



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 08:01 AM UTC

PDB ID : 2Q4I / pdb_00002q4i
Title : Ensemble refinement of the protein crystal structure of allene oxide cyclase from Arabidopsis thaliana At3g25770
Authors : Levin, E.J.; Kondrashov, D.A.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)
Deposited on : 2007-05-31
Resolution : 1.71 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:

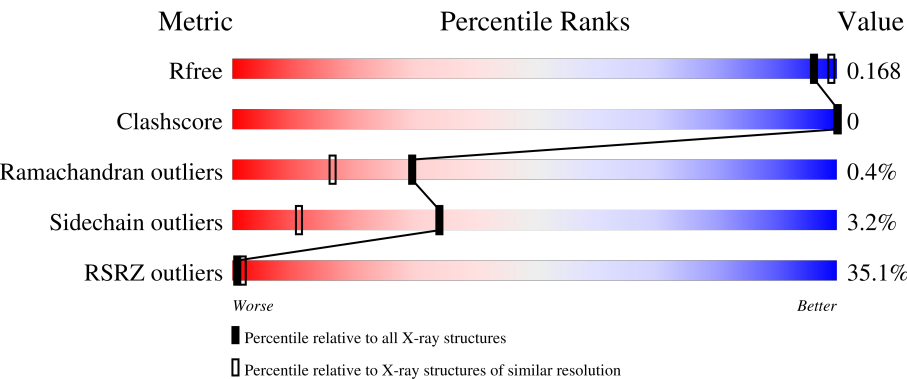
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.71 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.



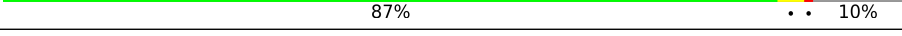
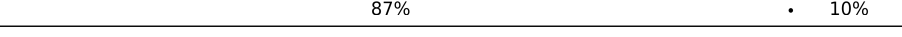
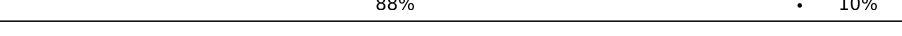
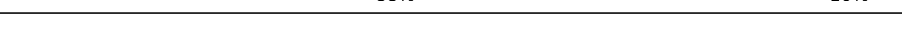
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1039 (1.72-1.72)
Clashscore	190562	1049 (1.72-1.72)
Ramachandran outliers	187476	1041 (1.72-1.72)
Sidechain outliers	187428	1041 (1.72-1.72)
RSRZ outliers	180081	1039 (1.72-1.72)

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	1-A	193	31% 88% 10%
1	1-B	193	32% 87% 10%
1	1-C	193	32% 88% 10%
1	2-A	193	87% 10%
1	2-B	193	87% 10%

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Mol	Chain	Length	Quality of chain
1	2-C	193	 88% 10%
1	3-A	193	 85% 5% 10%
1	3-B	193	 87% 10%
1	3-C	193	 88% 10%
1	4-A	193	 88% 10%
1	4-B	193	 87% 10%
1	4-C	193	 87% 10%
1	5-A	193	 88% 10%
1	5-B	193	 87% 10%
1	5-C	193	 87% 10%
1	6-A	193	 87% 10%
1	6-B	193	 87% 10%
1	6-C	193	 87% 10%
1	7-A	193	 88% 10%
1	7-B	193	 87% 10%
1	7-C	193	 87% 10%
1	8-A	193	 87% 10%
1	8-B	193	 86% 10%
1	8-C	193	 88% 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 38664 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 Allene oxide cyclase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-A	174	Total	C	N	O	S	Se	0	0	0
			1364	891	213	258	1	1			
1	2-A	174	Total	C	N	O	S	Se	0	0	0
			1364	891	213	258	1	1			
1	3-A	174	Total	C	N	O	S	Se	0	0	0
			1364	891	213	258	1	1			
1	4-A	174	Total	C	N	O	S	Se	0	0	0
			1364	891	213	258	1	1			
1	5-A	174	Total	C	N	O	S	Se	0	0	0
			1364	891	213	258	1	1			
1	6-A	174	Total	C	N	O	S	Se	0	0	0
			1364	891	213	258	1	1			
1	7-A	174	Total	C	N	O	S	Se	0	0	0
			1364	891	213	258	1	1			
1	8-A	174	Total	C	N	O	S	Se	0	0	0
			1364	891	213	258	1	1			
1	1-B	174	Total	C	N	O	S	Se	0	0	0
			1364	891	213	258	1	1			
1	2-B	174	Total	C	N	O	S	Se	0	0	0
			1364	891	213	258	1	1			
1	3-B	174	Total	C	N	O	S	Se	0	0	0
			1364	891	213	258	1	1			
1	4-B	174	Total	C	N	O	S	Se	0	0	0
			1364	891	213	258	1	1			
1	5-B	174	Total	C	N	O	S	Se	0	0	0
			1364	891	213	258	1	1			
1	6-B	174	Total	C	N	O	S	Se	0	0	0
			1364	891	213	258	1	1			
1	7-B	174	Total	C	N	O	S	Se	0	0	0
			1364	891	213	258	1	1			
1	8-B	174	Total	C	N	O	S	Se	0	0	0
			1364	891	213	258	1	1			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-C	174	Total	C	N	O	S	Se	0	0	0
			1364	891	213	258	1	1			
1	2-C	174	Total	C	N	O	S	Se	0	0	0
			1364	891	213	258	1	1			
1	3-C	174	Total	C	N	O	S	Se	0	0	0
			1364	891	213	258	1	1			
1	4-C	174	Total	C	N	O	S	Se	0	0	0
			1364	891	213	258	1	1			
1	5-C	174	Total	C	N	O	S	Se	0	0	0
			1364	891	213	258	1	1			
1	6-C	174	Total	C	N	O	S	Se	0	0	0
			1364	891	213	258	1	1			
1	7-C	174	Total	C	N	O	S	Se	0	0	0
			1364	891	213	258	1	1			
1	8-C	174	Total	C	N	O	S	Se	0	0	0
			1364	891	213	258	1	1			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP Q9LS02
A	47	MSE	MET	modified residue	UNP Q9LS02
B	1	SER	-	expression tag	UNP Q9LS02
B	47	MSE	MET	modified residue	UNP Q9LS02
C	1	SER	-	expression tag	UNP Q9LS02
C	47	MSE	MET	modified residue	UNP Q9LS02

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	1-A	248	Total	O	0	0
			248	248		
2	2-A	250	Total	O	0	0
			250	250		
2	3-A	246	Total	O	0	0
			246	246		
2	4-A	244	Total	O	0	0
			244	244		
2	5-A	243	Total	O	0	0
			243	243		
2	6-A	247	Total	O	0	0
			247	247		

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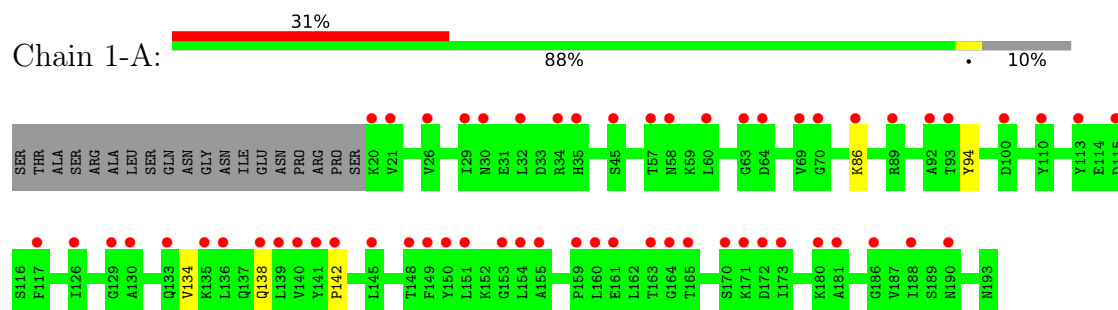
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	7-A	241	Total 241	O 241	0	0
2	8-A	251	Total 251	O 251	0	0
2	1-B	247	Total 247	O 247	0	0
2	2-B	248	Total 248	O 248	0	0
2	3-B	249	Total 249	O 249	0	0
2	4-B	254	Total 254	O 254	0	0
2	5-B	251	Total 251	O 251	0	0
2	6-B	250	Total 250	O 250	0	0
2	7-B	251	Total 251	O 251	0	0
2	8-B	249	Total 249	O 249	0	0
2	1-C	246	Total 246	O 246	0	0
2	2-C	243	Total 243	O 243	0	0
2	3-C	246	Total 246	O 246	0	0
2	4-C	243	Total 243	O 243	0	0
2	5-C	247	Total 247	O 247	0	0
2	6-C	244	Total 244	O 244	0	0
2	7-C	249	Total 249	O 249	0	0
2	8-C	241	Total 241	O 241	0	0

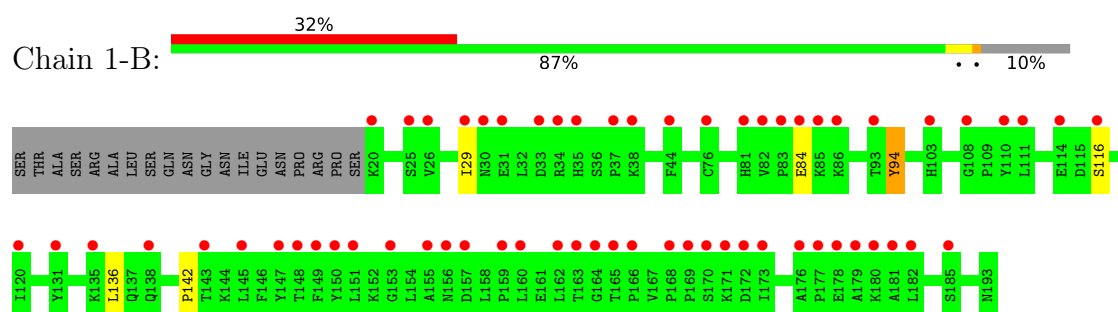
3 Residue-property plots [i](#)

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.

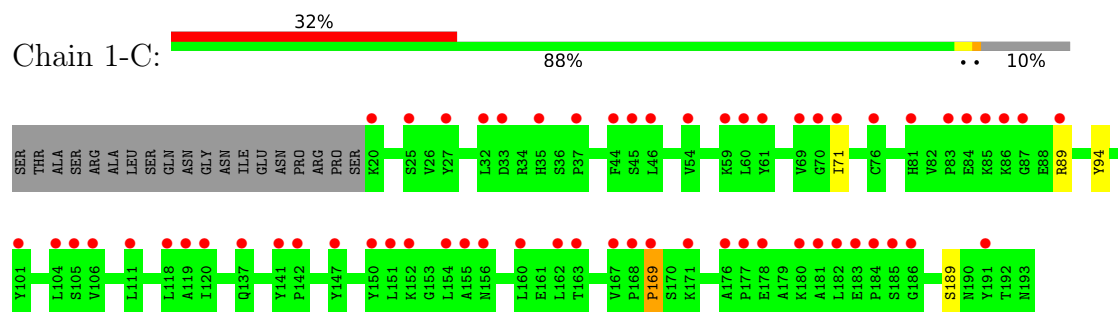
• Molecule 1: Allene oxide cyclase 2



• Molecule 1: Allene oxide cyclase 2

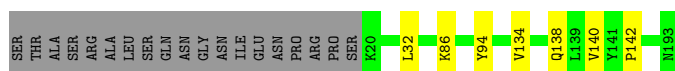


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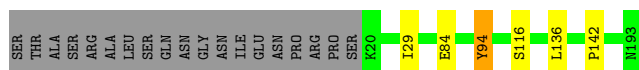
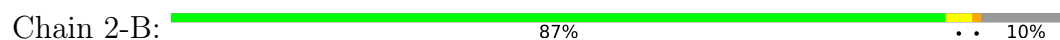


• Molecule 1: Allene oxide cyclase 2

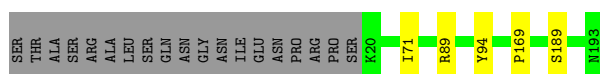
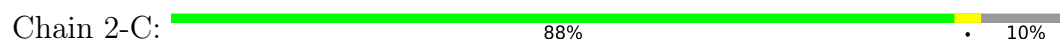




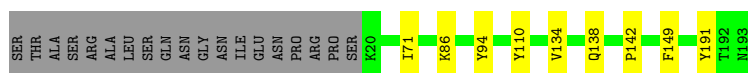
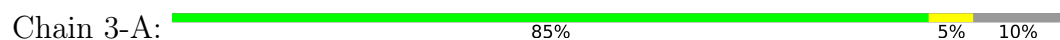
- Molecule 1: Allene oxide cyclase 2



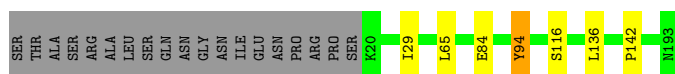
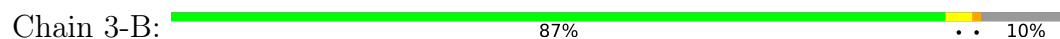
- Molecule 1: Allene oxide cyclase 2



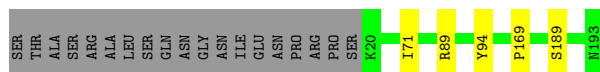
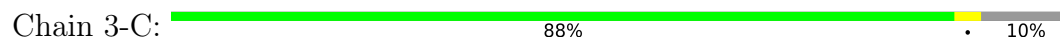
- Molecule 1: Allene oxide cyclase 2



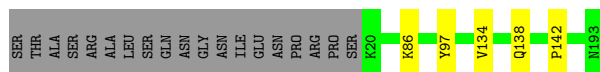
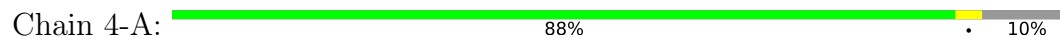
- Molecule 1: Allene oxide cyclase 2



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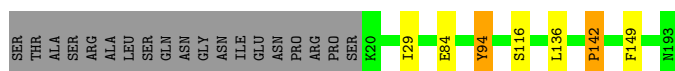


- Molecule 1: Allene oxide cyclase 2



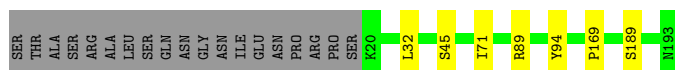
- Molecule 1: Allene oxide cyclase 2





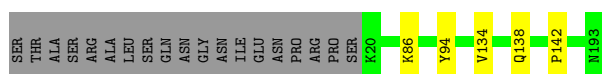
- Molecule 1: Allene oxide cyclase 2

Chain 4-C: 87% 10%



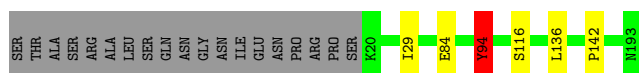
- Molecule 1: Allene oxide cyclase 2

Chain 5-A: 88% 10%



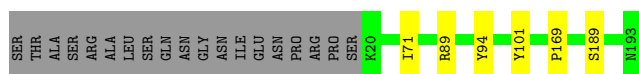
- Molecule 1: Allene oxide cyclase 2

Chain 5-B: 87% 10%



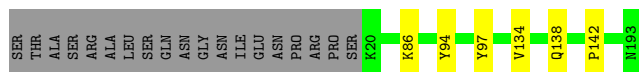
- Molecule 1: Allene oxide cyclase 2

Chain 5-C: 87% 10%



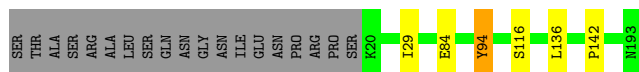
- Molecule 1: Allene oxide cyclase 2

Chain 6-A: 87% 10%



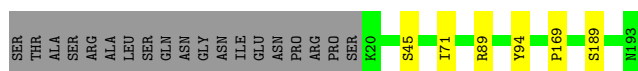
- Molecule 1: Allene oxide cyclase 2

Chain 6-B: 87% 10%



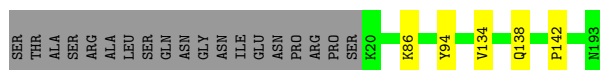
- Molecule 1: Allene oxide cyclase 2

Chain 6-C: 87% 10%



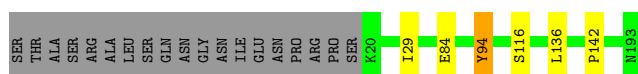
- Molecule 1: Allene oxide cyclase 2

Chain 7-A: 88% 10%



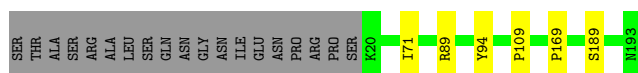
- Molecule 1: Allene oxide cyclase 2

Chain 7-B: 87% 10%



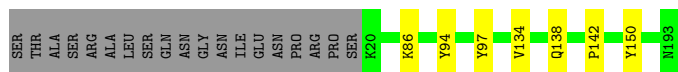
- Molecule 1: Allene oxide cyclase 2

Chain 7-C: 87% 10%



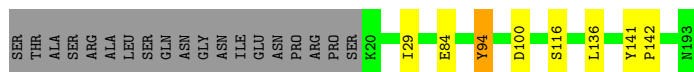
- Molecule 1: Allene oxide cyclase 2

Chain 8-A: 87% 10%



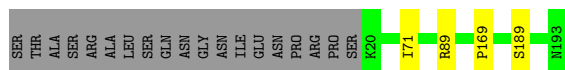
- Molecule 1: Allene oxide cyclase 2

Chain 8-B: 86% 10%



- Molecule 1: Allene oxide cyclase 2

Chain 8-C: 88% 10%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.41Å 100.01Å 105.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.17 – 1.71 48.17 – 1.71	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.17-1.71) 99.9 (48.17-1.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.53 (at 1.71Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.132 , 0.172 0.130 , 0.168	Depositor DCC
R_{free} test set	3725 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	11.3	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.04 , 57.4	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	0.87	EDS
Total number of atoms	38664	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% 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

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	1-A	0.51	0/1399	0.47	0/1897
1	1-B	0.50	0/1399	0.48	0/1897
1	1-C	0.49	0/1399	0.48	0/1897
1	2-A	0.51	0/1399	0.47	0/1897
1	2-B	0.50	0/1399	0.48	0/1897
1	2-C	0.49	0/1399	0.48	0/1897
1	3-A	0.51	0/1399	0.47	0/1897
1	3-B	0.50	0/1399	0.48	0/1897
1	3-C	0.49	0/1399	0.48	0/1897
1	4-A	0.51	0/1399	0.47	0/1897
1	4-B	0.50	0/1399	0.48	0/1897
1	4-C	0.49	0/1399	0.48	0/1897
1	5-A	0.51	0/1399	0.47	0/1897
1	5-B	0.50	0/1399	0.48	0/1897
1	5-C	0.49	0/1399	0.48	0/1897
1	6-A	0.51	0/1399	0.47	0/1897
1	6-B	0.50	0/1399	0.48	0/1897
1	6-C	0.49	0/1399	0.48	0/1897
1	7-A	0.51	0/1399	0.47	0/1897
1	7-B	0.50	0/1399	0.48	0/1897
1	7-C	0.49	0/1399	0.48	0/1897
1	8-A	0.51	0/1399	0.47	0/1897
1	8-B	0.50	0/1399	0.48	0/1897
1	8-C	0.49	0/1399	0.48	0/1897
All	All	0.50	0/33576	0.48	0/45528

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	1-A	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	1-B	0	1
1	1-C	0	1
1	2-A	0	1
1	2-B	0	1
1	2-C	0	1
1	3-A	0	2
1	3-B	0	1
1	3-C	0	1
1	4-A	0	1
1	4-B	0	1
1	4-C	0	1
1	5-A	0	1
1	5-B	0	1
1	5-C	0	2
1	6-A	0	2
1	6-B	0	1
1	6-C	0	1
1	7-A	0	1
1	7-B	0	1
1	7-C	0	1
1	8-A	0	3
1	8-B	0	2
All	All	0	29

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (29) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	94	TYR	Sidechain
1	1-B	94	TYR	Sidechain
1	1-C	94	TYR	Sidechain
1	2-A	94	TYR	Sidechain
1	2-B	94	TYR	Sidechain
1	2-C	94	TYR	Sidechain
1	3-A	110	TYR	Sidechain
1	3-A	94	TYR	Sidechain
1	3-B	94	TYR	Sidechain
1	3-C	94	TYR	Sidechain
1	4-A	97	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	4-B	94	TYR	Sidechain
1	4-C	94	TYR	Sidechain
1	5-A	94	TYR	Sidechain
1	5-B	94	TYR	Sidechain
1	5-C	101	TYR	Sidechain
1	5-C	94	TYR	Sidechain
1	6-A	94	TYR	Sidechain
1	6-A	97	TYR	Sidechain
1	6-B	94	TYR	Sidechain
1	6-C	94	TYR	Sidechain
1	7-A	94	TYR	Sidechain
1	7-B	94	TYR	Sidechain
1	7-C	94	TYR	Sidechain
1	8-A	150	TYR	Sidechain
1	8-A	94	TYR	Sidechain
1	8-A	97	TYR	Sidechain
1	8-B	141	TYR	Sidechain
1	8-B	94	TYR	Sidechain

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	1-A	1364	0	1356	0	0
1	1-B	1364	0	1356	0	0
1	1-C	1364	0	1356	0	0
1	2-A	1364	0	1356	0	0
1	2-B	1364	0	1356	0	0
1	2-C	1364	0	1356	0	0
1	3-A	1364	0	1356	0	0
1	3-B	1364	0	1356	0	0
1	3-C	1364	0	1356	0	0
1	4-A	1364	0	1356	0	0
1	4-B	1364	0	1356	0	0
1	4-C	1364	0	1356	0	0
1	5-A	1364	0	1356	0	0
1	5-B	1364	0	1356	0	0
1	5-C	1364	0	1356	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	6-A	1364	0	1356	0	0
1	6-B	1364	0	1356	0	0
1	6-C	1364	0	1356	0	0
1	7-A	1364	0	1356	0	0
1	7-B	1364	0	1356	0	0
1	7-C	1364	0	1356	0	0
1	8-A	1364	0	1356	0	0
1	8-B	1364	0	1356	0	0
1	8-C	1364	0	1356	0	0
2	1-A	248	0	0	0	0
2	1-B	247	0	0	0	0
2	1-C	246	0	0	0	0
2	2-A	250	0	0	0	0
2	2-B	248	0	0	0	0
2	2-C	243	0	0	0	0
2	3-A	246	0	0	0	0
2	3-B	249	0	0	0	0
2	3-C	246	0	0	0	0
2	4-A	244	0	0	0	0
2	4-B	254	0	0	0	0
2	4-C	243	0	0	0	0
2	5-A	243	0	0	0	0
2	5-B	251	0	0	0	0
2	5-C	247	0	0	0	0
2	6-A	247	0	0	0	0
2	6-B	250	0	0	0	0
2	6-C	244	0	0	0	0
2	7-A	241	0	0	0	0
2	7-B	251	0	0	0	0
2	7-C	249	0	0	0	0
2	8-A	251	0	0	0	0
2	8-B	249	0	0	0	0
2	8-C	241	0	0	0	0
All	All	38664	0	32544	0	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 0.

There are no clashes within the asymmetric unit.

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	1-A	172/193 (89%)	166 (96%)	6 (4%)	0	100	100
1	1-B	172/193 (89%)	165 (96%)	7 (4%)	0	100	100
1	1-C	172/193 (89%)	162 (94%)	9 (5%)	1 (1%)	21	9
1	2-A	172/193 (89%)	157 (91%)	13 (8%)	2 (1%)	10	2
1	2-B	172/193 (89%)	161 (94%)	11 (6%)	0	100	100
1	2-C	172/193 (89%)	161 (94%)	11 (6%)	0	100	100
1	3-A	172/193 (89%)	154 (90%)	15 (9%)	3 (2%)	7	1
1	3-B	172/193 (89%)	158 (92%)	13 (8%)	1 (1%)	21	9
1	3-C	172/193 (89%)	164 (95%)	8 (5%)	0	100	100
1	4-A	172/193 (89%)	165 (96%)	7 (4%)	0	100	100
1	4-B	172/193 (89%)	166 (96%)	4 (2%)	2 (1%)	10	2
1	4-C	172/193 (89%)	159 (92%)	11 (6%)	2 (1%)	10	2
1	5-A	172/193 (89%)	165 (96%)	7 (4%)	0	100	100
1	5-B	172/193 (89%)	162 (94%)	9 (5%)	1 (1%)	21	9
1	5-C	172/193 (89%)	167 (97%)	5 (3%)	0	100	100
1	6-A	172/193 (89%)	168 (98%)	4 (2%)	0	100	100
1	6-B	172/193 (89%)	162 (94%)	10 (6%)	0	100	100
1	6-C	172/193 (89%)	168 (98%)	3 (2%)	1 (1%)	21	9
1	7-A	172/193 (89%)	165 (96%)	7 (4%)	0	100	100
1	7-B	172/193 (89%)	167 (97%)	5 (3%)	0	100	100
1	7-C	172/193 (89%)	163 (95%)	8 (5%)	1 (1%)	21	9
1	8-A	172/193 (89%)	161 (94%)	11 (6%)	0	100	100
1	8-B	172/193 (89%)	165 (96%)	6 (4%)	1 (1%)	21	9
1	8-C	172/193 (89%)	162 (94%)	10 (6%)	0	100	100
All	All	4128/4632 (89%)	3913 (95%)	200 (5%)	15 (0%)	30	16

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2-A	32	LEU
1	3-A	191	TYR
1	3-B	65	LEU
1	4-C	32	LEU
1	4-C	45	SER
1	3-A	71	ILE
1	4-B	149	PHE
1	3-A	149	PHE
1	6-C	45	SER
1	5-B	94	TYR
1	8-B	100	ASP
1	7-C	109	PRO
1	1-C	169	PRO
1	2-A	140	VAL
1	4-B	142	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	1-A	147/162 (91%)	143 (97%)	4 (3%)	39	17
1	1-B	147/162 (91%)	141 (96%)	6 (4%)	27	7
1	1-C	147/162 (91%)	143 (97%)	4 (3%)	39	17
1	2-A	147/162 (91%)	143 (97%)	4 (3%)	39	17
1	2-B	147/162 (91%)	141 (96%)	6 (4%)	27	7
1	2-C	147/162 (91%)	143 (97%)	4 (3%)	39	17
1	3-A	147/162 (91%)	143 (97%)	4 (3%)	39	17
1	3-B	147/162 (91%)	141 (96%)	6 (4%)	27	7
1	3-C	147/162 (91%)	143 (97%)	4 (3%)	39	17
1	4-A	147/162 (91%)	143 (97%)	4 (3%)	39	17
1	4-B	147/162 (91%)	141 (96%)	6 (4%)	27	7
1	4-C	147/162 (91%)	143 (97%)	4 (3%)	39	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	5-A	147/162 (91%)	143 (97%)	4 (3%)	39	17
1	5-B	147/162 (91%)	141 (96%)	6 (4%)	27	7
1	5-C	147/162 (91%)	143 (97%)	4 (3%)	39	17
1	6-A	147/162 (91%)	143 (97%)	4 (3%)	39	17
1	6-B	147/162 (91%)	141 (96%)	6 (4%)	27	7
1	6-C	147/162 (91%)	143 (97%)	4 (3%)	39	17
1	7-A	147/162 (91%)	143 (97%)	4 (3%)	39	17
1	7-B	147/162 (91%)	141 (96%)	6 (4%)	27	7
1	7-C	147/162 (91%)	143 (97%)	4 (3%)	39	17
1	8-A	147/162 (91%)	143 (97%)	4 (3%)	39	17
1	8-B	147/162 (91%)	141 (96%)	6 (4%)	27	7
1	8-C	147/162 (91%)	143 (97%)	4 (3%)	39	17
All	All	3528/3888 (91%)	3416 (97%)	112 (3%)	34	11

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	86	LYS
1	1-A	134	VAL
1	1-A	138	GLN
1	1-A	142	PRO
1	1-B	29	ILE
1	1-B	84	GLU
1	1-B	94	TYR
1	1-B	116	SER
1	1-B	136	LEU
1	1-B	142	PRO
1	1-C	71	ILE
1	1-C	89	ARG
1	1-C	169	PRO
1	1-C	189	SER
1	2-A	86	LYS
1	2-A	134	VAL
1	2-A	138	GLN
1	2-A	142	PRO
1	2-B	29	ILE
1	2-B	84	GLU
1	2-B	94	TYR

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Mol	Chain	Res	Type
1	2-B	116	SER
1	2-B	136	LEU
1	2-B	142	PRO
1	2-C	71	ILE
1	2-C	89	ARG
1	2-C	169	PRO
1	2-C	189	SER
1	3-A	86	LYS
1	3-A	134	VAL
1	3-A	138	GLN
1	3-A	142	PRO
1	3-B	29	ILE
1	3-B	84	GLU
1	3-B	94	TYR
1	3-B	116	SER
1	3-B	136	LEU
1	3-B	142	PRO
1	3-C	71	ILE
1	3-C	89	ARG
1	3-C	169	PRO
1	3-C	189	SER
1	4-A	86	LYS
1	4-A	134	VAL
1	4-A	138	GLN
1	4-A	142	PRO
1	4-B	29	ILE
1	4-B	84	GLU
1	4-B	94	TYR
1	4-B	116	SER
1	4-B	136	LEU
1	4-B	142	PRO
1	4-C	71	ILE
1	4-C	89	ARG
1	4-C	169	PRO
1	4-C	189	SER
1	5-A	86	LYS
1	5-A	134	VAL
1	5-A	138	GLN
1	5-A	142	PRO
1	5-B	29	ILE
1	5-B	84	GLU
1	5-B	94	TYR

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Mol	Chain	Res	Type
1	5-B	116	SER
1	5-B	136	LEU
1	5-B	142	PRO
1	5-C	71	ILE
1	5-C	89	ARG
1	5-C	169	PRO
1	5-C	189	SER
1	6-A	86	LYS
1	6-A	134	VAL
1	6-A	138	GLN
1	6-A	142	PRO
1	6-B	29	ILE
1	6-B	84	GLU
1	6-B	94	TYR
1	6-B	116	SER
1	6-B	136	LEU
1	6-B	142	PRO
1	6-C	71	ILE
1	6-C	89	ARG
1	6-C	169	PRO
1	6-C	189	SER
1	7-A	86	LYS
1	7-A	134	VAL
1	7-A	138	GLN
1	7-A	142	PRO
1	7-B	29	ILE
1	7-B	84	GLU
1	7-B	94	TYR
1	7-B	116	SER
1	7-B	136	LEU
1	7-B	142	PRO
1	7-C	71	ILE
1	7-C	89	ARG
1	7-C	169	PRO
1	7-C	189	SER
1	8-A	86	LYS
1	8-A	134	VAL
1	8-A	138	GLN
1	8-A	142	PRO
1	8-B	29	ILE
1	8-B	84	GLU
1	8-B	94	TYR

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Mol	Chain	Res	Type
1	8-B	116	SER
1	8-B	136	LEU
1	8-B	142	PRO
1	8-C	71	ILE
1	8-C	89	ARG
1	8-C	169	PRO
1	8-C	189	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	58	ASN
1	1-A	133	GLN
1	1-A	137	GLN
1	1-B	103	HIS
1	1-B	138	GLN
1	1-B	156	ASN
1	1-B	190	ASN
1	1-C	138	GLN
1	2-A	58	ASN
1	2-A	107	GLN
1	2-A	138	GLN
1	2-B	35	HIS
1	2-B	42	ASN
1	2-B	138	GLN
1	2-B	190	ASN
1	3-B	107	GLN
1	3-B	138	GLN
1	3-B	190	ASN
1	3-C	58	ASN
1	3-C	138	GLN
1	4-A	58	ASN
1	4-B	22	GLN
1	4-B	103	HIS
1	4-B	138	GLN
1	4-B	190	ASN
1	4-C	42	ASN
1	4-C	103	HIS
1	4-C	133	GLN
1	5-A	138	GLN
1	5-A	190	ASN
1	5-B	58	ASN

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Mol	Chain	Res	Type
1	5-B	107	GLN
1	5-B	190	ASN
1	5-C	138	GLN
1	6-A	137	GLN
1	6-A	138	GLN
1	6-A	190	ASN
1	6-B	35	HIS
1	6-B	103	HIS
1	6-B	138	GLN
1	6-B	190	ASN
1	6-C	42	ASN
1	6-C	137	GLN
1	6-C	138	GLN
1	7-A	138	GLN
1	7-B	138	GLN
1	7-B	190	ASN
1	7-C	58	ASN
1	8-C	58	ASN

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](#)

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 ⓘ

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	1-A	173/193 (89%)	1.67	59 (34%) ⓘ ⓘ	0, 1, 2, 4	173 (100%)
1	1-B	173/193 (89%)	1.85	62 (35%) ⓘ ⓘ	0, 1, 2, 4	173 (100%)
1	1-C	173/193 (89%)	1.72	61 (35%) ⓘ ⓘ	0, 1, 2, 4	173 (100%)
1	2-A	0/193	-	-	-	-
1	2-B	0/193	-	-	-	-
1	2-C	0/193	-	-	-	-
1	3-A	0/193	-	-	-	-
1	3-B	0/193	-	-	-	-
1	3-C	0/193	-	-	-	-
1	4-A	0/193	-	-	-	-
1	4-B	0/193	-	-	-	-
1	4-C	0/193	-	-	-	-
1	5-A	0/193	-	-	-	-
1	5-B	0/193	-	-	-	-
1	5-C	0/193	-	-	-	-
1	6-A	0/193	-	-	-	-
1	6-B	0/193	-	-	-	-
1	6-C	0/193	-	-	-	-
1	7-A	0/193	-	-	-	-
1	7-B	0/193	-	-	-	-
1	7-C	0/193	-	-	-	-
1	8-A	0/193	-	-	-	-
1	8-B	0/193	-	-	-	-
1	8-C	0/193	-	-	-	-
All	All	519/4632 (11%)	1.74	182 (35%) ⓘ ⓘ	0, 1, 2, 4	519 (100%)

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-B	108	GLY	7.9
1	1-C	83	PRO	7.3

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Mol	Chain	Res	Type	RSRZ
1	1-B	148	THR	7.2
1	1-A	160	LEU	7.1
1	1-C	168	PRO	7.0
1	1-B	84	GLU	6.4
1	1-C	71	ILE	6.1
1	1-A	117	PHE	6.0
1	1-C	44	PHE	5.7
1	1-B	177	PRO	5.6
1	1-B	29	ILE	5.5
1	1-A	139	LEU	5.4
1	1-A	142	PRO	5.2
1	1-A	150	TYR	5.2
1	1-A	148	THR	5.1
1	1-C	160	LEU	5.1
1	1-B	82	VAL	5.1
1	1-B	83	PRO	5.0
1	1-B	172	ASP	4.9
1	1-A	151	LEU	4.8
1	1-B	37	PRO	4.7
1	1-B	150	TYR	4.7
1	1-C	169	PRO	4.7
1	1-C	105	SER	4.4
1	1-B	151	LEU	4.4
1	1-B	86	LYS	4.4
1	1-A	141	TYR	4.4
1	1-B	180	LYS	4.4
1	1-B	165	THR	4.3
1	1-A	138	GLN	4.3
1	1-B	81	HIS	4.3
1	1-B	149	PHE	4.2
1	1-C	167	VAL	4.0
1	1-C	35	HIS	4.0
1	1-C	180	LYS	3.9
1	1-B	110	TYR	3.9
1	1-A	32	LEU	3.9
1	1-C	70	GLY	3.9
1	1-B	168	PRO	3.8
1	1-B	155	ALA	3.8
1	1-B	85	LYS	3.7
1	1-B	160	LEU	3.7
1	1-A	26	VAL	3.7
1	1-B	143	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	1-C	147	TYR	3.7
1	1-B	178	GLU	3.7
1	1-A	165	THR	3.7
1	1-A	57	THR	3.6
1	1-B	182	LEU	3.6
1	1-C	20	LYS	3.6
1	1-A	155	ALA	3.6
1	1-C	101	TYR	3.5
1	1-B	116	SER	3.5
1	1-C	46	LEU	3.5
1	1-C	181	ALA	3.5
1	1-C	163	THR	3.4
1	1-B	164	GLY	3.3
1	1-A	140	VAL	3.3
1	1-C	84	GLU	3.3
1	1-A	163	THR	3.3
1	1-A	159	PRO	3.3
1	1-C	182	LEU	3.3
1	1-B	33	ASP	3.3
1	1-B	181	ALA	3.3
1	1-C	60	LEU	3.2
1	1-A	170	SER	3.2
1	1-A	34	ARG	3.2
1	1-A	164	GLY	3.2
1	1-C	185	SER	3.2
1	1-B	30	ASN	3.1
1	1-C	155	ALA	3.1
1	1-C	120	ILE	3.1
1	1-A	171	LYS	3.1
1	1-B	156	ASN	3.1
1	1-A	129	GLY	3.1
1	1-B	114	GLU	3.1
1	1-B	166	PRO	3.0
1	1-A	135	LYS	3.0
1	1-A	89	ARG	3.0
1	1-B	93	THR	3.0
1	1-B	170	SER	3.0
1	1-A	186	GLY	3.0
1	1-C	183	GLU	3.0
1	1-C	61	TYR	2.9
1	1-C	178	GLU	2.9
1	1-C	118	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	1-B	179	ALA	2.9
1	1-C	177	PRO	2.9
1	1-C	25	SER	2.9
1	1-A	21	VAL	2.9
1	1-A	161	GLU	2.9
1	1-A	30	ASN	2.9
1	1-C	184	PRO	2.8
1	1-C	89	ARG	2.8
1	1-B	25	SER	2.8
1	1-B	20	LYS	2.8
1	1-B	44	PHE	2.7
1	1-B	76	CYS	2.7
1	1-C	191	TYR	2.7
1	1-A	115	ASP	2.7
1	1-B	35	HIS	2.7
1	1-C	150	TYR	2.7
1	1-C	186	GLY	2.7
1	1-B	171	LYS	2.7
1	1-A	63	GLY	2.6
1	1-A	70	GLY	2.6
1	1-A	145	LEU	2.6
1	1-C	141	TYR	2.6
1	1-C	86	LYS	2.6
1	1-C	69	VAL	2.6
1	1-B	185	SER	2.6
1	1-C	45	SER	2.6
1	1-A	20	LYS	2.5
1	1-B	169	PRO	2.5
1	1-B	176	ALA	2.5
1	1-C	87	GLY	2.5
1	1-B	131	TYR	2.5
1	1-C	152	LYS	2.5
1	1-B	159	PRO	2.5
1	1-A	93	THR	2.5
1	1-A	136	LEU	2.4
1	1-B	173	ILE	2.4
1	1-C	106	VAL	2.4
1	1-B	138	GLN	2.4
1	1-A	29	ILE	2.4
1	1-A	64	ASP	2.4
1	1-A	86	LYS	2.4
1	1-A	60	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	1-B	162	LEU	2.4
1	1-A	92	ALA	2.4
1	1-C	85	LYS	2.4
1	1-C	171	LYS	2.4
1	1-C	142	PRO	2.3
1	1-A	172	ASP	2.3
1	1-C	119	ALA	2.3
1	1-C	81	HIS	2.3
1	1-B	163	THR	2.3
1	1-A	181	ALA	2.3
1	1-B	111	LEU	2.3
1	1-A	190	ASN	2.3
1	1-B	120	ILE	2.3
1	1-A	133	GLN	2.3
1	1-A	113	TYR	2.3
1	1-A	126	ILE	2.3
1	1-C	156	ASN	2.2
1	1-A	100	ASP	2.2
1	1-C	37	PRO	2.2
1	1-A	154	LEU	2.2
1	1-A	69	VAL	2.2
1	1-A	180	LYS	2.2
1	1-C	54	VAL	2.2
1	1-C	33	ASP	2.2
1	1-C	76	CYS	2.2
1	1-A	153	GLY	2.2
1	1-C	111	LEU	2.2
1	1-C	154	LEU	2.2
1	1-B	103	HIS	2.2
1	1-C	176	ALA	2.1
1	1-B	34	ARG	2.1
1	1-A	35	HIS	2.1
1	1-A	149	PHE	2.1
1	1-C	137	GLN	2.1
1	1-A	173	ILE	2.1
1	1-A	188	ILE	2.1
1	1-B	26	VAL	2.1
1	1-B	153	GLY	2.1
1	1-B	145	LEU	2.1
1	1-C	32	LEU	2.1
1	1-C	104	LEU	2.1
1	1-B	31	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	1-B	157	ASP	2.1
1	1-B	38	LYS	2.1
1	1-B	135	LYS	2.1
1	1-C	59	LYS	2.1
1	1-A	58	ASN	2.0
1	1-A	130	ALA	2.0
1	1-A	45	SER	2.0
1	1-C	151	LEU	2.0
1	1-C	162	LEU	2.0
1	1-A	110	TYR	2.0
1	1-B	147	TYR	2.0
1	1-C	27	TYR	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.