



wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 08:00 pm BST

PDB ID : 5XMD
Title : Crystal structure of epoxide hydrolase VrEH1 from Vigna radiata
Authors : Kong, X.D.; Xu, J.H.; Zhou, J.H.
Deposited on : 2017-05-14
Resolution : 2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

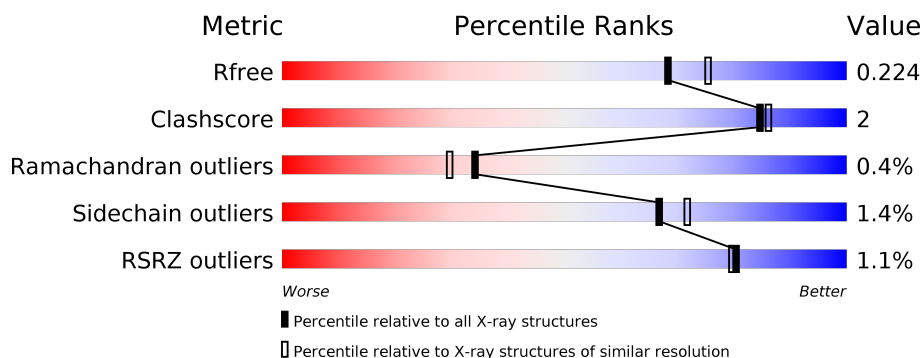
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 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	353	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>5%</div> <div>9%</div> </div> </div>
1	B	353	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>7%</div> <div>9%</div> </div> </div>
1	C	353	<div> <div>%</div> <div> <div></div> <div>80%</div> <div>7%</div> <div>14%</div> </div> </div>
1	D	353	<div> <div></div> <div> <div></div> <div>82%</div> <div>5%</div> <div>13%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10544 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 Epoxide hydrolase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	2	0
			2549	1647	426	468	8			
1	B	322	Total	C	N	O	S	0	0	0
			2550	1647	428	467	8			
1	C	305	Total	C	N	O	S	0	0	0
			2429	1576	403	442	8			
1	D	308	Total	C	N	O	S	0	2	0
			2473	1599	413	453	8			

There are 140 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-33	MET	-	expression tag	UNP E5L4L1
A	-32	GLY	-	expression tag	UNP E5L4L1
A	-31	SER	-	expression tag	UNP E5L4L1
A	-30	SER	-	expression tag	UNP E5L4L1
A	-29	HIS	-	expression tag	UNP E5L4L1
A	-28	HIS	-	expression tag	UNP E5L4L1
A	-27	HIS	-	expression tag	UNP E5L4L1
A	-26	HIS	-	expression tag	UNP E5L4L1
A	-25	HIS	-	expression tag	UNP E5L4L1
A	-24	HIS	-	expression tag	UNP E5L4L1
A	-23	SER	-	expression tag	UNP E5L4L1
A	-22	SER	-	expression tag	UNP E5L4L1
A	-21	GLY	-	expression tag	UNP E5L4L1
A	-20	LEU	-	expression tag	UNP E5L4L1
A	-19	VAL	-	expression tag	UNP E5L4L1
A	-18	PRO	-	expression tag	UNP E5L4L1
A	-17	ARG	-	expression tag	UNP E5L4L1
A	-16	GLY	-	expression tag	UNP E5L4L1
A	-15	SER	-	expression tag	UNP E5L4L1
A	-14	HIS	-	expression tag	UNP E5L4L1
A	-13	MET	-	expression tag	UNP E5L4L1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	ALA	-	expression tag	UNP E5L4L1
A	-11	SER	-	expression tag	UNP E5L4L1
A	-10	MET	-	expression tag	UNP E5L4L1
A	-9	THR	-	expression tag	UNP E5L4L1
A	-8	GLY	-	expression tag	UNP E5L4L1
A	-7	GLY	-	expression tag	UNP E5L4L1
A	-6	GLN	-	expression tag	UNP E5L4L1
A	-5	GLN	-	expression tag	UNP E5L4L1
A	-4	MET	-	expression tag	UNP E5L4L1
A	-3	GLY	-	expression tag	UNP E5L4L1
A	-2	ARG	-	expression tag	UNP E5L4L1
A	-1	GLY	-	expression tag	UNP E5L4L1
A	0	SER	-	expression tag	UNP E5L4L1
A	285	PRO	HIS	see sequence details	UNP E5L4L1
B	-33	MET	-	expression tag	UNP E5L4L1
B	-32	GLY	-	expression tag	UNP E5L4L1
B	-31	SER	-	expression tag	UNP E5L4L1
B	-30	SER	-	expression tag	UNP E5L4L1
B	-29	HIS	-	expression tag	UNP E5L4L1
B	-28	HIS	-	expression tag	UNP E5L4L1
B	-27	HIS	-	expression tag	UNP E5L4L1
B	-26	HIS	-	expression tag	UNP E5L4L1
B	-25	HIS	-	expression tag	UNP E5L4L1
B	-24	HIS	-	expression tag	UNP E5L4L1
B	-23	SER	-	expression tag	UNP E5L4L1
B	-22	SER	-	expression tag	UNP E5L4L1
B	-21	GLY	-	expression tag	UNP E5L4L1
B	-20	LEU	-	expression tag	UNP E5L4L1
B	-19	VAL	-	expression tag	UNP E5L4L1
B	-18	PRO	-	expression tag	UNP E5L4L1
B	-17	ARG	-	expression tag	UNP E5L4L1
B	-16	GLY	-	expression tag	UNP E5L4L1
B	-15	SER	-	expression tag	UNP E5L4L1
B	-14	HIS	-	expression tag	UNP E5L4L1
B	-13	MET	-	expression tag	UNP E5L4L1
B	-12	ALA	-	expression tag	UNP E5L4L1
B	-11	SER	-	expression tag	UNP E5L4L1
B	-10	MET	-	expression tag	UNP E5L4L1
B	-9	THR	-	expression tag	UNP E5L4L1
B	-8	GLY	-	expression tag	UNP E5L4L1
B	-7	GLY	-	expression tag	UNP E5L4L1
B	-6	GLN	-	expression tag	UNP E5L4L1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	GLN	-	expression tag	UNP E5L4L1
B	-4	MET	-	expression tag	UNP E5L4L1
B	-3	GLY	-	expression tag	UNP E5L4L1
B	-2	ARG	-	expression tag	UNP E5L4L1
B	-1	GLY	-	expression tag	UNP E5L4L1
B	0	SER	-	expression tag	UNP E5L4L1
B	285	PRO	HIS	see sequence details	UNP E5L4L1
C	-33	MET	-	expression tag	UNP E5L4L1
C	-32	GLY	-	expression tag	UNP E5L4L1
C	-31	SER	-	expression tag	UNP E5L4L1
C	-30	SER	-	expression tag	UNP E5L4L1
C	-29	HIS	-	expression tag	UNP E5L4L1
C	-28	HIS	-	expression tag	UNP E5L4L1
C	-27	HIS	-	expression tag	UNP E5L4L1
C	-26	HIS	-	expression tag	UNP E5L4L1
C	-25	HIS	-	expression tag	UNP E5L4L1
C	-24	HIS	-	expression tag	UNP E5L4L1
C	-23	SER	-	expression tag	UNP E5L4L1
C	-22	SER	-	expression tag	UNP E5L4L1
C	-21	GLY	-	expression tag	UNP E5L4L1
C	-20	LEU	-	expression tag	UNP E5L4L1
C	-19	VAL	-	expression tag	UNP E5L4L1
C	-18	PRO	-	expression tag	UNP E5L4L1
C	-17	ARG	-	expression tag	UNP E5L4L1
C	-16	GLY	-	expression tag	UNP E5L4L1
C	-15	SER	-	expression tag	UNP E5L4L1
C	-14	HIS	-	expression tag	UNP E5L4L1
C	-13	MET	-	expression tag	UNP E5L4L1
C	-12	ALA	-	expression tag	UNP E5L4L1
C	-11	SER	-	expression tag	UNP E5L4L1
C	-10	MET	-	expression tag	UNP E5L4L1
C	-9	THR	-	expression tag	UNP E5L4L1
C	-8	GLY	-	expression tag	UNP E5L4L1
C	-7	GLY	-	expression tag	UNP E5L4L1
C	-6	GLN	-	expression tag	UNP E5L4L1
C	-5	GLN	-	expression tag	UNP E5L4L1
C	-4	MET	-	expression tag	UNP E5L4L1
C	-3	GLY	-	expression tag	UNP E5L4L1
C	-2	ARG	-	expression tag	UNP E5L4L1
C	-1	GLY	-	expression tag	UNP E5L4L1
C	0	SER	-	expression tag	UNP E5L4L1
C	285	PRO	HIS	see sequence details	UNP E5L4L1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-33	MET	-	expression tag	UNP E5L4L1
D	-32	GLY	-	expression tag	UNP E5L4L1
D	-31	SER	-	expression tag	UNP E5L4L1
D	-30	SER	-	expression tag	UNP E5L4L1
D	-29	HIS	-	expression tag	UNP E5L4L1
D	-28	HIS	-	expression tag	UNP E5L4L1
D	-27	HIS	-	expression tag	UNP E5L4L1
D	-26	HIS	-	expression tag	UNP E5L4L1
D	-25	HIS	-	expression tag	UNP E5L4L1
D	-24	HIS	-	expression tag	UNP E5L4L1
D	-23	SER	-	expression tag	UNP E5L4L1
D	-22	SER	-	expression tag	UNP E5L4L1
D	-21	GLY	-	expression tag	UNP E5L4L1
D	-20	LEU	-	expression tag	UNP E5L4L1
D	-19	VAL	-	expression tag	UNP E5L4L1
D	-18	PRO	-	expression tag	UNP E5L4L1
D	-17	ARG	-	expression tag	UNP E5L4L1
D	-16	GLY	-	expression tag	UNP E5L4L1
D	-15	SER	-	expression tag	UNP E5L4L1
D	-14	HIS	-	expression tag	UNP E5L4L1
D	-13	MET	-	expression tag	UNP E5L4L1
D	-12	ALA	-	expression tag	UNP E5L4L1
D	-11	SER	-	expression tag	UNP E5L4L1
D	-10	MET	-	expression tag	UNP E5L4L1
D	-9	THR	-	expression tag	UNP E5L4L1
D	-8	GLY	-	expression tag	UNP E5L4L1
D	-7	GLY	-	expression tag	UNP E5L4L1
D	-6	GLN	-	expression tag	UNP E5L4L1
D	-5	GLN	-	expression tag	UNP E5L4L1
D	-4	MET	-	expression tag	UNP E5L4L1
D	-3	GLY	-	expression tag	UNP E5L4L1
D	-2	ARG	-	expression tag	UNP E5L4L1
D	-1	GLY	-	expression tag	UNP E5L4L1
D	0	SER	-	expression tag	UNP E5L4L1
D	285	PRO	HIS	see sequence details	UNP E5L4L1

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	169	Total O 169 169	0	0
2	B	141	Total O 141 141	0	0

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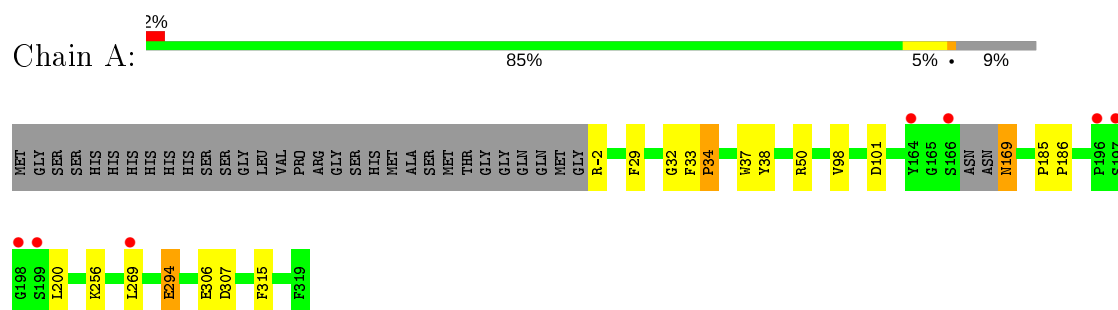
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	111	Total 111	O 111	0	0
2	D	122	Total 122	O 122	0	0

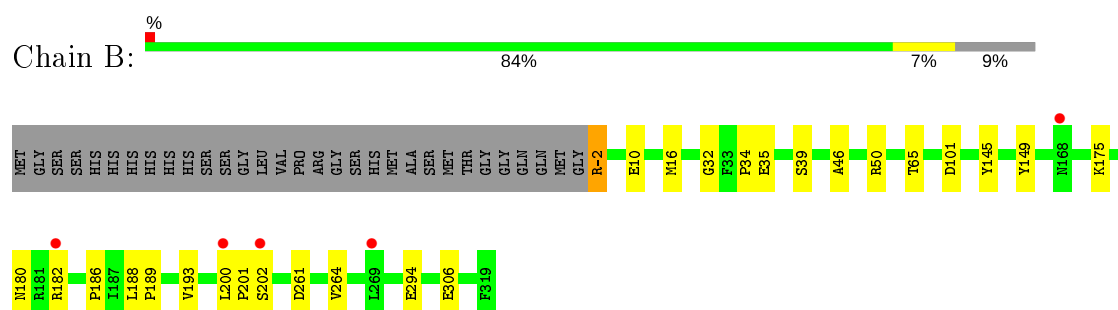
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

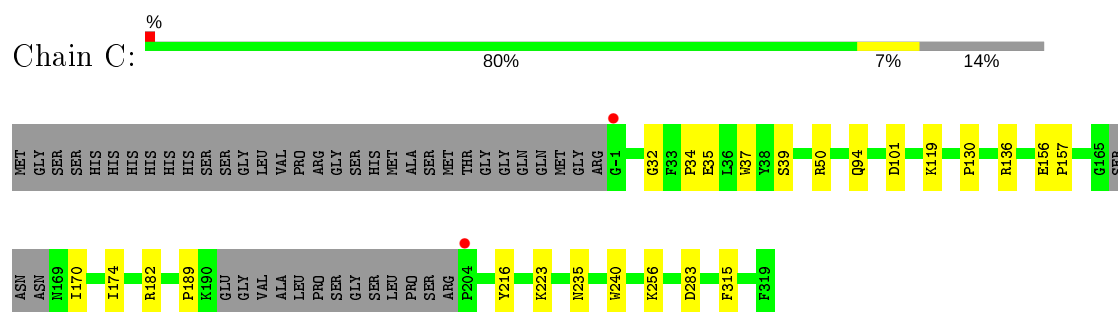
- Molecule 1: Epoxide hydrolase A



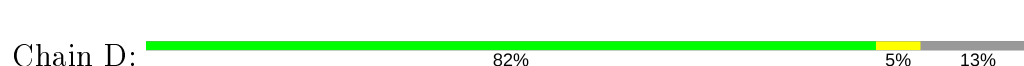
- Molecule 1: Epoxide hydrolase A



- Molecule 1: Epoxide hydrolase A



- Molecule 1: Epoxide hydrolase A





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.69Å 51.89Å 124.29Å 90.00° 94.27° 90.00°	Depositor
Resolution (Å)	41.32 – 2.00 41.32 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.4 (41.32-2.00) 93.2 (41.32-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.179 , 0.223 0.181 , 0.224	Depositor DCC
R_{free} test set	4128 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	29.8	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10544	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.50% 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](#)

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	0.41	0/2619	0.54	0/3559
1	B	0.40	0/2621	0.52	0/3564
1	C	0.38	0/2496	0.51	0/3390
1	D	0.38	0/2541	0.50	0/3453
All	All	0.39	0/10277	0.52	0/13966

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 [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	2549	0	2515	12	0
1	B	2550	0	2519	14	0
1	C	2429	0	2398	10	0
1	D	2473	0	2436	9	0
2	A	169	0	0	4	0
2	B	141	0	0	2	1
2	C	111	0	0	2	0
2	D	122	0	0	0	1
All	All	10544	0	9868	45	1

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.

The worst 5 of 45 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:B:202:SER:O	2:B:401:HOH:O	2.01	0.79
1:C:223:LYS:NZ	2:C:401:HOH:O	2.28	0.65
1:A:294:GLU:H	1:A:294:GLU:CD	2.01	0.61
1:D:32:GLY:HA3	1:D:101:ASP:HB3	1.83	0.59
1:D:10:GLU:HG2	1:D:15:LYS:HD3	1.84	0.59

All (1) 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)
2:B:475:HOH:O	2:D:512:HOH:O[2_444]	2.18	0.02

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	318/353 (90%)	311 (98%)	6 (2%)	1 (0%)	41	37
1	B	320/353 (91%)	308 (96%)	11 (3%)	1 (0%)	41	37
1	C	299/353 (85%)	286 (96%)	11 (4%)	2 (1%)	22	16
1	D	306/353 (87%)	296 (97%)	9 (3%)	1 (0%)	41	37
All	All	1243/1412 (88%)	1201 (97%)	37 (3%)	5 (0%)	34	30

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	189	PRO
1	B	34	PRO
1	D	34	PRO

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Mol	Chain	Res	Type
1	A	34	PRO
1	C	34	PRO

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	272/296 (92%)	268 (98%)	4 (2%)	65	69
1	B	272/296 (92%)	268 (98%)	4 (2%)	65	69
1	C	258/296 (87%)	254 (98%)	4 (2%)	62	67
1	D	264/296 (89%)	261 (99%)	3 (1%)	73	78
All	All	1066/1184 (90%)	1051 (99%)	15 (1%)	67	72

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	193	VAL
1	B	306	GLU
1	D	119	LYS
1	B	10	GLU
1	C	182	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	235	ASN
1	D	155	GLN

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	320/353 (90%)	-0.38	7 (2%) 62 60	17, 28, 47, 66	0
1	B	322/353 (91%)	-0.32	5 (1%) 72 70	18, 29, 51, 65	0
1	C	305/353 (86%)	-0.10	2 (0%) 87 87	19, 34, 56, 70	0
1	D	308/353 (87%)	-0.37	0 100 100	19, 34, 51, 69	0
All	All	1255/1412 (88%)	-0.30	14 (1%) 80 79	17, 31, 52, 70	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	-1	GLY	4.4
1	B	202	SER	3.8
1	A	269	LEU	3.5
1	A	199	SER	3.2
1	A	196	PRO	3.2

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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.