Full wwPDB X-ray Structure Validation Report (i)

Mar 13, 2024 – 04:30 PM JST

PDB ID	:	5EWU
Title	:	Crystal structure of the Arabidopsis thaliana C-terminal Chlh at 1.25A
Authors	:	Chen, Z.; Zhang, X.; Liu, Y.; Jiang, L.
Deposited on	:	2015-11-21
Resolution	:	1.25 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

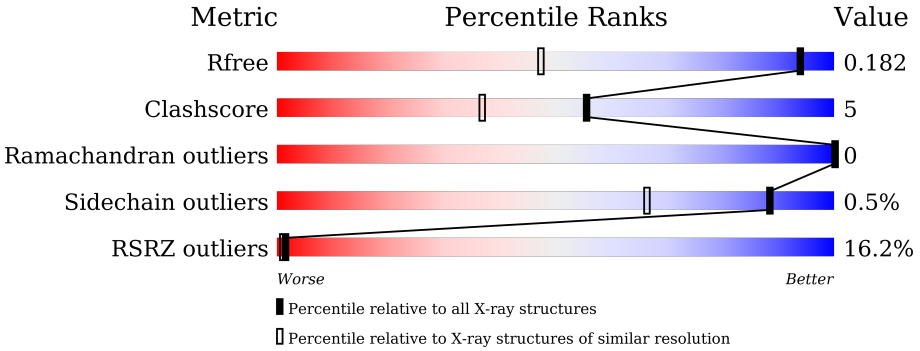
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.25 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	1023 (1.28-1.24)
Clashscore	141614	1060 (1.28-1.24)
Ramachandran outliers	138981	1029 (1.28-1.24)
Sidechain outliers	138945	1028 (1.28-1.24)
RSRZ outliers	127900	1004 (1.28-1.24)

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 of 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 <=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	388	11% 91% 7% •
1	B	388	21% 87% 10% • •

2 Entry composition (i)

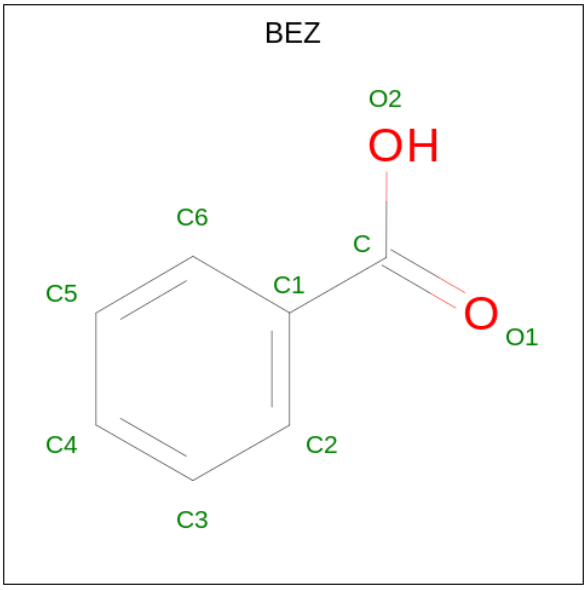
There are 4 unique types of molecules in this entry. The entry contains 7148 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Magnesium-chelatase subunit ChlH, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	383	3004	1896	504	588	16	0	9	0
1	B	377	2893	1823	490	566	14	0	2	0

- Molecule 2 is BENZOIC ACID (three-letter code: BEZ) (formula: $C_7H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	9	7	2	0	0
2	B	1	9	7	2	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	2	2	2	0	0
			Total	Mg		
3	B	3	3	3	0	0

- Molecule 4 is water.

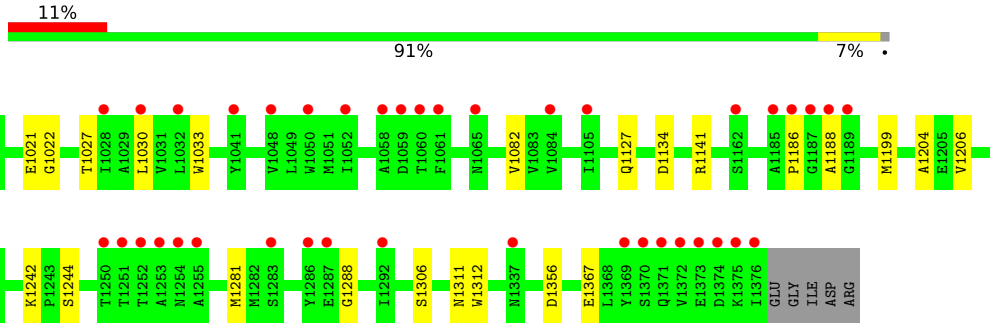
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	634	634	634	0	0
			Total	O		
4	B	594	594	594	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

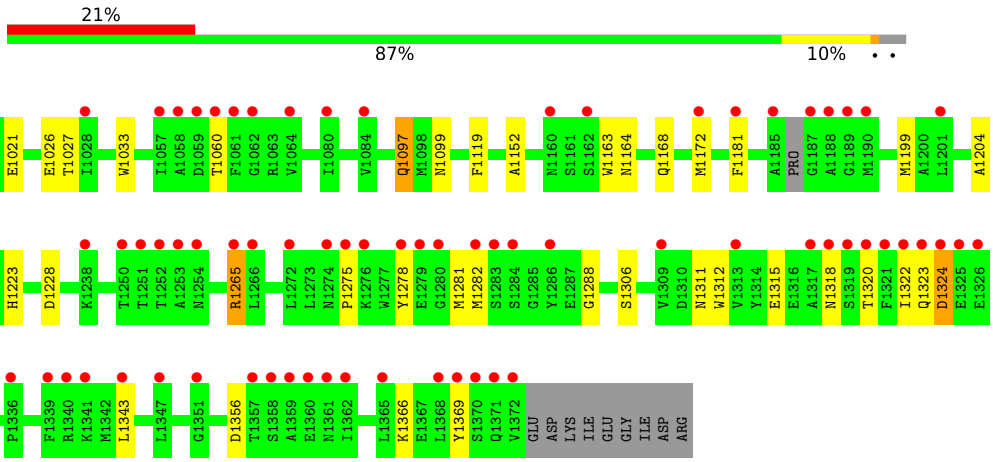
• Molecule 1: Magnesium-chelatase subunit ChlH, chloroplastic

Chain A:



• Molecule 1: Magnesium-chelatase subunit ChlH, chloroplastic

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	69.10Å 72.78Å 72.91Å 90.00° 109.76° 90.00°	Depositor
Resolution (Å)	50.00 – 1.25 27.16 – 1.25	Depositor EDS
% Data completeness (in resolution range)	89.8 (50.00-1.25) 89.7 (27.16-1.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 1.25Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.169 , 0.184 0.165 , 0.182	Depositor DCC
R_{free} test set	8309 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	11.6	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 64.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	7148	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.59% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.37	0/3080	0.56	0/4170
1	B	0.39	0/2947	0.60	2/3993 (0.1%)
All	All	0.38	0/6027	0.58	2/8163 (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	B	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	1199	MET	CG-SD-CE	-8.56	86.50	100.20
1	B	1324	ASP	N-CA-C	-7.01	92.08	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1323	GLN	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	3004	0	2925	21	1
1	B	2893	0	2786	38	1
2	A	9	0	5	1	0
2	B	9	0	5	0	0
3	A	2	0	0	0	0
3	B	3	0	0	0	0
4	A	634	0	0	6	1
4	B	594	0	0	13	0
All	All	7148	0	5721	59	2

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 (59) 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:1327:MET:HE3	4:B:1953:HOH:O	1.20	1.30
1:A:1082:VAL:HB	4:A:1784:HOH:O	1.65	0.93
1:A:1311:ASN:HD21	1:A:1356:ASP:H	1.09	0.93
1:B:1311:ASN:HD21	1:B:1356:ASP:H	1.11	0.92
1:B:1366:LYS:HA	4:B:1617:HOH:O	1.71	0.89
2:A:1401:BEZ:H2	4:A:1506:HOH:O	1.73	0.88
1:B:1164:ASN:H	1:B:1168:GLN:NE2	1.72	0.87
1:A:1186:PRO:HA	4:A:1505:HOH:O	1.77	0.83
1:B:1324:ASP:HB2	4:B:1503:HOH:O	1.85	0.75
1:A:1134:ASP:OD1	4:A:1501:HOH:O	2.04	0.74
1:B:1164:ASN:H	1:B:1168:GLN:HE22	1.35	0.73
1:A:1188:ALA:HB3	4:A:1887:HOH:O	1.89	0.71
1:B:1311:ASN:ND2	1:B:1356:ASP:H	1.89	0.70
1:B:1322:ILE:HD13	4:B:1506:HOH:O	1.93	0.67
1:B:1343:LEU:HD13	1:B:1369:TYR:HA	1.78	0.65
1:B:1324:ASP:CB	4:B:1503:HOH:O	2.44	0.63
1:A:1311:ASN:ND2	1:A:1356:ASP:H	1.89	0.63
1:A:1033:TRP:HE1	1:A:1209:GLN:HE21	1.49	0.60
1:B:1311:ASN:HD21	1:B:1356:ASP:N	1.92	0.59
1:B:1033:TRP:HE1	1:B:1209:GLN:HE21	1.48	0.58
1:B:1369:TYR:HB2	4:B:1617:HOH:O	2.06	0.56
1:B:1281:MET:O	1:B:1288:GLY:HA3	2.06	0.56
1:A:1231:ASN:HD21	1:A:1242:LYS:HZ2	1.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1324:ASP:O	1:B:1327:MET:HG2	2.08	0.54
1:B:1163:TRP:HA	1:B:1168:GLN:HE22	1.73	0.54
1:B:1278:TYR:O	1:B:1282:MET:HG2	2.09	0.52
1:B:995:ALA:N	4:B:1505:HOH:O	2.43	0.51
1:B:1327:MET:HE3	4:B:1804:HOH:O	2.11	0.51
1:A:1311:ASN:HD21	1:A:1356:ASP:N	1.93	0.51
1:B:1275:PRO:HA	1:B:1278:TYR:CZ	2.47	0.49
1:A:1033:TRP:HE1	1:A:1209:GLN:NE2	2.11	0.48
1:B:1033:TRP:HE1	1:B:1209:GLN:NE2	2.12	0.48
1:B:1315:GLU:HG3	4:B:1501:HOH:O	2.14	0.47
1:A:1027:THR:HB	1:A:1204:ALA:HA	1.96	0.47
1:B:1282:MET:HG3	4:B:1953:HOH:O	2.14	0.47
1:A:1312:TRP:CE2	1:B:1021:GLU:HG3	2.50	0.46
1:A:1017:LYS:HG2	1:A:1022:GLY:HA2	1.96	0.46
1:A:1281:MET:O	1:A:1288:GLY:HA3	2.16	0.46
1:B:1324:ASP:HB3	1:B:1327:MET:HG3	1.99	0.45
1:B:1327:MET:CE	4:B:1804:HOH:O	2.64	0.44
1:A:1231:ASN:ND2	1:A:1242:LYS:HZ2	2.16	0.43
1:A:1127:GLN:HA	1:A:1199:MET:HE1	2.01	0.43
1:A:1021:GLU:O	1:A:1021:GLU:HG3	2.19	0.42
1:B:1152:ALA:O	1:B:1172[B]:MET:HG2	2.19	0.42
1:B:1318:ASN:ND2	4:B:1502:HOH:O	2.39	0.42
1:B:1278:TYR:CE2	1:B:1320:THR:HG21	2.54	0.42
1:A:1030:LEU:HG	4:A:1784:HOH:O	2.19	0.42
1:B:1221:VAL:HG21	1:B:1223:HIS:CE1	2.54	0.41
1:B:1228:ASP:OD2	1:B:1306:SER:HB3	2.20	0.41
1:B:1265:ARG:HB2	1:B:1312:TRP:HZ2	1.84	0.41
1:B:1369:TYR:CB	4:B:1617:HOH:O	2.64	0.41
1:B:1097:GLN:HE21	1:B:1097:GLN:H	1.68	0.41
1:B:1026:GLU:HA	1:B:1119:PHE:CD2	2.56	0.41
1:A:1082:VAL:O	1:A:1141:ARG:HD2	2.20	0.41
1:B:1099:ASN:HD22	1:B:1181:PHE:HE1	1.67	0.41
1:A:1206:VAL:HA	1:A:1244:SER:O	2.21	0.41
1:B:1027:THR:HB	1:B:1204:ALA:HA	2.03	0.41
1:A:1228:ASP:OD2	1:A:1306:SER:HB3	2.21	0.40
1:B:1343:LEU:HD13	1:B:1369:TYR:CA	2.48	0.40

All (2) 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:B:1060:THR:O	1:B:1168:GLN:NE2[2_656]	2.08	0.12
1:A:1367:GLU:OE2	4:A:1501:HOH:O[1_455]	2.11	0.09

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	390/388 (100%)	384 (98%)	6 (2%)	0	100	100
1	B	375/388 (97%)	365 (97%)	10 (3%)	0	100	100
All	All	765/776 (99%)	749 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	321/337 (95%)	320 (100%)	1 (0%)	92	79
1	B	300/337 (89%)	298 (99%)	2 (1%)	84	57
All	All	621/674 (92%)	618 (100%)	3 (0%)	88	66

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1011	ARG
1	B	1097	GLN

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Mol	Chain	Res	Type
1	B	1265	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1097	GLN
1	A	1099	ASN
1	A	1209	GLN
1	A	1231	ASN
1	A	1311	ASN
1	A	1361	ASN
1	B	1020	ASN
1	B	1097	GLN
1	B	1099	ASN
1	B	1168	GLN
1	B	1209	GLN
1	B	1256	GLN
1	B	1311	ASN
1	B	1361	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 5 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
2	BEZ	A	1401	-	9,9,9	0.96	1 (11%)	11,11,11	1.45	2 (18%)
2	BEZ	B	1401	-	9,9,9	0.75	0	11,11,11	1.07	2 (18%)

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
2	BEZ	A	1401	-	-	0/4/4/4	0/1/1/1
2	BEZ	B	1401	-	-	0/4/4/4	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1401	BEZ	O2-C	-2.21	1.23	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1401	BEZ	O2-C-C1	3.25	123.29	114.85
2	A	1401	BEZ	O2-C-O1	-3.00	116.69	123.35
2	B	1401	BEZ	O2-C-C1	2.46	121.22	114.85
2	B	1401	BEZ	O2-C-O1	-2.23	118.41	123.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1401	BEZ	1	0

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 (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	383/388 (98%)	0.87	43 (11%)	5	3	6, 12, 24, 34	0
1	B	377/388 (97%)	1.28	80 (21%)	0	0	6, 15, 29, 37	10 (2%)
All	All	760/776 (97%)	1.07	123 (16%)	1	1	6, 13, 27, 37	10 (1%)

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1188	ALA	13.1
1	B	1061	PHE	11.1
1	B	1060	THR	10.7
1	A	1188	ALA	9.6
1	A	1060	THR	9.1
1	A	1186	PRO	8.6
1	A	1187	GLY	8.4
1	B	1365	LEU	7.6
1	B	1189	GLY	7.5
1	B	1187	GLY	7.4
1	A	1376	ILE	7.1
1	A	1252	THR	6.8
1	A	1018	LEU	6.6
1	B	1185	ALA	6.5
1	A	1253	ALA	6.2
1	B	1275	PRO	6.2
1	B	1322	ILE	6.0
1	A	1254	ASN	5.9
1	A	1255	ALA	5.8
1	B	1328	LEU	5.5
1	B	1190	MET	5.5
1	A	1374	ASP	5.5
1	B	1329	ASN	5.4
1	B	1347	LEU	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	1185	ALA	5.2
1	B	1181	PHE	5.1
1	B	1018	LEU	5.0
1	B	1057	ILE	5.0
1	B	1253	ALA	5.0
1	B	1286	TYR	4.9
1	B	1058	ALA	4.8
1	A	1061	PHE	4.8
1	B	1283	SER	4.8
1	A	1372	VAL	4.8
1	A	1250	THR	4.7
1	B	1280	GLY	4.7
1	B	1372	VAL	4.6
1	B	1359	ALA	4.6
1	B	1327	MET	4.5
1	B	1252	THR	4.5
1	B	1278	TYR	4.4
1	B	1162	SER	4.4
1	B	1282	MET	4.4
1	B	1339	PHE	4.3
1	A	1251	THR	4.3
1	A	1373	GLU	4.2
1	B	1062	GLY	4.0
1	B	995	ALA	3.9
1	B	1238	LYS	3.9
1	A	1041	TYR	3.9
1	A	1375	LYS	3.9
1	A	1369	TYR	3.7
1	B	1360	GLU	3.7
1	B	1059	ASP	3.7
1	B	1276	LYS	3.6
1	B	1320	THR	3.5
1	B	1369	TYR	3.5
1	B	1370	SER	3.4
1	B	1279	GLU	3.4
1	A	995	ALA	3.4
1	B	1251	THR	3.4
1	A	1337	ASN	3.3
1	B	1326	GLU	3.2
1	A	1189	GLY	3.2
1	B	1254	ASN	3.2
1	B	1317	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	1323	GLN	3.2
1	B	1357	THR	3.2
1	B	1265	ARG	3.1
1	B	1343	LEU	3.0
1	B	1358	SER	3.0
1	B	1336	PRO	3.0
1	B	1319	SER	3.0
1	B	1019	GLU	3.0
1	A	994	GLN	2.8
1	B	1160	ASN	2.7
1	B	1362	ILE	2.7
1	B	1064	VAL	2.7
1	A	1286	TYR	2.7
1	B	1321	PHE	2.7
1	B	1250	THR	2.6
1	A	1058	ALA	2.6
1	A	1105	ILE	2.6
1	B	1080	ILE	2.6
1	B	1272	LEU	2.6
1	A	1065	ASN	2.5
1	B	1331	LEU	2.5
1	B	1341	LYS	2.5
1	B	1266	LEU	2.5
1	A	1028	ILE	2.5
1	B	1028	ILE	2.5
1	B	1284	SER	2.5
1	A	1048	VAL	2.5
1	A	1052	ILE	2.5
1	B	1274	ASN	2.4
1	A	1370	SER	2.4
1	B	1325	GLU	2.4
1	B	1332	MET	2.4
1	A	1030	LEU	2.4
1	A	1162	SER	2.4
1	B	1084	VAL	2.3
1	A	1292	ILE	2.3
1	B	1371	GLN	2.3
1	B	1368	LEU	2.3
1	A	1283	SER	2.3
1	A	1059	ASP	2.2
1	A	1287	GLU	2.2
1	A	1050[A]	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	1351	GLY	2.2
1	B	1340	ARG	2.2
1	B	1214	SER	2.2
1	B	1361	ASN	2.2
1	B	1318	ASN	2.2
1	A	1371	GLN	2.2
1	B	1172[A]	MET	2.2
1	B	1324	ASP	2.1
1	A	1238	LYS	2.1
1	B	1309	VAL	2.1
1	A	1032	LEU	2.0
1	B	1201	LEU	2.0
1	A	1084	VAL	2.0
1	B	1313	VAL	2.0
1	B	996	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 monosaccharides 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(Å^2)	Q<0.9
2	BEZ	A	1401	9/9	0.92	0.12	14,14,16,16	0
2	BEZ	B	1401	9/9	0.94	0.12	11,14,15,16	0
3	MG	B	1402	1/1	0.98	0.18	24,24,24,24	0
3	MG	A	1402	1/1	0.99	0.23	23,23,23,23	0
3	MG	B	1404	1/1	0.99	0.08	22,22,22,22	0
3	MG	B	1403	1/1	1.00	0.15	10,10,10,10	0
3	MG	A	1403	1/1	1.00	0.13	11,11,11,11	0

6.5 Other polymers (i)

There are no such residues in this entry.