



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:48 AM UTC

PDB ID : 5VG2 / pdb_00005vg2
Title : Intradiol ring-cleavage Dioxygenase from *Tetranychus urticae*
Authors : Schlachter, C.; Klapper, V.; Chruszcz, M.
Deposited on : 2017-04-10
Resolution : 2.46 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

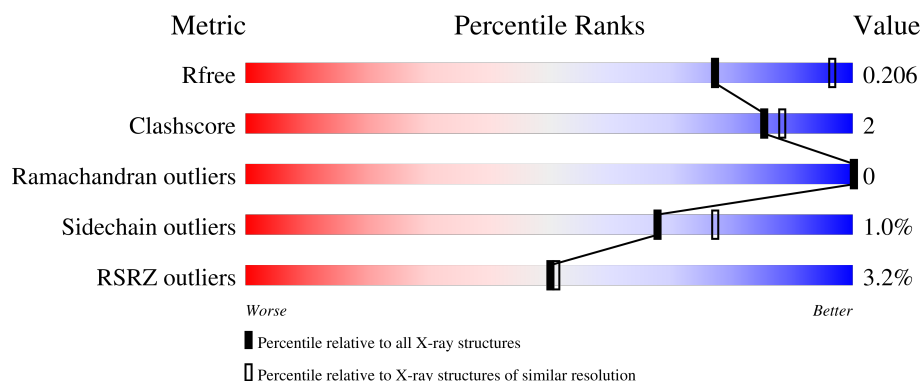
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.46 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	229	2% 85% • 11%
1	B	229	4% 82% 5% • 12%
1	C	229	83% 5% 11%
1	U	229	5% 83% 6% 11%

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
3	CAC	C	302	-	X	-	-
3	CAC	C	303	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6649 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 Intradiol ring-cleavage Dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	U	203	Total	C	N	O	S	0	0	0
			1618	1026	284	302	6			
1	A	204	Total	C	N	O	S	0	0	0
			1633	1034	287	306	6			
1	B	201	Total	C	N	O	S	0	0	0
			1594	1012	279	297	6			
1	C	204	Total	C	N	O	S	0	0	0
			1615	1025	283	301	6			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	260	ALA	-	expression tag	UNP T1K8P1
U	261	GLY	-	expression tag	UNP T1K8P1
U	262	GLU	-	expression tag	UNP T1K8P1
U	263	ASN	-	expression tag	UNP T1K8P1
U	264	LEU	-	expression tag	UNP T1K8P1
U	265	TYR	-	expression tag	UNP T1K8P1
U	266	PHE	-	expression tag	UNP T1K8P1
U	267	GLN	-	expression tag	UNP T1K8P1
U	268	SER	-	expression tag	UNP T1K8P1
U	269	ALA	-	expression tag	UNP T1K8P1
U	270	GLY	-	expression tag	UNP T1K8P1
U	271	HIS	-	expression tag	UNP T1K8P1
U	272	HIS	-	expression tag	UNP T1K8P1
U	273	HIS	-	expression tag	UNP T1K8P1
U	274	HIS	-	expression tag	UNP T1K8P1
U	275	HIS	-	expression tag	UNP T1K8P1
U	276	HIS	-	expression tag	UNP T1K8P1
A	260	ALA	-	expression tag	UNP T1K8P1
A	261	GLY	-	expression tag	UNP T1K8P1
A	262	GLU	-	expression tag	UNP T1K8P1
A	263	ASN	-	expression tag	UNP T1K8P1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	264	LEU	-	expression tag	UNP T1K8P1
A	265	TYR	-	expression tag	UNP T1K8P1
A	266	PHE	-	expression tag	UNP T1K8P1
A	267	GLN	-	expression tag	UNP T1K8P1
A	268	SER	-	expression tag	UNP T1K8P1
A	269	ALA	-	expression tag	UNP T1K8P1
A	270	GLY	-	expression tag	UNP T1K8P1
A	271	HIS	-	expression tag	UNP T1K8P1
A	272	HIS	-	expression tag	UNP T1K8P1
A	273	HIS	-	expression tag	UNP T1K8P1
A	274	HIS	-	expression tag	UNP T1K8P1
A	275	HIS	-	expression tag	UNP T1K8P1
A	276	HIS	-	expression tag	UNP T1K8P1
B	260	ALA	-	expression tag	UNP T1K8P1
B	261	GLY	-	expression tag	UNP T1K8P1
B	262	GLU	-	expression tag	UNP T1K8P1
B	263	ASN	-	expression tag	UNP T1K8P1
B	264	LEU	-	expression tag	UNP T1K8P1
B	265	TYR	-	expression tag	UNP T1K8P1
B	266	PHE	-	expression tag	UNP T1K8P1
B	267	GLN	-	expression tag	UNP T1K8P1
B	268	SER	-	expression tag	UNP T1K8P1
B	269	ALA	-	expression tag	UNP T1K8P1
B	270	GLY	-	expression tag	UNP T1K8P1
B	271	HIS	-	expression tag	UNP T1K8P1
B	272	HIS	-	expression tag	UNP T1K8P1
B	273	HIS	-	expression tag	UNP T1K8P1
B	274	HIS	-	expression tag	UNP T1K8P1
B	275	HIS	-	expression tag	UNP T1K8P1
B	276	HIS	-	expression tag	UNP T1K8P1
C	260	ALA	-	expression tag	UNP T1K8P1
C	261	GLY	-	expression tag	UNP T1K8P1
C	262	GLU	-	expression tag	UNP T1K8P1
C	263	ASN	-	expression tag	UNP T1K8P1
C	264	LEU	-	expression tag	UNP T1K8P1
C	265	TYR	-	expression tag	UNP T1K8P1
C	266	PHE	-	expression tag	UNP T1K8P1
C	267	GLN	-	expression tag	UNP T1K8P1
C	268	SER	-	expression tag	UNP T1K8P1
C	269	ALA	-	expression tag	UNP T1K8P1
C	270	GLY	-	expression tag	UNP T1K8P1
C	271	HIS	-	expression tag	UNP T1K8P1

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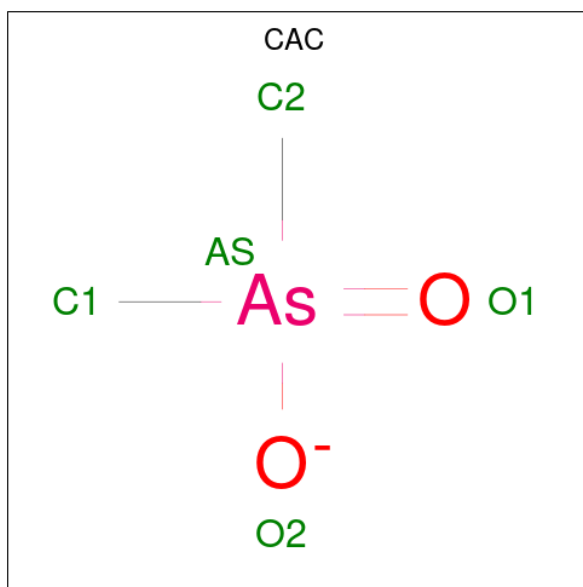
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Chain	Residue	Modelled	Actual	Comment	Reference
C	272	HIS	-	expression tag	UNP T1K8P1
C	273	HIS	-	expression tag	UNP T1K8P1
C	274	HIS	-	expression tag	UNP T1K8P1
C	275	HIS	-	expression tag	UNP T1K8P1
C	276	HIS	-	expression tag	UNP T1K8P1

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	U	1	Total Fe 1 1	0	0
2	A	1	Total Fe 1 1	0	0
2	B	1	Total Fe 1 1	0	0
2	C	1	Total Fe 1 1	0	0

- Molecule 3 is CACODYLATE ION (CCD ID: CAC) (formula: C₂H₆AsO₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	U	1	Total As C O 5 1 2 2	0	0
3	A	1	Total As C O 5 1 2 2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total 5	As 1	C 2	O 2	0	0
3	B	1	Total 5	As 1	C 2	O 2	0	0
3	C	1	Total 5	As 1	C 2	O 2	0	0
3	C	1	Total 5	As 1	C 2	O 2	0	0
3	C	1	Total 5	As 1	C 2	O 2	0	0
3	C	1	Total 5	As 1	C 2	O 2	0	0
3	C	1	Total 5	As 1	C 2	O 2	0	0

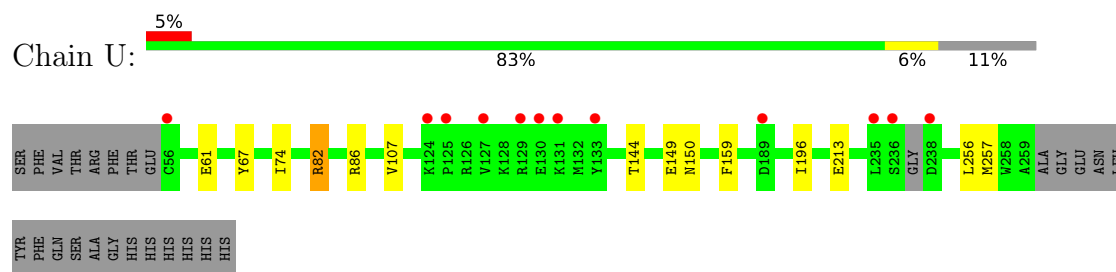
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	U	39	Total 39	O 39	0	0
4	A	44	Total 44	O 44	0	0
4	B	27	Total 27	O 27	0	0
4	C	30	Total 30	O 30	0	0

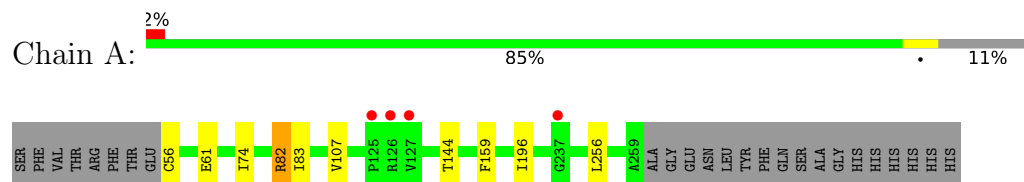
3 Residue-property plots [i](#)

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.

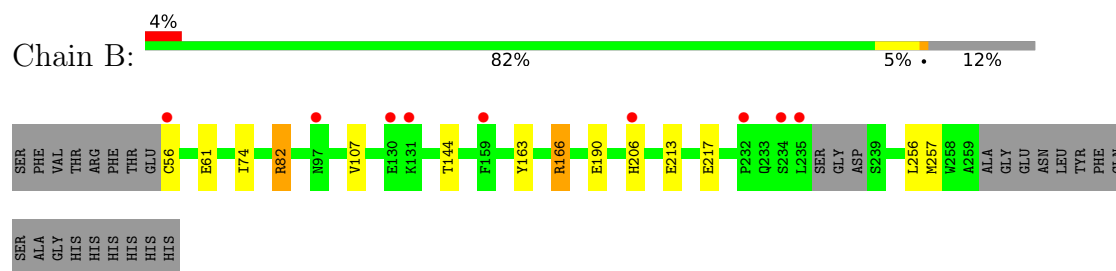
- Molecule 1: Intradiol ring-cleavage Dioxygenase



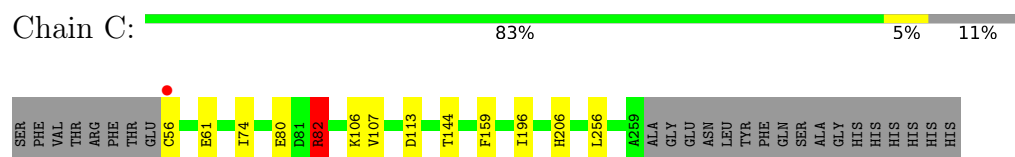
- Molecule 1: Intradiol ring-cleavage Dioxygenase



- Molecule 1: Intradiol ring-cleavage Dioxygenase



- Molecule 1: Intradiol ring-cleavage Dioxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	60.49Å 43.07Å 165.71Å 90.00° 95.18° 90.00°	Depositor
Resolution (Å)	50.01 – 2.46 50.01 – 2.46	Depositor EDS
% Data completeness (in resolution range)	95.0 (50.01-2.46) 95.2 (50.01-2.46)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.191 , 0.231 (Not available) , 0.206	Depositor DCC
R_{free} test set	1414 reflections (4.47%)	wwPDB-VP
Wilson B-factor (Å ²)	37.3	Xtriage
Anisotropy	0.856	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6649	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.30% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	1.02	1/1675 (0.1%)	0.99	0/2271
1	B	0.97	0/1635	0.99	1/2219 (0.0%)
1	C	0.95	1/1657 (0.1%)	1.01	2/2249 (0.1%)
1	U	0.96	0/1659	0.95	2/2250 (0.1%)
All	All	0.97	2/6626 (0.0%)	0.98	5/8989 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	80	GLU	CA-C	5.23	1.58	1.53
1	A	83	ILE	C-O	-5.04	1.19	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	206	HIS	N-CA-C	7.23	119.16	111.28
1	C	206	HIS	N-CA-C	5.45	117.30	111.36
1	C	82	ARG	NE-CZ-NH1	-5.39	116.11	121.50
1	U	86	ARG	NE-CZ-NH2	5.10	123.79	119.20
1	U	67	TYR	N-CA-C	5.02	118.94	112.41

There are no chirality outliers.

There are no planarity outliers.

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	1633	0	1574	6	0
1	B	1594	0	1519	8	0
1	C	1615	0	1548	8	0
1	U	1618	0	1551	8	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	U	1	0	0	0	0
3	A	5	0	0	0	0
3	B	10	0	0	0	0
3	C	25	0	0	1	0
3	U	5	0	0	0	0
4	A	44	0	0	0	0
4	B	27	0	0	0	0
4	C	30	0	0	1	0
4	U	39	0	0	0	0
All	All	6649	0	6192	28	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 (28) 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:U:74:ILE:HB	1:C:74:ILE:HB	1.78	0.64
1:A:74:ILE:HB	1:B:74:ILE:HB	1.80	0.64
1:U:149:GLU:OE1	1:U:150:ASN:ND2	2.41	0.54
1:U:61:GLU:HB3	1:U:256:LEU:HD12	1.91	0.52
1:U:159:PHE:CD1	1:U:196:ILE:HG21	2.48	0.48
1:A:159:PHE:CD1	1:A:196:ILE:HG21	2.49	0.48
1:U:82:ARG:N	1:U:82:ARG:HD2	2.29	0.48
1:C:159:PHE:CD1	1:C:196:ILE:HG21	2.48	0.47
1:B:190:GLU:OE1	1:B:190:GLU:HA	2.15	0.47
1:B:61:GLU:HB3	1:B:256:LEU:HD12	1.95	0.47
1:U:213:GLU:CD	1:U:213:GLU:H	2.24	0.46
1:C:61:GLU:HB3	1:C:256:LEU:HD12	1.97	0.45
1:B:213:GLU:CD	1:B:213:GLU:H	2.24	0.45
1:C:56:CYS:O	1:C:56:CYS:SG	2.74	0.45
1:C:106:LYS:NZ	3:C:302:CAC:O1	2.50	0.45
1:C:82:ARG:N	1:C:82:ARG:HD2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ARG:N	1:A:82:ARG:HD2	2.31	0.45
1:C:113:ASP:HB2	4:C:410:HOH:O	2.17	0.44
1:A:56:CYS:SG	1:A:56:CYS:O	2.76	0.43
1:B:82:ARG:N	1:B:82:ARG:HD2	2.34	0.42
1:B:107:VAL:O	1:B:144:THR:HA	2.20	0.41
1:U:257:MET:HE3	1:U:257:MET:HB3	1.92	0.41
1:B:56:CYS:SG	1:B:56:CYS:O	2.79	0.41
1:A:107:VAL:O	1:A:144:THR:HA	2.20	0.41
1:A:61:GLU:HB3	1:A:256:LEU:HD12	2.03	0.41
1:B:163:TYR:CE2	1:B:166:ARG:HG3	2.55	0.41
1:C:107:VAL:O	1:C:144:THR:HA	2.21	0.40
1:U:107:VAL:O	1:U:144:THR:HA	2.20	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	202/229 (88%)	196 (97%)	6 (3%)	0	100	100
1	B	197/229 (86%)	192 (98%)	5 (2%)	0	100	100
1	C	202/229 (88%)	196 (97%)	6 (3%)	0	100	100
1	U	199/229 (87%)	194 (98%)	5 (2%)	0	100	100
All	All	800/916 (87%)	778 (97%)	22 (3%)	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	180/204 (88%)	179 (99%)	1 (1%)	78	86
1	B	173/204 (85%)	169 (98%)	4 (2%)	44	59
1	C	176/204 (86%)	175 (99%)	1 (1%)	78	86
1	U	177/204 (87%)	176 (99%)	1 (1%)	78	86
All	All	706/816 (86%)	699 (99%)	7 (1%)	68	77

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	82	ARG
1	A	82	ARG
1	B	82	ARG
1	B	166	ARG
1	B	217	GLU
1	B	257	MET
1	C	82	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	U	92	ASN
1	U	145	GLN
1	U	150	ASN
1	U	177	ASN
1	U	197	GLN
1	A	92	ASN
1	A	145	GLN
1	A	197	GLN
1	A	229	ASN
1	B	92	ASN
1	B	145	GLN
1	B	197	GLN
1	C	92	ASN
1	C	145	GLN
1	C	150	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 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	CAC	A	302	-	2,4,4	2.93	2 (100%)	4,6,6	2.21	1 (25%)
3	CAC	B	303	-	2,4,4	2.84	2 (100%)	4,6,6	1.59	1 (25%)
3	CAC	C	304	-	2,4,4	2.75	2 (100%)	4,6,6	1.79	1 (25%)
3	CAC	C	305	-	2,4,4	2.85	2 (100%)	4,6,6	1.58	1 (25%)
3	CAC	U	302	-	2,4,4	2.82	2 (100%)	4,6,6	1.59	1 (25%)
3	CAC	C	306	-	2,4,4	2.85	2 (100%)	4,6,6	1.15	0
3	CAC	B	302	-	2,4,4	3.01	2 (100%)	4,6,6	1.54	1 (25%)
3	CAC	C	303	-	2,4,4	2.60	2 (100%)	4,6,6	2.48	3 (75%)
3	CAC	C	302	-	2,4,4	2.70	2 (100%)	4,6,6	2.07	2 (50%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	CAC	AS-C2	3.06	1.97	1.90
3	B	302	CAC	AS-C2	3.06	1.97	1.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	302	CAC	AS-C2	3.02	1.97	1.90
3	B	302	CAC	AS-C1	2.96	1.97	1.90
3	C	305	CAC	AS-C1	2.88	1.97	1.90
3	C	306	CAC	AS-C2	2.88	1.97	1.90
3	B	303	CAC	AS-C2	2.85	1.97	1.90
3	C	304	CAC	AS-C1	2.83	1.97	1.90
3	B	303	CAC	AS-C1	2.83	1.97	1.90
3	C	302	CAC	AS-C1	2.82	1.97	1.90
3	C	305	CAC	AS-C2	2.82	1.97	1.90
3	C	306	CAC	AS-C1	2.81	1.97	1.90
3	A	302	CAC	AS-C1	2.79	1.96	1.90
3	C	303	CAC	AS-C2	2.74	1.96	1.90
3	C	304	CAC	AS-C2	2.67	1.96	1.90
3	U	302	CAC	AS-C1	2.59	1.96	1.90
3	C	302	CAC	AS-C2	2.58	1.96	1.90
3	C	303	CAC	AS-C1	2.45	1.96	1.90

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	CAC	O1-AS-C1	-3.76	106.83	111.50
3	C	303	CAC	O1-AS-C2	-3.69	106.91	111.50
3	U	302	CAC	O1-AS-C1	-2.71	108.13	111.50
3	C	302	CAC	O1-AS-C1	-2.61	108.26	111.50
3	C	302	CAC	O2-AS-C1	2.44	111.75	105.84
3	B	303	CAC	O1-AS-C2	-2.20	108.76	111.50
3	C	303	CAC	O2-AS-C2	2.17	111.10	105.84
3	C	303	CAC	O1-AS-C1	-2.15	108.82	111.50
3	C	304	CAC	O1-AS-C1	-2.12	108.87	111.50
3	C	305	CAC	O1-AS-C2	-2.08	108.92	111.50
3	B	302	CAC	O1-AS-C1	-2.06	108.94	111.50

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	C	302	CAC	1	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, 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	204/229 (89%)	0.01	4 (1%) 65 66	31, 48, 80, 106	0
1	B	201/229 (87%)	0.20	9 (4%) 38 37	33, 54, 88, 123	0
1	C	204/229 (89%)	0.17	1 (0%) 87 88	35, 55, 95, 123	0
1	U	203/229 (88%)	0.21	12 (5%) 28 25	35, 55, 101, 131	0
All	All	812/916 (88%)	0.15	26 (3%) 50 51	31, 53, 93, 131	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	U	238	ASP	3.7
1	U	127	VAL	3.6
1	B	131	LYS	3.6
1	B	235	LEU	3.3
1	A	127	VAL	3.2
1	B	56	CYS	3.1
1	B	232	PRO	2.7
1	A	125	PRO	2.6
1	U	56	CYS	2.5
1	C	56	CYS	2.5
1	U	236	SER	2.4
1	B	130	GLU	2.4
1	U	189	ASP	2.3
1	U	131	LYS	2.2
1	U	125	PRO	2.2
1	B	234	SER	2.2
1	U	124	LYS	2.2
1	B	206	HIS	2.2
1	A	126	ARG	2.2
1	B	159	PHE	2.2
1	B	97	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	U	133	TYR	2.1
1	U	130	GLU	2.1
1	U	129	ARG	2.1
1	A	237	GLY	2.1
1	U	235	LEU	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(Å ²)	Q<0.9
3	CAC	C	306	5/5	0.58	0.25	147,154,158,159	0
3	CAC	A	302	5/5	0.64	0.21	125,127,128,133	0
3	CAC	B	302	5/5	0.66	0.23	106,121,124,132	0
3	CAC	U	302	5/5	0.70	0.21	124,125,131,135	0
3	CAC	C	304	5/5	0.74	0.14	149,149,157,160	0
3	CAC	B	303	5/5	0.75	0.21	125,126,140,145	0
3	CAC	C	302	5/5	0.76	0.20	132,137,138,141	0
3	CAC	C	303	5/5	0.76	0.16	148,149,156,160	0
3	CAC	C	305	5/5	0.77	0.20	130,137,146,151	0
2	FE	B	301	1/1	0.97	0.05	53,53,53,53	0
2	FE	C	301	1/1	0.98	0.07	58,58,58,58	0
2	FE	A	301	1/1	0.99	0.03	46,46,46,46	0
2	FE	U	301	1/1	0.99	0.05	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.