Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2023 – 10:42 PM EDT

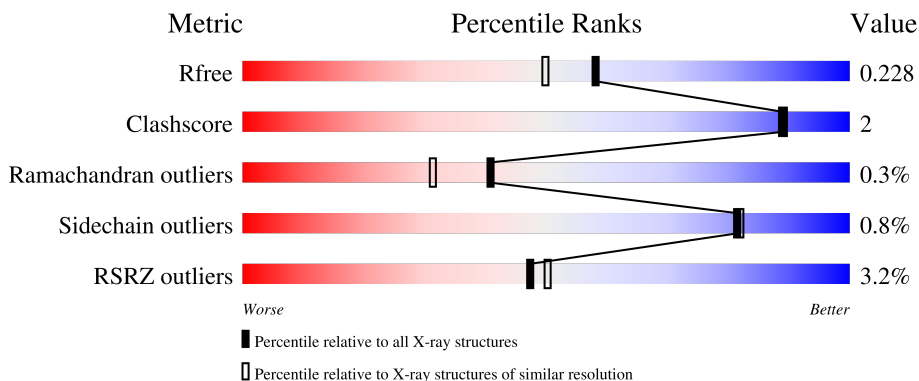|		
PDB ID	:	3PL2
Title	:	Crystal structure of a 5-keto-2-deoxygluconokinase (NCgl0155, Cgl0158) from Corynebacterium glutamicum ATCC 13032 KITASATO at 1.89 A resolution
Authors	:	Joint Center for Structural Genomics (JCSG)
Deposited on	:	2010-11-12
Resolution	:	1.89 Å(reported)

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 1.89 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		0.228
Clashscore		2
Ramachandran outliers		0.3%
Sidechain outliers		0.8%
RSRZ outliers		3.2%

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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	319	4% / 91% / 6% ··
1	B	319	3% / 91% / 6% ·
1	C	319	2% / 92% / 6% ·
1	D	319	4% / 90% / 7% ·

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 10314 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 Sugar kinase, ribokinase family.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	Se	0	8	0
			2428	1539	409	470	4	6			
1	B	310	Total	C	N	O	S	Se	0	14	0
			2443	1547	408	478	4	6			
1	C	310	Total	C	N	O	S	Se	0	12	0
			2445	1547	413	475	4	6			
1	D	309	Total	C	N	O	S	Se	0	7	0
			2408	1523	407	467	4	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q8NTZ3
B	0	GLY	-	expression tag	UNP Q8NTZ3
C	0	GLY	-	expression tag	UNP Q8NTZ3
D	0	GLY	-	expression tag	UNP Q8NTZ3

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).

CIT

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total 13	C 6	O 7	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	128	Total 128	O 128	0	0
3	B	164	Total 164	O 164	0	0
3	C	162	Total 162	O 162	0	0
3	D	123	Total 123	O 123	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.
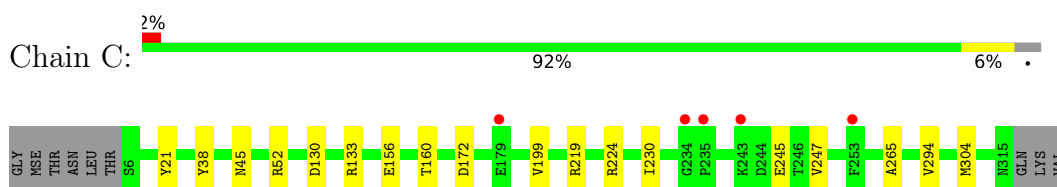
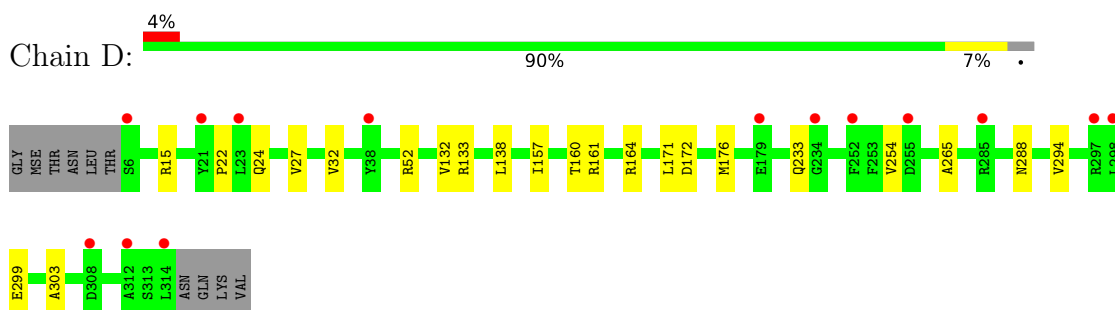• Molecule 1: Sugar kinase, ribokinase family
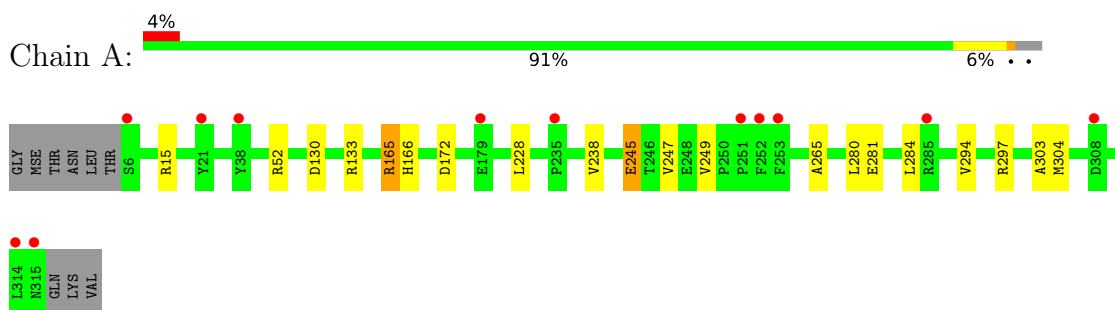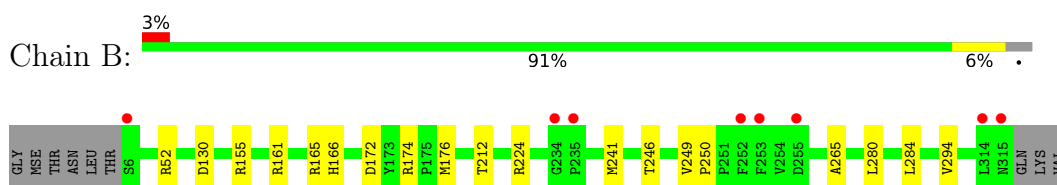
Chain A:

• Molecule 1: Sugar kinase, ribokinase family

Chain B:

• Molecule 1: Sugar kinase, ribokinase family

Chain C:

• Molecule 1: Sugar kinase, ribokinase family

Chain D:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	45.91Å 79.49Å 81.70Å 101.86° 95.72° 92.11°	Depositor
Resolution (Å)	37.80 – 1.89 37.80 – 1.89	Depositor EDS
% Data completeness (in resolution range)	97.0 (37.80-1.89) 96.8 (37.80-1.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.10 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.180 , 0.225 0.186 , 0.228	Depositor DCC
R_{free} test set	4384 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	25.3	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 37.4	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.006 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10314	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.42% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.74	0/2505	0.80	3/3401 (0.1%)
1	B	0.79	0/2533	0.84	4/3438 (0.1%)
1	C	0.75	0/2534	0.81	5/3442 (0.1%)
1	D	0.74	0/2480	0.81	3/3366 (0.1%)
All	All	0.76	0/10052	0.81	15/13647 (0.1%)

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	D	0	1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	161	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	C	133	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	A	15	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	C	224	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	B	52	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	C	219	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	D	15	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	B	130	ASP	CB-CG-OD1	5.42	123.17	118.30
1	A	165	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	D	133	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	D	52	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	15	ARG	NE-CZ-NH2	-5.13	117.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	52	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	C	224	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	B	155	ARG	NE-CZ-NH1	5.08	122.84	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	171	LEU	Peptide

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	2428	0	2369	10	0
1	B	2443	0	2387	9	0
1	C	2445	0	2386	6	0
1	D	2408	0	2357	12	0
2	B	13	0	5	0	0
3	A	128	0	0	0	0
3	B	164	0	0	0	0
3	C	162	0	0	0	0
3	D	123	0	0	0	0
All	All	10314	0	9504	37	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 2.

All (37) 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:D:27[B]:VAL:HG13	1:D:32:VAL:HG22	1.70	0.73
1:B:280:LEU:O	1:B:284:LEU:HD13	1.96	0.65
1:D:27[A]:VAL:HG23	1:D:32:VAL:HG22	1.83	0.58
1:C:156:GLU:O	1:C:160:THR:HG23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:VAL:HG22	1:A:284:LEU:HD11	1.89	0.54
1:C:265:ALA:HB2	1:C:294:VAL:HG21	1.90	0.54
1:A:249:VAL:HG23	1:A:284:LEU:HD23	1.89	0.54
1:C:21[B]:TYR:CE1	1:C:38:TYR:CE2	2.95	0.53
1:B:265:ALA:HB2	1:B:294:VAL:HG21	1.91	0.52
1:A:245:GLU:HG3	1:A:247:VAL:HG23	1.92	0.51
1:A:247:VAL:HG11	1:A:281:GLU:HA	1.94	0.49
1:A:265:ALA:HB2	1:A:294:VAL:HG21	1.93	0.49
1:D:27[B]:VAL:HG13	1:D:32:VAL:CG2	2.41	0.49
1:B:176[B]:MSE:HE3	1:B:176[B]:MSE:H	1.80	0.46
1:C:199:VAL:HG22	1:C:230:ILE:HD12	1.98	0.46
1:B:241[B]:MSE:HG2	1:B:246:THR:HG23	1.97	0.45
1:D:27[B]:VAL:CG1	1:D:32:VAL:HG22	2.41	0.45
1:D:299:GLU:HB2	1:D:303:ALA:HB2	2.00	0.44
1:D:265:ALA:HB2	1:D:294:VAL:HG21	1.99	0.44
1:D:132:VAL:CG1	1:D:157:ILE:HG23	2.48	0.44
1:A:228:LEU:HD11	1:A:280:LEU:HD11	1.99	0.43
1:D:22:PRO:HB3	1:D:32:VAL:HG11	2.00	0.43
1:D:176[C]:MSE:HB2	1:D:176[C]:MSE:HE2	1.72	0.43
1:D:161:ARG:NH2	1:D:164:ARG:HD3	2.34	0.42
1:C:245:GLU:HG2	1:C:247:VAL:HG23	2.01	0.42
1:B:224[A]:ARG:HG3	1:B:224[A]:ARG:NH1	2.35	0.42
1:B:249:VAL:HG12	1:B:250:PRO:O	2.20	0.42
1:B:224[A]:ARG:HG3	1:B:224[A]:ARG:HH11	1.85	0.41
1:D:24:GLN:O	1:D:27[B]:VAL:HG12	2.20	0.41
1:B:165:ARG:HA	1:B:166:HIS:HA	1.92	0.41
1:B:174[B]:ARG:HE	1:B:176[B]:MSE:SE	2.54	0.41
1:A:52:ARG:HG3	1:A:304:MSE:HB2	2.02	0.40
1:A:165:ARG:HA	1:A:166:HIS:HA	1.96	0.40
1:A:130:ASP:OD1	1:A:133[A]:ARG:NH2	2.54	0.40
1:A:297[A]:ARG:HD2	1:A:303:ALA:HB1	2.04	0.40
1:C:45:ASN:HB3	1:C:304:MSE:HE3	2.03	0.40
1:D:24:GLN:HB2	1:D:27[B]:VAL:HG11	2.03	0.40

There are no symmetry-related clashes.

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	317/319 (99%)	311 (98%)	5 (2%)	1 (0%)	41	31
1	B	322/319 (101%)	316 (98%)	5 (2%)	1 (0%)	41	31
1	C	321/319 (101%)	317 (99%)	3 (1%)	1 (0%)	41	31
1	D	315/319 (99%)	311 (99%)	3 (1%)	1 (0%)	41	31
All	All	1275/1276 (100%)	1255 (98%)	16 (1%)	4 (0%)	41	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	172	ASP
1	B	172	ASP
1	C	172	ASP
1	D	172	ASP

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	258/255 (101%)	257 (100%)	1 (0%)	91	91
1	B	263/255 (103%)	262 (100%)	1 (0%)	91	91
1	C	262/255 (103%)	261 (100%)	1 (0%)	91	91
1	D	257/255 (101%)	252 (98%)	5 (2%)	57	53
All	All	1040/1020 (102%)	1032 (99%)	8 (1%)	81	82

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	245	GLU
1	B	212	THR
1	C	130	ASP
1	D	138	LEU
1	D	160	THR
1	D	233	GLN
1	D	254	VAL
1	D	288	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

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	$\#|Z| > 2$
2	CIT	B	400	-	12,12,12	1.02	0	17,17,17	1.47	2 (11%)

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	CIT	B	400	-	-	5/16/16/16	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	400	CIT	O4-C5-O3	-3.31	115.05	123.30
2	B	400	CIT	O6-C6-C3	3.06	118.37	113.05

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	400	CIT	C4-C3-C6-O6
2	B	400	CIT	O7-C3-C6-O6
2	B	400	CIT	C4-C3-C6-O5
2	B	400	CIT	C2-C3-C6-O6
2	B	400	CIT	C2-C3-C6-O5

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, 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(Å²)	Q<0.9
1	A	306/319 (95%)	0.07	12 (3%)	39	42	25, 37, 64, 84	0
1	B	306/319 (95%)	-0.08	8 (2%)	56	58	20, 30, 49, 61	0
1	C	306/319 (95%)	0.03	5 (1%)	72	74	21, 34, 58, 74	0
1	D	305/319 (95%)	0.06	14 (4%)	32	35	24, 36, 63, 77	0
All	All	1223/1276 (95%)	0.02	39 (3%)	47	50	20, 34, 60, 84	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	253	PHE	7.7
1	D	252	PHE	6.7
1	B	235	PRO	5.3
1	A	314	LEU	5.3
1	A	253	PHE	5.2
1	A	315	ASN	5.1
1	C	235	PRO	5.0
1	A	252	PHE	4.5
1	D	234	GLY	4.4
1	B	253	PHE	4.0
1	A	235	PRO	3.5
1	D	38	TYR	3.5
1	D	298	LEU	3.3
1	D	312	ALA	3.1
1	C	234	GLY	3.0
1	B	234	GLY	2.9
1	A	38	TYR	2.9
1	A	21[A]	TYR	2.7
1	D	314	LEU	2.7
1	D	308	ASP	2.7
1	D	297	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	315	ASN	2.5
1	A	6	SER	2.5
1	D	6	SER	2.5
1	D	255	ASP	2.4
1	C	243	LYS	2.4
1	B	314	LEU	2.4
1	D	285	ARG	2.4
1	D	21	TYR	2.3
1	B	252	PHE	2.3
1	A	308	ASP	2.3
1	B	255	ASP	2.3
1	A	251	PRO	2.3
1	A	179	GLU	2.3
1	B	6	SER	2.3
1	D	179	GLU	2.3
1	C	179	GLU	2.2
1	D	23	LEU	2.1
1	A	285	ARG	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 monosaccharides 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. 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	CIT	B	400	13/13	0.88	0.13	32,38,43,43	0

6.5 Other polymers ⓘ

There are no such residues in this entry.