B:357:ASP:CA	1.84	1.07
1:B:356:THR:CB	1:B:357:ASP:HA	1.85	1.05
1:A:393:GLN:NE2	1:A:405:TYR:HE2	1.58	1.02
1:B:337:ASP:O	1:B:340:THR:HG23	1.68	0.92
1:B:356:THR:HB	1:B:357:ASP:HA	0.92	0.90
1:A:393:GLN:NE2	1:A:405:TYR:CE2	2.48	0.76
1:A:359:VAL:HG12	1:A:361:LEU:CD1	2.16	0.75
1:C:312:ASN:ND2	1:C:314:LEU:H	1.84	0.75
1:B:367:GLN:HE21	1:B:367:GLN:HA	1.52	0.72
1:B:247:ARG:HB2	1:B:376:VAL:HG12	1.71	0.70
1:A:333:HIS:O	1:A:336:THR:CG2	2.39	0.70
1:B:247:ARG:HB2	1:B:376:VAL:CG1	2.21	0.70
1:A:367:GLN:O	1:A:367:GLN:HG3	1.91	0.70
1:B:307:SER:OG	1:B:330:HIS:HD2	1.74	0.70
1:C:321:ILE:HD12	1:C:361:LEU:HD12	1.73	0.70
1:C:326:PHE:O	1:C:329:VAL:HG13	1.93	0.69
1:B:333:HIS:O	1:B:336:THR:CG2	2.40	0.68
1:A:393:GLN:HE21	1:A:405:TYR:HE2	1.43	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237[A]:HIS:CE1	3:C:138:HOH:O	2.49	0.66
1:B:279:LYS:HG3	1:B:282:GLU:OE1	1.95	0.65
1:C:231:PRO:HB3	1:C:234:GLN:HB2	1.78	0.65
1:C:327:GLY:O	1:C:331:LYS:HG3	1.97	0.65
1:C:307:SER:OG	1:C:330:HIS:HD2	1.80	0.65
1:C:312:ASN:HD22	1:C:314:LEU:H	1.43	0.64
1:A:359:VAL:HG12	1:A:361:LEU:HD12	1.79	0.64
1:A:365:ASN:HD22	1:A:366:PRO:HD2	1.62	0.64
1:C:364:ASP:OD1	1:C:364:ASP:N	2.31	0.63
1:A:359:VAL:HG12	1:A:361:LEU:HD11	1.78	0.63
1:A:272:GLN:HE22	1:C:404:GLN:HE22	1.48	0.61
1:B:387:ASN:OD1	1:B:388:GLY:N	2.28	0.60
1:C:328:ASP:HA	1:C:331:LYS:HE2	1.83	0.60
1:A:333:HIS:O	1:A:336:THR:HG22	2.00	0.60
1:B:351:LYS:H	1:B:351:LYS:HE3	1.67	0.59
1:B:333:HIS:O	1:B:336:THR:HG23	2.02	0.59
1:B:312:ASN:HD22	1:B:314:LEU:H	1.50	0.59
1:B:268:LEU:HD13	1:B:321:ILE:HG23	1.86	0.57
1:A:333:HIS:O	1:A:336:THR:HG23	2.05	0.57
1:B:312:ASN:ND2	1:B:314:LEU:H	2.03	0.57
1:A:353:LYS:O	1:A:356:THR:HG22	2.05	0.57
1:B:365:ASN:HD22	1:B:366:PRO:HD2	1.68	0.57
1:B:286:VAL:HG13	1:B:345:LEU:HG	1.87	0.56
1:C:263:ARG:HD3	1:C:284:ASP:OD1	2.05	0.56
1:C:292:VAL:CG1	1:C:394:MET:HE1	2.36	0.56
1:C:295:ILE:HB	1:C:308:ILE:HB	1.87	0.56
1:B:385:LYS:O	1:B:387:ASN:O	2.24	0.54
1:C:247:ARG:HG2	1:C:248:LYS:HG3	1.90	0.54
1:B:307:SER:OG	1:B:330:HIS:CD2	2.59	0.52
1:B:251:VAL:HG23	1:B:255:GLU:HG2	1.91	0.52
1:B:333:HIS:O	1:B:336:THR:HG22	2.10	0.51
1:A:407:VAL:HG13	1:C:276:ALA:CB	2.41	0.51
1:C:365:ASN:OD1	1:C:367:GLN:HB2	2.10	0.51
1:B:386:LYS:HD2	1:B:387:ASN:N	2.24	0.51
1:C:237[A]:HIS:HE1	3:C:138:HOH:O	1.87	0.49
1:B:314:LEU:HA	1:B:317:LEU:HD13	1.94	0.48
1:A:272:GLN:NE2	1:C:404:GLN:HE22	2.12	0.48
1:A:260:MET:SD	1:A:286:VAL:HG11	2.54	0.48
1:B:365:ASN:HD22	1:B:366:PRO:CD	2.25	0.48
1:A:359:VAL:CG1	1:A:361:LEU:HD11	2.45	0.47
1:C:321:ILE:CD1	1:C:361:LEU:HD12	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:245:ARG:O	1:C:376:VAL:HG13	2.15	0.47
1:C:389:ASP:HB2	1:C:390:PRO:CD	2.44	0.47
1:B:341:VAL:HG22	1:B:372:MET:HB2	1.97	0.46
1:C:389:ASP:CB	1:C:390:PRO:CD	2.92	0.46
1:B:351:LYS:H	1:B:351:LYS:CE	2.28	0.46
1:C:365:ASN:HB3	1:C:368:LYS:HG3	1.98	0.46
1:A:310:ARG:HH21	1:A:310:ARG:HG3	1.82	0.45
1:C:329:VAL:HG21	1:C:363:VAL:HG23	1.97	0.45
1:A:354:GLU:CD	1:A:354:GLU:N	2.71	0.44
1:A:335:LYS:HD3	1:B:346:ASN:CG	2.39	0.43
1:A:250[B]:ARG:HH21	1:B:367:GLN:CD	2.21	0.43
1:B:256:MET:O	1:B:260:MET:HG2	2.18	0.43
1:B:365:ASN:HA	1:B:366:PRO:HD3	1.93	0.43
1:B:367:GLN:NE2	1:B:367:GLN:HA	2.29	0.42
1:A:342:ILE:HG13	1:A:342:ILE:O	2.18	0.42
1:C:296:THR:HG23	1:C:307:SER:HB3	2.02	0.41
1:C:231:PRO:CB	1:C:234:GLN:HB2	2.46	0.41
1:C:239:GLU:HG3	1:C:242:SER:OG	2.20	0.41
1:C:256:MET:O	1:C:260:MET:HG2	2.20	0.41
1:A:318:ASP:HB3	1:A:404:GLN:HE22	1.86	0.41
1:C:271:LEU:HD13	1:C:361:LEU:HD11	2.02	0.40
1:C:394:MET:HE2	1:C:394:MET:HB2	1.73	0.40
1:C:247:ARG:NH1	1:C:374:ASP:OD2	2.54	0.40
1:C:263:ARG:HD3	1:C:284:ASP:CG	2.42	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	168/200 (84%)	162 (96%)	5 (3%)	1 (1%)	30 36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	162/200 (81%)	157 (97%)	5 (3%)	0	100 100
1	C	172/200 (86%)	168 (98%)	2 (1%)	2 (1%)	16 16
All	All	502/600 (84%)	487 (97%)	12 (2%)	3 (1%)	30 36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	418	ARG
1	A	354	GLU
1	C	232	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	153/179 (86%)	138 (90%)	15 (10%)	10 11
1	B	150/179 (84%)	128 (85%)	22 (15%)	4 3
1	C	156/179 (87%)	139 (89%)	17 (11%)	8 9
All	All	459/537 (86%)	405 (88%)	54 (12%)	6 7

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	235	GLN
1	A	267	ARG
1	A	295	ILE
1	A	305	THR
1	A	328	ASP
1	A	336	THR
1	A	354	GLU
1	A	363	VAL
1	A	367	GLN
1	A	382	LYS
1	A	394	MET

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Mol	Chain	Res	Type
1	A	395	VAL
1	A	397	LEU
1	A	404	GLN
1	A	408	GLN
1	B	238	VAL
1	B	251	VAL
1	B	252	SER
1	B	254	SER
1	B	255	GLU
1	B	268	LEU
1	B	279	LYS
1	B	296	THR
1	B	305	THR
1	B	307	SER
1	B	310	ARG
1	B	317	LEU
1	B	319	LYS
1	B	329	VAL
1	B	336	THR
1	B	340	THR
1	B	341	VAL
1	B	351	LYS
1	B	356	THR
1	B	367	GLN
1	B	370	LEU
1	B	386	LYS
1	C	239	GLU
1	C	267	ARG
1	C	270	GLN
1	C	281	GLU
1	C	290	VAL
1	C	307	SER
1	C	317	LEU
1	C	329	VAL
1	C	332	GLU
1	C	364	ASP
1	C	367	GLN
1	C	370	LEU
1	C	376	VAL
1	C	389	ASP
1	C	395	VAL
1	C	397	LEU

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Mol	Chain	Res	Type
1	C	410	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	272	GLN
1	A	330	HIS
1	A	365	ASN
1	B	312	ASN
1	B	330	HIS
1	B	365	ASN
1	B	367	GLN
1	C	273	ASN
1	C	312	ASN
1	C	330	HIS
1	C	398	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

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

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

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	172/200 (86%)	0.33	8 (4%) 35 44	40, 52, 70, 77	7 (4%)
1	B	166/200 (83%)	0.60	17 (10%) 9 13	45, 56, 73, 82	3 (1%)
1	C	177/200 (88%)	0.64	14 (7%) 15 22	43, 56, 72, 79	7 (3%)
All	All	515/600 (85%)	0.52	39 (7%) 17 24	40, 54, 72, 82	17 (3%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	356	THR	14.1
1	B	355	GLY	7.9
1	C	231	PRO	6.9
1	B	356	THR	6.3
1	C	355	GLY	6.2
1	C	387	ASN	5.4
1	B	386	LYS	5.2
1	B	352	PRO	5.1
1	C	390	PRO	4.7
1	C	417	LYS	4.5
1	A	411	TYR	4.3
1	B	408	GLN	4.2
1	A	413	LYS	4.1
1	C	389	ASP	4.1
1	B	280	LEU	3.6
1	C	357	ASP	3.5
1	C	297	PRO	3.4
1	B	354	GLU	3.3
1	C	232	VAL	3.2
1	B	237	HIS	3.2
1	B	387	ASN	3.2
1	B	357	ASP	3.1
1	C	388	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	416	SER	3.0
1	A	364	ASP	2.8
1	B	385	LYS	2.8
1	A	296	THR	2.7
1	C	234	GLN	2.6
1	B	353	LYS	2.6
1	A	410	GLN	2.5
1	B	388	GLY	2.5
1	B	358	GLU	2.4
1	C	296	THR	2.4
1	A	412	LYS	2.3
1	B	295	ILE	2.3
1	B	389	ASP	2.1
1	A	408	GLN	2.1
1	A	295	ILE	2.1
1	B	351	LYS	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)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	ZN	B	501	1/1	1.00	0.13	-0.36	49,49,49,49	0
2	ZN	A	500	1/1	0.99	0.12	-0.84	41,41,41,41	0
2	ZN	C	502	1/1	1.00	0.10	-1.67	50,50,50,50	0

6.5 Other polymers (i)

There are no such residues in this entry.