



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:32 AM UTC

PDB ID : 2JGP / pdb_00002jgp
Title : Structure of the TycC5-6 PCP-C bidomain of the tyrocidine synthetase TycC
Authors : Samel, S.A.; Schoenafinger, G.; Knappe, T.A.; Marahiel, M.A.; Essen, L.-O.
Deposited on : 2007-02-13
Resolution : 1.85 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

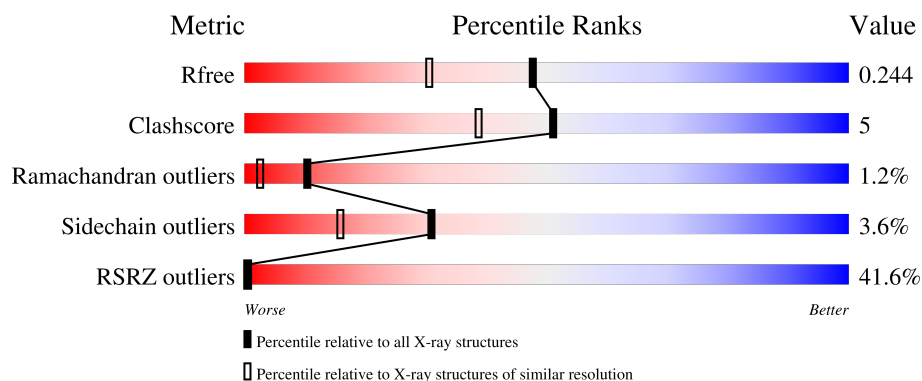
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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 $\leq 5\%$. 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	520	41% 87% 12%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4477 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.

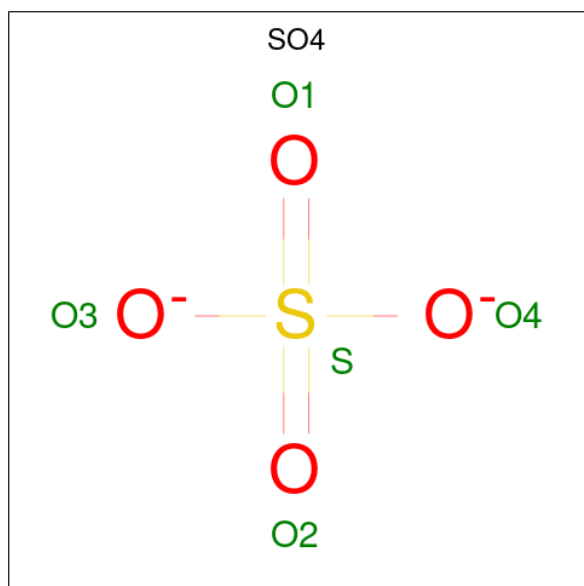
- Molecule 1 is a protein called TYROCIDINE SYNTHETASE 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	520	4161	2655	695	795	16	35	2	0

There is a discrepancy between the modelled and reference sequences:

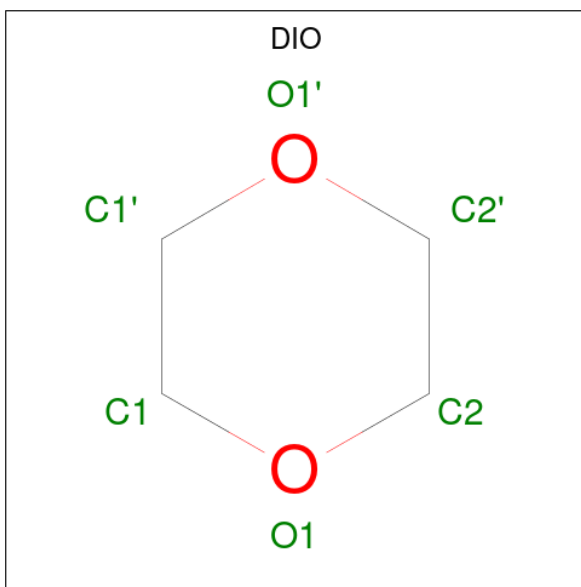
Chain	Residue	Modelled	Actual	Comment	Reference
A	183	GLU	GLN	conflict	UNP O30409

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0

- Molecule 3 is 1,4-DIETHYLENE DIOXIDE (CCD ID: DIO) (formula: C₄H₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	4	2		
3	A	1	Total	C	O	0	0
			6	4	2		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		

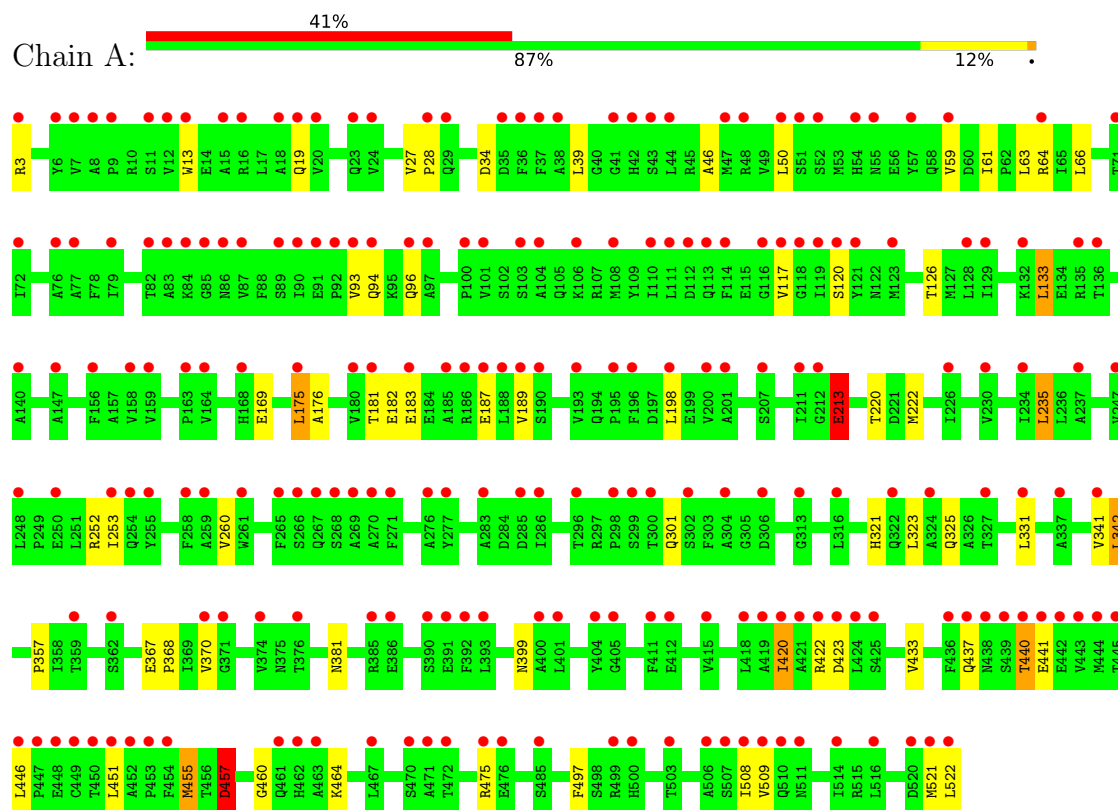
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	293	Total	O	0	0
			293	293		

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: TYROCIDINE SYNTHETASE 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	84.97Å 84.97Å 164.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.81 – 1.85 19.81 – 1.85	Depositor EDS
% Data completeness (in resolution range)	98.6 (19.81-1.85) 98.5 (19.81-1.85)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.208 , 0.238 0.214 , 0.244	Depositor DCC
R_{free} test set	1766 reflections (2.63%)	wwPDB-VP
Wilson B-factor (Å ²)	33.6	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 53.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4477	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: SO4, DIO, NA

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	0.49	2/4259 (0.0%)	0.83	6/5783 (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	A	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	460	GLY	C-N	-12.13	1.15	1.33
1	A	455	MET	C-N	7.29	1.45	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	455	MET	O-C-N	-30.46	87.04	122.68
1	A	457	ASP	CB-CG-OD2	-11.20	92.63	118.40
1	A	460	GLY	CA-C-N	9.85	138.37	121.14
1	A	460	GLY	C-N-CA	9.85	138.37	121.14
1	A	460	GLY	O-C-N	-6.64	114.06	122.70
1	A	457	ASP	CB-CG-OD1	5.91	132.00	118.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	455	MET	Mainchain
1	A	457	ASP	Sidechain

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	4161	0	4084	43	0
2	A	10	0	0	0	0
3	A	12	0	16	1	0
4	A	1	0	0	0	0
5	A	293	0	0	1	0
All	All	4477	0	4100	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)
1:A:508:ILE:HD12	1:A:509:VAL:N	2.01	0.76
1:A:117:VAL:HG12	1:A:120:SER:HB3	1.72	0.71
1:A:117:VAL:CG1	1:A:120:SER:HB3	2.21	0.70
1:A:323:LEU:CD2	1:A:508:ILE:HD13	2.23	0.69
1:A:117:VAL:HG12	1:A:117:VAL:O	1.95	0.65
1:A:175:LEU:C	1:A:175:LEU:HD23	2.24	0.62
1:A:220:THR:HG21	3:A:1525:DIO:H22	1.82	0.61
1:A:252:ARG:NH1	1:A:253:ILE:HD11	2.15	0.61
1:A:508:ILE:HD12	1:A:508:ILE:C	2.26	0.60
1:A:420:ILE:HG23	1:A:422:ARG:HB2	1.83	0.60
1:A:521:MET:O	1:A:522:LEU:HB2	2.05	0.57
1:A:446:LEU:HD13	1:A:451:LEU:HD11	1.85	0.57
1:A:3:ARG:NH2	1:A:28:PRO:O	2.38	0.55
1:A:3:ARG:NH2	1:A:27:VAL:HG12	2.22	0.53
1:A:126:THR:HG21	1:A:189:VAL:HG11	1.90	0.53
1:A:175:LEU:HD23	1:A:176:ALA:C	2.34	0.53
1:A:175:LEU:HD23	1:A:176:ALA:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:GLN:NE2	5:A:2020:HOH:O	2.43	0.52
1:A:342:LEU:HD13	1:A:497:PHE:CZ	2.47	0.49
1:A:3:ARG:NH2	1:A:27:VAL:CG1	2.77	0.48
1:A:126:THR:HG21	1:A:189:VAL:CG1	2.44	0.47
1:A:321:HIS:CE1	1:A:331:LEU:HD22	2.49	0.47
1:A:13:TRP:CH2	1:A:59:VAL:HG21	2.50	0.47
1:A:50:LEU:HD22	1:A:61:ILE:O	2.14	0.47
1:A:213:GLU:N	1:A:213:GLU:CD	2.73	0.46
1:A:175:LEU:C	1:A:175:LEU:CD2	2.88	0.46
1:A:381:ASN:ND2	1:A:399:ASN:HD22	2.14	0.45
1:A:117:VAL:CG1	1:A:117:VAL:O	2.63	0.45
1:A:446:LEU:CD1	1:A:451:LEU:HD11	2.46	0.45
1:A:222:MET:HE1	1:A:235:LEU:HD23	1.99	0.45
1:A:213:GLU:CD	1:A:213:GLU:H	2.25	0.45
1:A:50:LEU:HD11	1:A:63:LEU:HA	2.00	0.44
1:A:301:GLN:NE2	1:A:464:LYS:O	2.50	0.44
1:A:34:ASP:HB3	1:A:39:LEU:HD11	2.00	0.44
1:A:367:GLU:N	1:A:368:PRO:CD	2.82	0.43
1:A:323:LEU:HD22	1:A:508:ILE:HD13	2.00	0.42
1:A:181:THR:HG22	1:A:182:GLU:N	2.35	0.41
1:A:46:ALA:HB1	1:A:66:LEU:HD23	2.02	0.41
1:A:440:THR:O	1:A:440:THR:HG22	2.20	0.41
1:A:181:THR:HG22	1:A:183:GLU:H	1.85	0.40
1:A:357:PRO:HD3	1:A:433:VAL:HG13	2.02	0.40
1:A:93:VAL:HG11	1:A:260:VAL:HB	2.04	0.40
1:A:235:LEU:CD1	1:A:370:VAL:HG21	2.50	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	520/520 (100%)	489 (94%)	25 (5%)	6 (1%)	10 2

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	213	GLU
1	A	440	THR
1	A	441	GLU
1	A	133	LEU
1	A	475	ARG
1	A	423	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	452/450 (100%)	436 (96%)	16 (4%)	32 16

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	ARG
1	A	94	GLN
1	A	96	GLN
1	A	133	LEU
1	A	169	GLU
1	A	175	LEU
1	A	187	GLU
1	A	198	LEU
1	A	213	GLU
1	A	235	LEU
1	A	325	GLN
1	A	341	VAL
1	A	342	LEU
1	A	420	ILE
1	A	437	GLN

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Mol	Chain	Res	Type
1	A	457	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	143	GLN
1	A	241	GLN
1	A	267	GLN
1	A	280	GLN
1	A	290	ASN
1	A	301	GLN
1	A	325	GLN
1	A	381	ASN
1	A	437	GLN
1	A	500	HIS
1	A	510	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	$\# Z > 2$
3	DIO	A	1525	-	6,6,6	0.49	0	6,6,6	0.49	0
3	DIO	A	1526	-	6,6,6	0.49	0	6,6,6	0.54	0
2	SO4	A	1524	-	4,4,4	0.25	0	6,6,6	0.15	0
2	SO4	A	1523	-	4,4,4	0.20	0	6,6,6	0.14	0

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
3	DIO	A	1525	-	-	-	0/1/1/1
3	DIO	A	1526	-	-	-	0/1/1/1

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1525	DIO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	460:GLY	C	461:GLN	N	1.15

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(Å ²)	Q<0.9
1	A	515/520 (99%)	1.96	214 (41%) 0 0	38, 62, 75, 87	2 (0%)

All (214) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	443	VAL	8.9
1	A	420	ILE	7.1
1	A	419	ALA	6.0
1	A	449	CYS	5.0
1	A	439	SER	5.0
1	A	476	GLU	4.6
1	A	451	LEU	4.6
1	A	422	ARG	4.3
1	A	12	VAL	4.3
1	A	117	VAL	4.2
1	A	15	ALA	4.1
1	A	94	GLN	4.0
1	A	445	THR	4.0
1	A	448	GLU	3.9
1	A	418	LEU	3.8
1	A	101	VAL	3.7
1	A	446	LEU	3.7
1	A	259	ALA	3.7
1	A	187	GLU	3.6
1	A	421	ALA	3.6
1	A	147	ALA	3.6
1	A	116	GLY	3.5
1	A	188	LEU	3.5
1	A	114	PHE	3.5
1	A	507	SER	3.4
1	A	424	LEU	3.4
1	A	475	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	423	ASP	3.4
1	A	19	GLN	3.4
1	A	18	ALA	3.4
1	A	6	TYR	3.3
1	A	175	LEU	3.3
1	A	119	ILE	3.3
1	A	84[A]	LYS	3.3
1	A	454	PHE	3.3
1	A	121	TYR	3.2
1	A	83	ALA	3.2
1	A	7	VAL	3.2
1	A	442	GLU	3.2
1	A	118	GLY	3.2
1	A	87	VAL	3.2
1	A	158	VAL	3.2
1	A	111	LEU	3.2
1	A	140	ALA	3.1
1	A	324	ALA	3.1
1	A	462	HIS	3.1
1	A	472	THR	3.1
1	A	438	ASN	3.1
1	A	452	ALA	3.1
1	A	509	VAL	3.0
1	A	437	GLN	3.0
1	A	359	THR	3.0
1	A	440	THR	3.0
1	A	516	LEU	3.0
1	A	374	VAL	3.0
1	A	503	THR	3.0
1	A	520	ASP	3.0
1	A	51	SER	2.9
1	A	270	ALA	2.9
1	A	254[A]	GLN	2.9
1	A	85	GLY	2.9
1	A	277	TYR	2.9
1	A	9	PRO	2.9
1	A	97	ALA	2.9
1	A	269	ALA	2.9
1	A	522	LEU	2.9
1	A	371	GLY	2.9
1	A	28	PRO	2.8
1	A	77	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	265	PHE	2.8
1	A	47	MET	2.8
1	A	180	VAL	2.8
1	A	57	TYR	2.8
1	A	8	ALA	2.8
1	A	136	THR	2.8
1	A	129	ILE	2.8
1	A	450	THR	2.8
1	A	207	SER	2.7
1	A	64	ARG	2.7
1	A	271	PHE	2.7
1	A	392	PHE	2.7
1	A	391	GLU	2.7
1	A	401	LEU	2.7
1	A	110	ILE	2.7
1	A	508	ILE	2.7
1	A	48	ARG	2.7
1	A	189	VAL	2.7
1	A	55	ASN	2.7
1	A	38	ALA	2.7
1	A	283	ALA	2.7
1	A	112	ASP	2.7
1	A	268	SER	2.7
1	A	267	GLN	2.7
1	A	159	VAL	2.7
1	A	200	VAL	2.7
1	A	196	PHE	2.6
1	A	447	PRO	2.6
1	A	467	LEU	2.6
1	A	306	ASP	2.6
1	A	11	SER	2.6
1	A	13	TRP	2.6
1	A	36	PHE	2.6
1	A	86	ASN	2.6
1	A	195	PRO	2.6
1	A	234	ILE	2.6
1	A	253	ILE	2.6
1	A	514	ILE	2.6
1	A	298	PRO	2.6
1	A	248	LEU	2.6
1	A	316	LEU	2.6
1	A	90	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	286	ILE	2.6
1	A	52	SER	2.6
1	A	3	ARG	2.5
1	A	404	TYR	2.5
1	A	461	GLN	2.5
1	A	128	LEU	2.5
1	A	198	LEU	2.5
1	A	261	TRP	2.5
1	A	237	ALA	2.5
1	A	20	VAL	2.5
1	A	193	VAL	2.5
1	A	82	THR	2.5
1	A	23	GLN	2.5
1	A	41	GLY	2.5
1	A	181	THR	2.5
1	A	44	LEU	2.5
1	A	72	ILE	2.5
1	A	183	GLU	2.5
1	A	444	MET	2.5
1	A	164	VAL	2.5
1	A	285	ASP	2.5
1	A	212	GLY	2.4
1	A	89	SER	2.4
1	A	470	SER	2.4
1	A	71	THR	2.4
1	A	250	GLU	2.4
1	A	441	GLU	2.4
1	A	190	SER	2.4
1	A	104	ALA	2.4
1	A	59	VAL	2.4
1	A	230	VAL	2.4
1	A	299	SER	2.4
1	A	76	ALA	2.4
1	A	92	PRO	2.4
1	A	100	PRO	2.4
1	A	113	GLN	2.4
1	A	54	HIS	2.4
1	A	43	SER	2.4
1	A	16	ARG	2.3
1	A	91	GLU	2.3
1	A	327	THR	2.3
1	A	226	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	50	LEU	2.3
1	A	96	GLN	2.3
1	A	300	THR	2.3
1	A	201	ALA	2.3
1	A	211	ILE	2.3
1	A	385	ARG	2.3
1	A	376	THR	2.3
1	A	436	PHE	2.3
1	A	341	VAL	2.3
1	A	132	LYS	2.3
1	A	156	PHE	2.2
1	A	302	SER	2.2
1	A	390	SER	2.2
1	A	485	SER	2.2
1	A	79	ILE	2.2
1	A	103	SER	2.2
1	A	120	SER	2.2
1	A	106	LYS	2.2
1	A	393	LEU	2.2
1	A	337	ALA	2.2
1	A	471	ALA	2.2
1	A	37	PHE	2.2
1	A	255	TYR	2.2
1	A	510	GLN	2.2
1	A	42	HIS	2.1
1	A	386	GLU	2.1
1	A	296	THR	2.1
1	A	405	GLY	2.1
1	A	135	ARG	2.1
1	A	163	PRO	2.1
1	A	108	MET	2.1
1	A	500	HIS	2.1
1	A	276	ALA	2.1
1	A	258	PHE	2.1
1	A	411	PHE	2.1
1	A	35	ASP	2.1
1	A	123	MET	2.1
1	A	331	LEU	2.1
1	A	453	PRO	2.1
1	A	511	ASN	2.1
1	A	29	GLN	2.1
1	A	266	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	168	HIS	2.1
1	A	93	VAL	2.1
1	A	415	VAL	2.1
1	A	322	GLN	2.1
1	A	304	ALA	2.1
1	A	400	ALA	2.1
1	A	506	ALA	2.1
1	A	186	ARG	2.1
1	A	499	ARG	2.1
1	A	362	SER	2.0
1	A	24	VAL	2.0
1	A	247	VAL	2.0
1	A	185	ALA	2.0
1	A	463	ALA	2.0
1	A	412	GLU	2.0
1	A	425	SER	2.0
1	A	521	MET	2.0
1	A	313	GLY	2.0
1	A	370	VAL	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	DIO	A	1525	6/6	0.78	0.15	55,56,56,56	0
3	DIO	A	1526	6/6	0.78	0.18	79,79,79,79	0
4	NA	A	1527	1/1	0.80	0.33	69,69,69,69	0
2	SO4	A	1523	5/5	0.83	0.15	69,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	1524	5/5	0.89	0.15	57,57,58,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.