Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:15 PM GMT

PDB ID	:	3TE5
Title	:	structure of the regulatory fragment of sacchromyces cerevisiae ampk in complex with NADH
Authors	:	Mayer, F.V.; Heath, R.; Underwood, E.; Sanders, M.J.; Carmena, D.; McCartney, R.; Leiper, F.C.; Xiao, B.; Jing, C.; Walker, P.A.; Haire, L.F.; Ogrodowicz, R.; Martin, S.R.; Schmidt, M.C.; Gamblin, S.J.; Carling, D.
Deposited on	:	2011-08-12
Resolution	:	2.50 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:

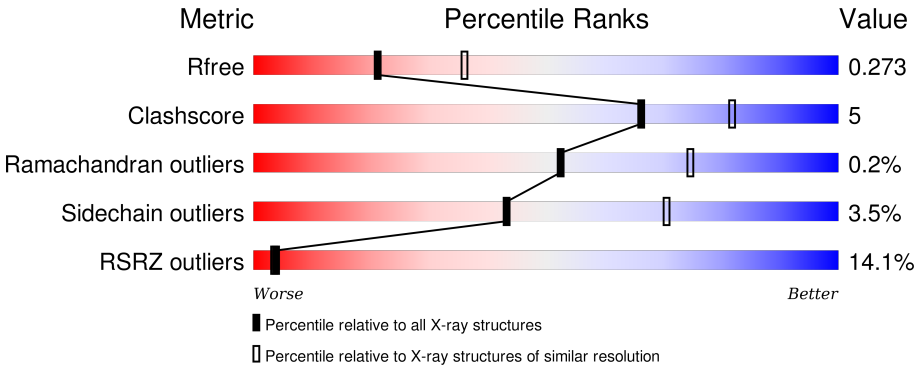
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	179	14% 68% 9% 23%
2	B	113	30% 82% 8% • 9%
3	C	323	6% 83% 12% • •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4623 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 Carbon catabolite-derepressing protein kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	138	Total	C	N	O	S	0	0	0
			1102	722	184	191	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	455	GLY	-	EXPRESSION TAG	UNP P06782
A	456	PRO	-	EXPRESSION TAG	UNP P06782

- Molecule 2 is a protein called SNF1 protein kinase subunit beta-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	103	Total	C	N	O	S	0	0	0
			825	536	133	154	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	303	MET	-	EXPRESSION TAG	UNP P34164

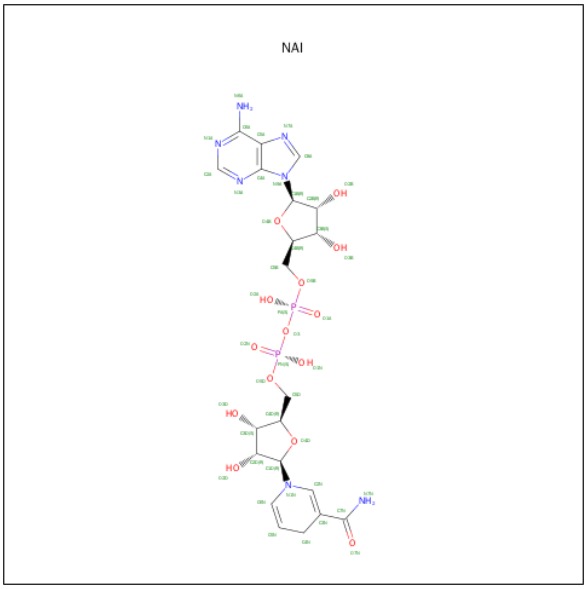
- Molecule 3 is a protein called Nuclear protein SNF4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	313	Total	C	N	O	S	0	0	0
			2438	1555	412	461	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	EXPRESSION TAG	UNP P12904
C	2	ALA	-	EXPRESSION TAG	UNP P12904

- Molecule 4 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 5 is water.

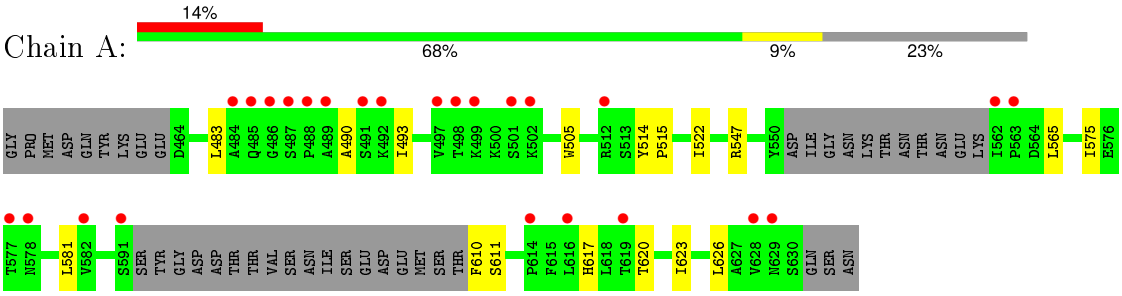
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	38	Total	O	0	0
			38	38		
5	B	40	Total	O	0	0
			40	40		
5	C	136	Total	O	0	0
			136	136		

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.

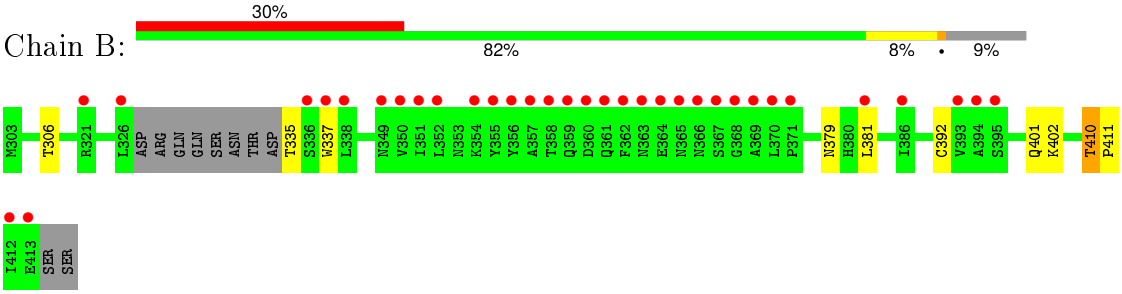
- Molecule 1: Carbon catabolite-derepressing protein kinase

Chain A:



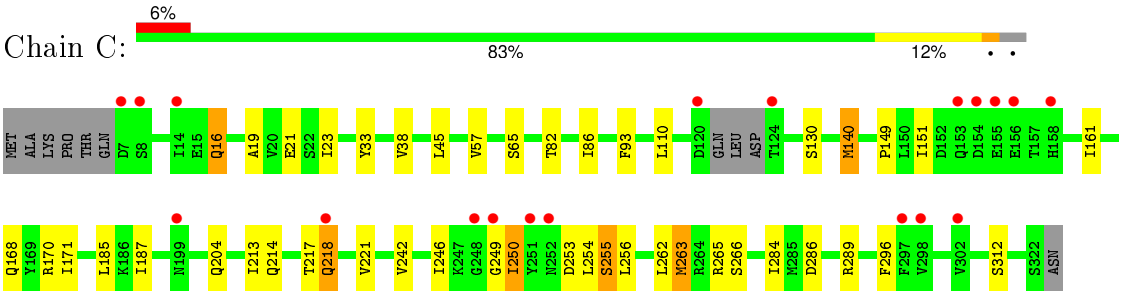
- Molecule 2: SNF1 protein kinase subunit beta-2

Chain B:



- Molecule 3: Nuclear protein SNF4

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	95.73Å 240.24Å 79.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.50 24.71 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (25.00-2.50) 99.9 (24.71-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.96 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.241 , 0.281 0.234 , 0.273	Depositor DCC
R_{free} test set	1617 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	48.1	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 44.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 31944 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4623	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% 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: NAI

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	0.33	0/1131	0.47	0/1533
2	B	0.36	0/848	0.52	0/1167
3	C	0.36	0/2472	0.53	0/3353
All	All	0.35	0/4451	0.51	0/6053

There are no bond length outliers.

There are no bond angle outliers.

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	1102	0	1113	14	0
2	B	825	0	807	7	0
3	C	2438	0	2487	30	0
4	C	44	0	27	3	0
5	A	38	0	0	1	0
5	B	40	0	0	0	0
5	C	136	0	0	2	0
All	All	4623	0	4434	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 5.

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)
3:C:16:GLN:HG3	3:C:187:ILE:HG13	1.72	0.71
3:C:242:VAL:O	3:C:246:ILE:HG22	1.98	0.63
3:C:93:PHE:HD1	3:C:254:LEU:HD13	1.64	0.62
1:A:611:SER:HB2	3:C:161:ILE:CG2	2.35	0.56
3:C:250:ILE:CG2	3:C:253:ASP:HB2	2.37	0.54
3:C:253:ASP:HA	3:C:256:LEU:HD13	1.91	0.52
1:A:505:TRP:HH2	2:B:392:CYS:HG	1.58	0.52
3:C:93:PHE:CD1	3:C:254:LEU:HD13	2.45	0.52
1:A:575:ILE:HD11	1:A:581:LEU:HB2	1.93	0.51
3:C:16:GLN:HG2	3:C:185:LEU:HA	1.93	0.51
2:B:402:LYS:HD2	3:C:38:VAL:HA	1.94	0.50
3:C:82:THR:O	3:C:86:ILE:HG12	2.12	0.49
2:B:335:THR:HG23	2:B:337:TRP:CD1	2.47	0.49
3:C:149:PRO:HB2	3:C:151:ILE:CD1	2.42	0.49
3:C:250:ILE:HG23	3:C:253:ASP:HB2	1.94	0.49
3:C:19:ALA:O	3:C:23:ILE:HG12	2.12	0.49
1:A:483:LEU:HG	1:A:490:ALA:HB1	1.94	0.49
2:B:410:THR:HG22	2:B:411:PRO:HD2	1.96	0.48
3:C:140:MET:HE1	3:C:171:ILE:HD12	1.96	0.48
1:A:493:ILE:CG2	3:C:263:MET:HB2	2.45	0.47
3:C:214:GLN:O	3:C:218:GLN:HB2	2.14	0.47
1:A:610:PHE:N	5:A:38:HOH:O	2.47	0.47
1:A:623:ILE:HD11	2:B:381:LEU:HD21	1.98	0.46
3:C:286:ASP:OD1	3:C:289:ARG:NH2	2.46	0.46
2:B:402:LYS:HG2	3:C:33:TYR:CE1	2.51	0.45
1:A:610:PHE:HZ	2:B:379:ASN:OD1	2.00	0.45
3:C:246:ILE:HA	5:C:435:HOH:O	2.17	0.45
1:A:522:ILE:HA	1:A:626:LEU:HD21	1.99	0.45
1:A:547:ARG:HG2	1:A:565:LEU:HB3	1.99	0.44
3:C:284:ILE:HG23	3:C:296:PHE:CE2	2.53	0.44
1:A:617:HIS:O	1:A:620:THR:HB	2.18	0.44
3:C:16:GLN:NE2	5:C:409:HOH:O	2.51	0.44
1:A:514:TYR:HB3	1:A:515:PRO:HD2	1.99	0.43
3:C:168:GLN:HE22	3:C:312:SER:HB3	1.82	0.43
1:A:611:SER:HB2	3:C:161:ILE:HG21	2.01	0.43
1:A:611:SER:HB2	3:C:161:ILE:HG22	2.01	0.42
3:C:254:LEU:HD12	3:C:255:SER:N	2.35	0.41
3:C:312:SER:HB3	4:C:324:NAI:H52N	2.02	0.41
3:C:221:VAL:HG12	4:C:324:NAI:H51A	2.02	0.41
3:C:86:ILE:HG23	3:C:213:ILE:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:324:NAI:O2A	4:C:324:NAI:H8A	2.20	0.41
3:C:262:LEU:O	3:C:265:ARG:HB2	2.20	0.41
3:C:45:LEU:HD21	3:C:57:VAL:HG11	2.03	0.41

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	132/179 (74%)	128 (97%)	4 (3%)	0	100	100
2	B	99/113 (88%)	96 (97%)	3 (3%)	0	100	100
3	C	309/323 (96%)	303 (98%)	5 (2%)	1 (0%)	46	68
All	All	540/615 (88%)	527 (98%)	12 (2%)	1 (0%)	52	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	249	GLY

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	119/162 (74%)	119 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	94/108 (87%)	91 (97%)	3 (3%)	46 74
3	C	277/297 (93%)	263 (95%)	14 (5%)	29 52
All	All	490/567 (86%)	473 (96%)	17 (4%)	43 70

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	306	THR
2	B	401	GLN
2	B	410	THR
3	C	16	GLN
3	C	21	GLU
3	C	65	SER
3	C	110	LEU
3	C	130	SER
3	C	140	MET
3	C	170	ARG
3	C	204	GLN
3	C	217	THR
3	C	218	GLN
3	C	250	ILE
3	C	255	SER
3	C	263	MET
3	C	266	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	485	GLN
2	B	359	GLN
3	C	168	GLN
3	C	178	ASN
3	C	183	HIS

5.3.3 RNA

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

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	$\#\|Z\| > 2$
4	NAI	C	324	-	38,48,48	1.70	7 (18%)	48,73,73	2.55	6 (12%)

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
4	NAI	C	324	-	-	0/25/72/72	0/5/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	324	NAI	C4N-C5N	-4.03	1.40	1.49
4	C	324	NAI	C5A-C4A	-2.72	1.34	1.40
4	C	324	NAI	C2N-C3N	2.39	1.40	1.34
4	C	324	NAI	C2A-N1A	3.37	1.40	1.33
4	C	324	NAI	C6N-C5N	3.56	1.40	1.33
4	C	324	NAI	O4B-C1B	4.08	1.46	1.41
4	C	324	NAI	C2A-N3A	4.27	1.39	1.32

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	324	NAI	N3A-C2A-N1A	-14.86	117.52	128.89
4	C	324	NAI	O3-PA-O5B	-4.01	92.30	102.94
4	C	324	NAI	C1B-N9A-C4A	-3.75	121.28	126.94
4	C	324	NAI	PN-O3-PA	-2.84	124.75	132.73
4	C	324	NAI	O4D-C1D-N1N	2.89	114.16	108.07
4	C	324	NAI	C5N-C4N-C3N	3.11	121.09	112.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	324	NAI	3	0

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	138/179 (77%)	1.09	25 (18%) 2 2	32, 58, 77, 78	0
2	B	103/113 (91%)	1.64	34 (33%) 0 0	34, 60, 86, 89	0
3	C	313/323 (96%)	0.32	19 (6%) 25 27	26, 40, 60, 72	0
All	All	554/615 (90%)	0.76	78 (14%) 4 3	26, 45, 77, 89	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	368	GLY	12.1
2	B	369	ALA	8.4
2	B	358	THR	8.4
3	C	7	ASP	6.4
1	A	488	PRO	6.1
2	B	365	ASN	6.1
2	B	366	ASN	6.0
1	A	562	ILE	5.9
3	C	248	GLY	5.8
2	B	367	SER	5.7
2	B	326	LEU	5.6
1	A	502	LYS	5.3
1	A	501	SER	5.2
1	A	491	SER	5.0
1	A	497	VAL	4.9
2	B	362	PHE	4.7
3	C	251	TYR	4.7
1	A	487	SER	4.6
3	C	155	GLU	4.5
1	A	591	SER	4.4
2	B	359	GLN	4.4
3	C	158	HIS	4.3
1	A	499	LYS	4.2

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Mol	Chain	Res	Type	RSRZ
2	B	337	TRP	4.1
1	A	498	THR	3.9
2	B	370	LEU	3.9
1	A	628	VAL	3.8
2	B	354	LYS	3.8
2	B	355	TYR	3.8
3	C	153	GLN	3.8
3	C	8	SER	3.7
2	B	356	TYR	3.7
3	C	249	GLY	3.7
1	A	486	GLY	3.6
1	A	616	LEU	3.5
1	A	577	THR	3.5
1	A	563	PRO	3.4
3	C	14	ILE	3.2
1	A	578	ASN	3.2
3	C	120	ASP	3.2
2	B	363	ASN	3.1
2	B	371	PRO	3.1
2	B	350	VAL	3.1
2	B	361	GLN	3.1
2	B	364	GLU	3.1
3	C	218	GLN	3.0
2	B	386	ILE	3.0
1	A	512	ARG	3.0
1	A	619	THR	2.9
1	A	582	VAL	2.9
2	B	321	ARG	2.8
3	C	252	ASN	2.7
2	B	413	GLU	2.7
1	A	492	LYS	2.6
2	B	412	ILE	2.6
3	C	199	ASN	2.6
2	B	351	ILE	2.5
3	C	154	ASP	2.5
3	C	156	GLU	2.5
1	A	484	ALA	2.5
3	C	302	VAL	2.4
3	C	124	THR	2.4
1	A	485	GLN	2.4
2	B	357	ALA	2.3
2	B	349	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	381	LEU	2.2
2	B	393	VAL	2.2
3	C	297	PHE	2.1
2	B	360	ASP	2.1
1	A	629	ASN	2.1
2	B	394	ALA	2.1
1	A	614	PRO	2.1
2	B	336	SER	2.1
2	B	338	LEU	2.1
2	B	395	SER	2.1
2	B	352	LEU	2.1
1	A	489	ALA	2.0
3	C	298	VAL	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

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
4	NAI	C	324	44/44	0.93	0.15	-0.45	40,42,43,43	0

6.5 Other polymers

There are no such residues in this entry.