wwPDB X-ray Structure Validation Summary Report (i)

Aug 20, 2023 – 02:52 PM EDT

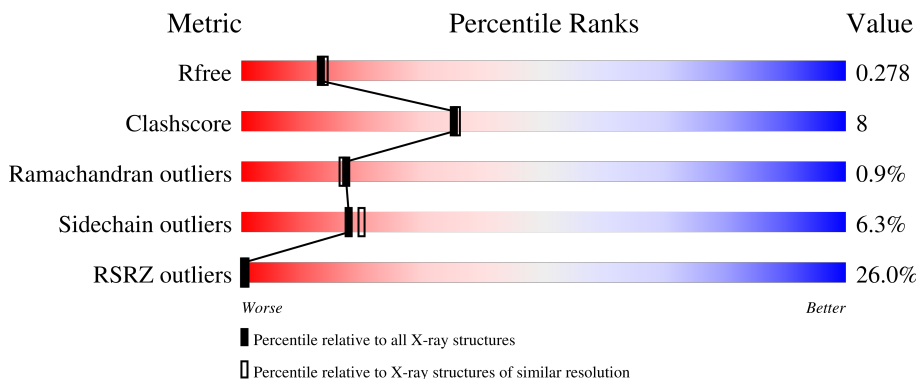|		
PDB ID	:	2I1W
Title	:	Crystal structure of NAD kinase 1 from Listeria monocytogenes
Authors	:	Poncet-Montange, G.; Assairi, L.; Arold, S.; Pochet, S.; Labesse, G.
Deposited on	:	2006-08-15
Resolution	:	2.34 Å(reported)

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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 2.34 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	Percentile Ranks	Value
Rfree		0.278
Clashscore		8
Ramachandran outliers		0.9%
Sidechain outliers		6.3%
RSRZ outliers		26.0%

Worse *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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	272	18% / 71% 20% · 6%
1	B	272	25% / 79% 14% ·· ·
1	C	272	31% / 78% 14% · 5%
1	D	272	24% / 70% 22% ·· 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	IOD	A	513	-	-	X	-
2	IOD	A	531	-	-	X	-
2	IOD	A	533	-	-	X	-
2	IOD	B	515	-	-	X	-
2	IOD	B	522	-	-	X	-

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 8538 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 Probable inorganic polyphosphate/ATP-NAD kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			2040	1309	341	381	9			
1	B	262	Total	C	N	O	S	0	0	0
			2069	1328	345	387	9			
1	C	258	Total	C	N	O	S	0	0	0
			2032	1305	341	377	9			
1	D	259	Total	C	N	O	S	0	0	0
			2016	1294	341	372	9			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	265	LEU	-	cloning artifact	UNP Q8Y8D7
A	266	GLU	-	cloning artifact	UNP Q8Y8D7
A	267	HIS	-	expression tag	UNP Q8Y8D7
A	268	HIS	-	expression tag	UNP Q8Y8D7
A	269	HIS	-	expression tag	UNP Q8Y8D7
A	270	HIS	-	expression tag	UNP Q8Y8D7
A	271	HIS	-	expression tag	UNP Q8Y8D7
A	272	HIS	-	expression tag	UNP Q8Y8D7
B	265	LEU	-	cloning artifact	UNP Q8Y8D7
B	266	GLU	-	cloning artifact	UNP Q8Y8D7
B	267	HIS	-	expression tag	UNP Q8Y8D7
B	268	HIS	-	expression tag	UNP Q8Y8D7
B	269	HIS	-	expression tag	UNP Q8Y8D7
B	270	HIS	-	expression tag	UNP Q8Y8D7
B	271	HIS	-	expression tag	UNP Q8Y8D7
B	272	HIS	-	expression tag	UNP Q8Y8D7
C	265	LEU	-	cloning artifact	UNP Q8Y8D7
C	266	GLU	-	cloning artifact	UNP Q8Y8D7
C	267	HIS	-	expression tag	UNP Q8Y8D7
C	268	HIS	-	expression tag	UNP Q8Y8D7
C	269	HIS	-	expression tag	UNP Q8Y8D7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	270	HIS	-	expression tag	UNP Q8Y8D7
C	271	HIS	-	expression tag	UNP Q8Y8D7
C	272	HIS	-	expression tag	UNP Q8Y8D7
D	265	LEU	-	cloning artifact	UNP Q8Y8D7
D	266	GLU	-	cloning artifact	UNP Q8Y8D7
D	267	HIS	-	expression tag	UNP Q8Y8D7
D	268	HIS	-	expression tag	UNP Q8Y8D7
D	269	HIS	-	expression tag	UNP Q8Y8D7
D	270	HIS	-	expression tag	UNP Q8Y8D7
D	271	HIS	-	expression tag	UNP Q8Y8D7
D	272	HIS	-	expression tag	UNP Q8Y8D7

- Molecule 2 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	8	Total 9	I 9	0	1
2	B	5	Total 6	I 6	0	1
2	C	2	Total 3	I 3	0	1
2	D	3	Total 4	I 4	0	1

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	101	Total 101	O 101	0	0
3	B	91	Total 91	O 91	0	0
3	C	76	Total 76	O 76	0	0
3	D	91	Total 91	O 91	0	0

3 Residue-property plots ⓘ

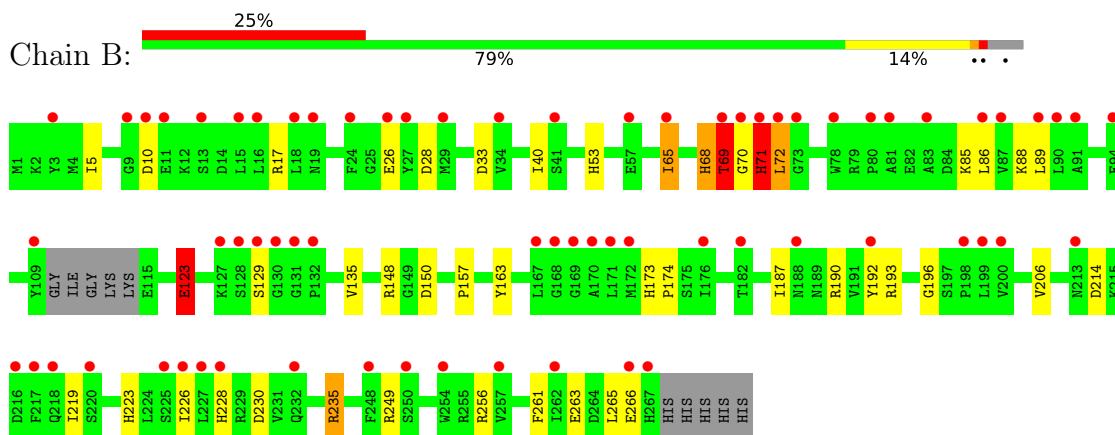These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.
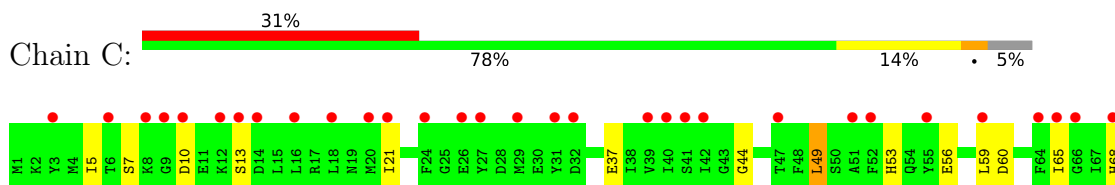
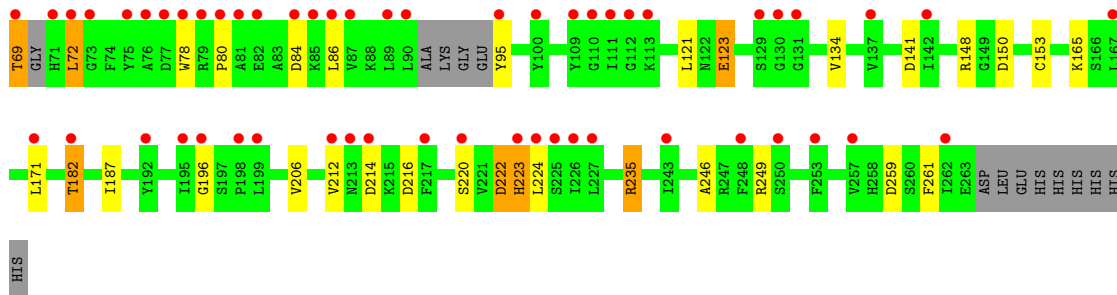• Molecule 1: Probable inorganic polyphosphate/ATP-NAD kinase 1

Chain A:

• Molecule 1: Probable inorganic polyphosphate/ATP-NAD kinase 1

Chain B:

• Molecule 1: Probable inorganic polyphosphate/ATP-NAD kinase 1

Chain C:

T69 GLY H71 L72 G73 F74 Y75 A76 D77 W78 R79 P80 A81 E82 A83 D84 K85 L86 V87 K88 L89 L90 ALA LYS GLY GLU Y95 Y100 Y109 G110 I111 G112 K113 L121 N122 E123 S129 G130 G131 V134 V137 D141 I142 R148 G149 D150 C153 K165 S166 L167

L171 T182 I187 Y192 I195 G196 S197 P198 L199 V206 V212 N213 D214 K215 D216 F217 S220 V221 D222 H223 L224 S225 I226 L227 R235 I243 A246 R247 F248 R249 S250 F253 V257 H258 D259 S260 F261 I262 E263 ASP LEU GLU HIS HIS HIS HIS HIS

HIS

• Molecule 1: Probable inorganic polyphosphate/ATP-NAD kinase 1

Chain D:

24%

70%   22%   5%

M1 I5 T6 D10 E11 K12 S13 D14 R17 L18 N19 M20 I21 F24 G25 E26 Y27 D28 M29 E30 Y31 D32 D33 V34 E35 P36 E37 I38 G43 G44 T47 A51 F52 H53 R58 L59 D60 E61 I62 A63 H68 T69 GLY H71 L72 D77 A83 D84 K85

L86 V87 K88 L89 L90 A91 K92 G93 E94 Y95 Q96 K97 Y100 P101 L102 Y109 G110 ILE GLY LYS K114 T117 Y118 L119 A120 E123 S124 T125 V126 K127 S128 S129 G130 G131 P132 F133 I139 N140 D141 D150 P157 Y163 N164 K165 S166 L167 G168 G169 A170 L171 P174

L181 R193 T194 I195 L199 K203 V206 P211 V212 N213 D214 K215 D216 F217 Q218 I219 S220 V221 D222 H223 L224 S225 I226 L227 H228 R229 D230 I234 K241 K242 I243 R247 F248 R249 P252 R256 V257 F261 I262 E263 ASP LEU GLU HIS HIS HIS HIS HIS

HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	66.61Å 119.02Å 67.94Å 90.00° 102.08° 90.00°	Depositor
Resolution (Å)	34.37 – 2.34 34.47 – 2.34	Depositor EDS
% Data completeness (in resolution range)	97.5 (34.37-2.34) 97.5 (34.47-2.34)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.38 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.194 , 0.257 0.220 , 0.278	Depositor DCC
R_{free} test set	1330 reflections (3.12%)	wwPDB-VP
Wilson B-factor (Å^2)	38.9	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 72.0	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.008 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8538	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.49% 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, 0.333 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: IOD

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	0.69	2/2088 (0.1%)	0.88	8/2820 (0.3%)
1	B	0.69	3/2120 (0.1%)	0.83	6/2870 (0.2%)
1	C	0.53	0/2081	0.80	8/2816 (0.3%)
1	D	0.58	1/2063 (0.0%)	0.83	10/2788 (0.4%)
All	All	0.62	6/8352 (0.1%)	0.84	32/11294 (0.3%)

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
1	B	0	2
1	C	1	0
1	D	0	6
All	All	1	9

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	26	GLU	CD-OE2	9.35	1.35	1.25
1	B	26	GLU	CD-OE1	8.52	1.35	1.25
1	A	259	ASP	CB-CG	6.58	1.65	1.51
1	A	263	GLU	C-O	5.99	1.34	1.23
1	D	94	GLU	N-CA	5.14	1.56	1.46

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	28	ASP	CB-CG-OD2	6.95	124.55	118.30
1	A	223	HIS	N-CA-C	6.40	128.27	111.00
1	A	60	ASP	CB-CG-OD2	6.37	124.03	118.30
1	B	10	ASP	CB-CG-OD2	6.34	124.01	118.30
1	A	15	LEU	CA-CB-CG	6.29	129.76	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	95	TYR	CA

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	222	ASP	Peptide
1	B	68	HIS	Peptide
1	B	69	THR	Peptide
1	D	60	ASP	Peptide
1	D	68	HIS	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	2040	0	1983	41	0
1	B	2069	0	1997	35	0
1	C	2032	0	1961	28	0
1	D	2016	0	1948	31	0
2	A	9	0	0	10	0
2	B	6	0	0	6	0
2	C	3	0	0	1	0
2	D	4	0	0	1	0
3	A	101	0	0	3	1
3	B	91	0	0	6	4
3	C	76	0	0	3	2
3	D	91	0	0	1	3
All	All	8538	0	7889	132	5

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 8.

The worst 5 of 132 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)
2:A:530:IOD:I	3:A:596:HOH:O	2.29	1.19
2:A:531:IOD:I	3:A:535:HOH:O	2.43	1.06
1:C:196:GLY:O	2:C:523:IOD:I	2.56	0.94
1:D:69:THR:O	1:D:71:HIS:N	2.00	0.93
1:B:256:ARG:HD3	3:B:559:HOH:O	1.70	0.91

All (5) 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)
3:B:611:HOH:O	3:C:584:HOH:O[1_556]	1.34	0.86
3:B:604:HOH:O	3:D:589:HOH:O[1_556]	1.63	0.57
3:B:613:HOH:O	3:D:586:HOH:O[1_556]	2.05	0.15
3:A:588:HOH:O	3:C:580:HOH:O[1_556]	2.11	0.09
3:B:612:HOH:O	3:D:587:HOH:O[1_556]	2.17	0.03

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	251/272 (92%)	238 (95%)	12 (5%)	1 (0%)	34	38
1	B	258/272 (95%)	243 (94%)	13 (5%)	2 (1%)	19	20
1	C	252/272 (93%)	240 (95%)	11 (4%)	1 (0%)	34	38
1	D	253/272 (93%)	231 (91%)	17 (7%)	5 (2%)	7	4
All	All	1014/1088 (93%)	952 (94%)	53 (5%)	9 (1%)	17	17

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	HIS
1	B	71	HIS
1	C	72	LEU
1	D	61	GLU
1	D	68	HIS

5.3.2 Protein sidechains ⓘ

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	219/237 (92%)	205 (94%)	14 (6%)	17	19
1	B	221/237 (93%)	210 (95%)	11 (5%)	24	30
1	C	216/237 (91%)	202 (94%)	14 (6%)	17	19
1	D	212/237 (90%)	196 (92%)	16 (8%)	13	14
All	All	868/948 (92%)	813 (94%)	55 (6%)	18	20

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	72	LEU
1	C	223	HIS
1	D	249	ARG
1	D	206	VAL
1	C	95	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	53	HIS
1	C	173	HIS
1	D	188	ASN
1	C	223	HIS
1	A	218	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 22 ligands modelled in this entry, 22 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 (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	257/272 (94%)	1.37	49 (19%)	1	2	33, 40, 51, 55	14 (5%)
1	B	262/272 (96%)	1.59	69 (26%)	0	0	31, 40, 48, 55	13 (4%)
1	C	258/272 (94%)	1.65	85 (32%)	0	0	35, 41, 47, 50	8 (3%)
1	D	259/272 (95%)	1.51	66 (25%)	0	1	35, 40, 47, 50	10 (3%)
All	All	1036/1088 (95%)	1.53	269 (25%)	0	1	31, 40, 48, 55	45 (4%)

The worst 5 of 269 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	227	LEU	7.3
1	B	91	ALA	6.6
1	B	130	GLY	6.3
1	C	9	GLY	6.1
1	A	217	PHE	6.0

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	IOD	A	534	1/1	0.93	0.42	39,39,39,39	1
2	IOD	B	515	1/1	0.93	0.15	49,49,49,49	1
2	IOD	A	530	1/1	0.94	0.48	45,45,45,45	1
2	IOD	A	531	1/1	0.96	0.21	46,46,46,46	1
2	IOD	B	522	1/1	0.96	0.06	40,40,40,40	1
2	IOD	C	523	1/1	0.96	0.15	40,40,40,40	1
2	IOD	A	533	1/1	0.97	0.38	48,48,48,48	1
2	IOD	A	513	1/1	0.97	0.17	49,49,49,49	1
2	IOD	B	535	1/1	0.97	0.09	33,33,33,33	1
2	IOD	A	532	1/1	0.97	0.28	41,41,41,41	1
2	IOD	B	528	1/1	0.98	0.25	31,31,31,31	1
2	IOD	A	502[A]	1/1	0.98	0.24	43,43,43,43	1
2	IOD	C	504[A]	1/1	0.98	0.06	33,33,33,33	1
2	IOD	C	504[B]	1/1	0.98	0.06	35,35,35,35	1
2	IOD	A	502[B]	1/1	0.98	0.24	35,35,35,35	1
2	IOD	D	506[A]	1/1	0.98	0.06	33,33,33,33	1
2	IOD	D	506[B]	1/1	0.98	0.06	39,39,39,39	1
2	IOD	D	520	1/1	0.98	0.05	41,41,41,41	1
2	IOD	B	508[A]	1/1	0.99	0.06	37,37,37,37	1
2	IOD	B	508[B]	1/1	0.99	0.06	41,41,41,41	1
2	IOD	D	510	1/1	0.99	0.07	40,40,40,40	1
2	IOD	A	501	1/1	0.99	0.23	36,36,36,36	1

6.5 Other polymers (i)

There are no such residues in this entry.