



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:51 PM UTC

PDB ID : 2Q49 / pdb_00002q49
Title : Ensemble refinement of the protein crystal structure of gene product from Arabidopsis thaliana At2g19940
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 : 2.19 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:

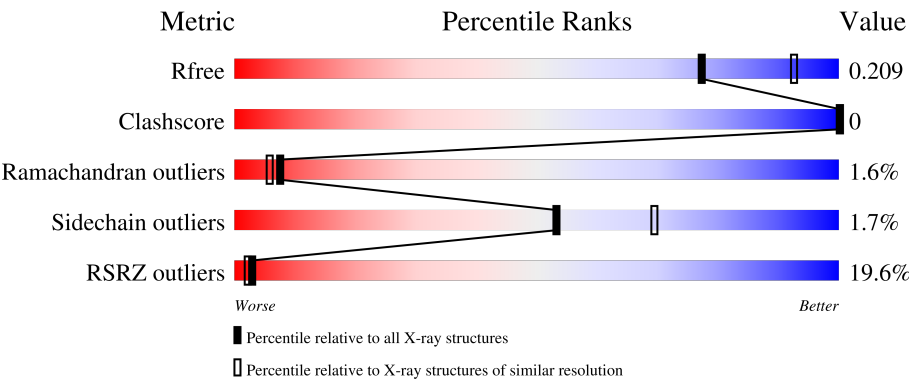
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.19 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.



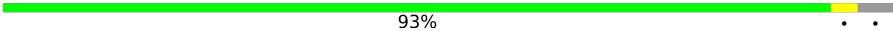
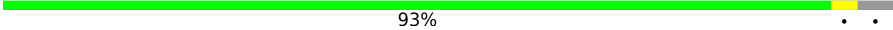
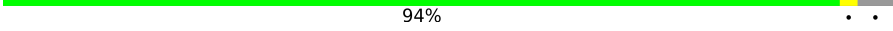
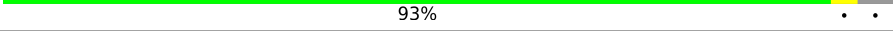
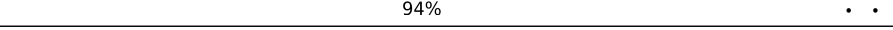
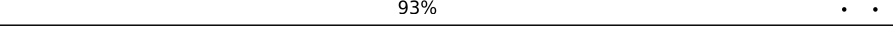
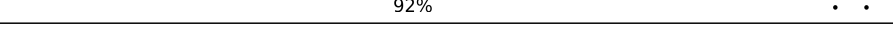
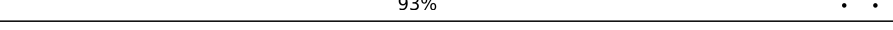
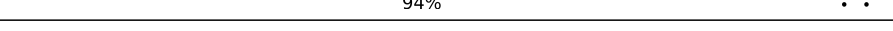
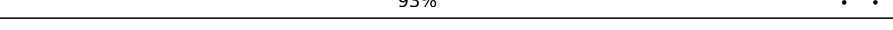
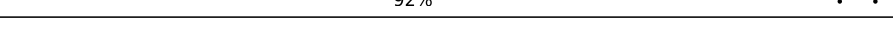
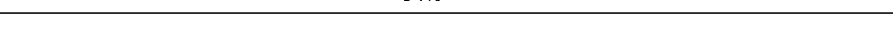
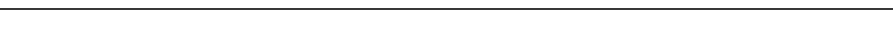
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	359	13% 93%
1	1-B	359	16% 92%
1	1-C	359	30% 93%
1	1-D	359	16% 93%
1	2-A	359	93%

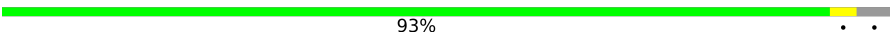
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Mol	Chain	Length	Quality of chain
1	2-B	359	 92% . .
1	2-C	359	 91% 5% .
1	2-D	359	 93% . .
1	3-A	359	 93% . .
1	3-B	359	 92% . .
1	3-C	359	 92% . .
1	3-D	359	 94% . .
1	4-A	359	 93% . .
1	4-B	359	 92% . .
1	4-C	359	 91% 5% .
1	4-D	359	 94% . .
1	5-A	359	 93% . .
1	5-B	359	 92% . .
1	5-C	359	 93% . .
1	5-D	359	 94% . .
1	6-A	359	 93% . .
1	6-B	359	 92% . .
1	6-C	359	 91% 5% .
1	6-D	359	 94% . .
1	7-A	359	 93% . .
1	7-B	359	 92% . .
1	7-C	359	 92% . .
1	7-D	359	 94% . .
1	8-A	359	 94% . .
1	8-B	359	 92% . .

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Mol	Chain	Length	Quality of chain
1	8-C	359	 92% • •
1	8-D	359	 93% • •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 93408 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 Probable N-acetyl-gamma-glutamyl-phosphate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	345	Total	C	N	O	S	0	0	0
			2680	1700	467	501	12			
1	2-A	345	Total	C	N	O	S	0	0	0
			2680	1700	467	501	12			
1	3-A	345	Total	C	N	O	S	0	0	0
			2680	1700	467	501	12			
1	4-A	345	Total	C	N	O	S	0	0	0
			2680	1700	467	501	12			
1	5-A	345	Total	C	N	O	S	0	0	0
			2680	1700	467	501	12			
1	6-A	345	Total	C	N	O	S	0	0	0
			2680	1700	467	501	12			
1	7-A	345	Total	C	N	O	S	0	0	0
			2680	1700	467	501	12			
1	8-A	345	Total	C	N	O	S	0	0	0
			2680	1700	467	501	12			
1	1-B	345	Total	C	N	O	S	0	0	0
			2680	1700	467	501	12			
1	2-B	345	Total	C	N	O	S	0	0	0
			2680	1700	467	501	12			
1	3-B	345	Total	C	N	O	S	0	0	0
			2680	1700	467	501	12			
1	4-B	345	Total	C	N	O	S	0	0	0
			2680	1700	467	501	12			
1	5-B	345	Total	C	N	O	S	0	0	0
			2680	1700	467	501	12			
1	6-B	345	Total	C	N	O	S	0	0	0
			2680	1700	467	501	12			
1	7-B	345	Total	C	N	O	S	0	0	0
			2680	1700	467	501	12			
1	8-B	345	Total	C	N	O	S	0	0	0
			2680	1700	467	501	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-C	345	Total	C	N	O	S	0	0	0
			2680	1700	467	501	12			
1	2-C	345	Total	C	N	O	S	0	0	0
			2680	1700	467	501	12			
1	3-C	345	Total	C	N	O	S	0	0	0
			2680	1700	467	501	12			
1	4-C	345	Total	C	N	O	S	0	0	0
			2680	1700	467	501	12			
1	5-C	345	Total	C	N	O	S	0	0	0
			2680	1700	467	501	12			
1	6-C	345	Total	C	N	O	S	0	0	0
			2680	1700	467	501	12			
1	7-C	345	Total	C	N	O	S	0	0	0
			2680	1700	467	501	12			
1	8-C	345	Total	C	N	O	S	0	0	0
			2680	1700	467	501	12			
1	1-D	345	Total	C	N	O	S	0	0	0
			2680	1700	467	501	12			
1	2-D	345	Total	C	N	O	S	0	0	0
			2680	1700	467	501	12			
1	3-D	345	Total	C	N	O	S	0	0	0
			2680	1700	467	501	12			
1	4-D	345	Total	C	N	O	S	0	0	0
			2680	1700	467	501	12			
1	5-D	345	Total	C	N	O	S	0	0	0
			2680	1700	467	501	12			
1	6-D	345	Total	C	N	O	S	0	0	0
			2680	1700	467	501	12			
1	7-D	345	Total	C	N	O	S	0	0	0
			2680	1700	467	501	12			
1	8-D	345	Total	C	N	O	S	0	0	0
			2680	1700	467	501	12			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	1-A	270	Total	O	0	0
			270	270		
2	2-A	263	Total	O	0	0
			263	263		
2	3-A	268	Total	O	0	0
			268	268		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	4-A	267	Total 267	O 267	0	0
2	5-A	262	Total 262	O 262	0	0
2	6-A	267	Total 267	O 267	0	0
2	7-A	269	Total 269	O 269	0	0
2	8-A	267	Total 267	O 267	0	0
2	1-B	225	Total 225	O 225	0	0
2	2-B	227	Total 227	O 227	0	0
2	3-B	216	Total 216	O 216	0	0
2	4-B	224	Total 224	O 224	0	0
2	5-B	223	Total 223	O 223	0	0
2	6-B	225	Total 225	O 225	0	0
2	7-B	223	Total 223	O 223	0	0
2	8-B	222	Total 222	O 222	0	0
2	1-C	220	Total 220	O 220	0	0
2	2-C	231	Total 231	O 231	0	0
2	3-C	228	Total 228	O 228	0	0
2	4-C	223	Total 223	O 223	0	0
2	5-C	229	Total 229	O 229	0	0
2	6-C	224	Total 224	O 224	0	0
2	7-C	224	Total 224	O 224	0	0
2	8-C	231	Total 231	O 231	0	0

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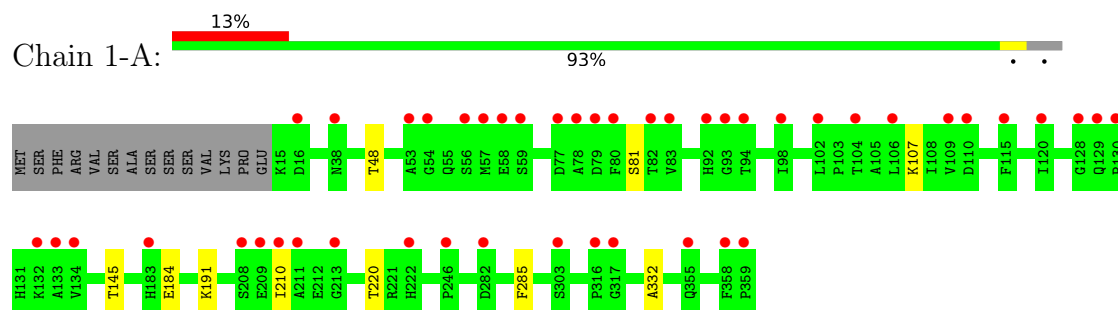
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	1-D	241	Total 241	O 241	0	0
2	2-D	235	Total 235	O 235	0	0
2	3-D	244	Total 244	O 244	0	0
2	4-D	242	Total 242	O 242	0	0
2	5-D	242	Total 242	O 242	0	0
2	6-D	240	Total 240	O 240	0	0
2	7-D	240	Total 240	O 240	0	0
2	8-D	236	Total 236	O 236	0	0

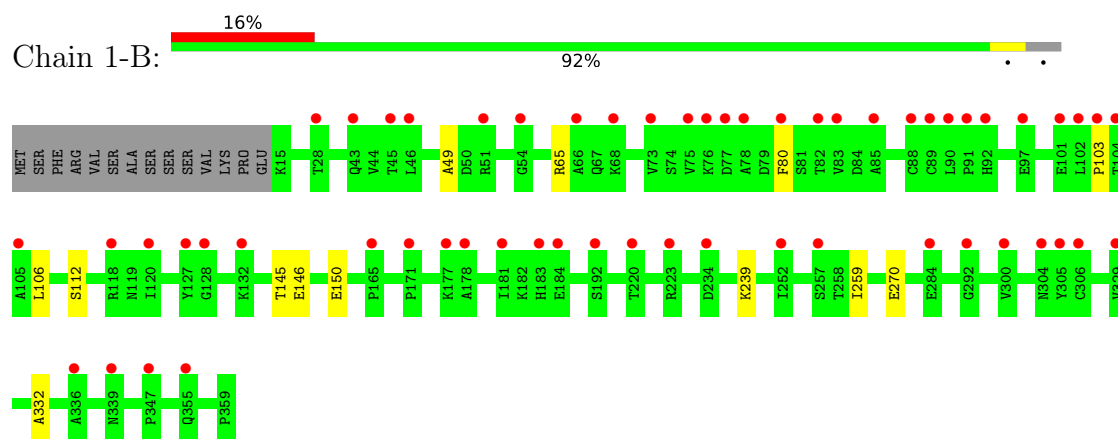
3 Residue-property plots [i](#)

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.

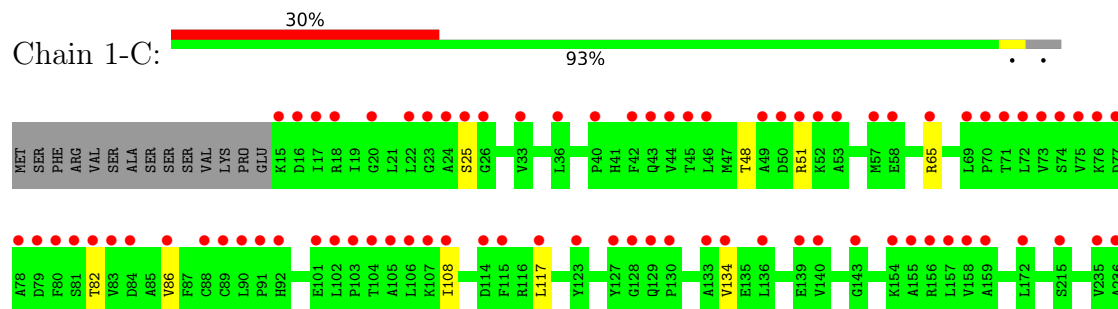
- Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

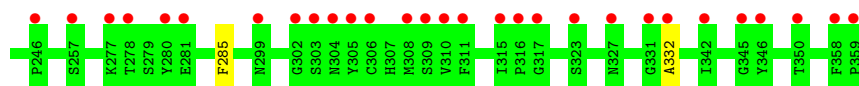


- Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

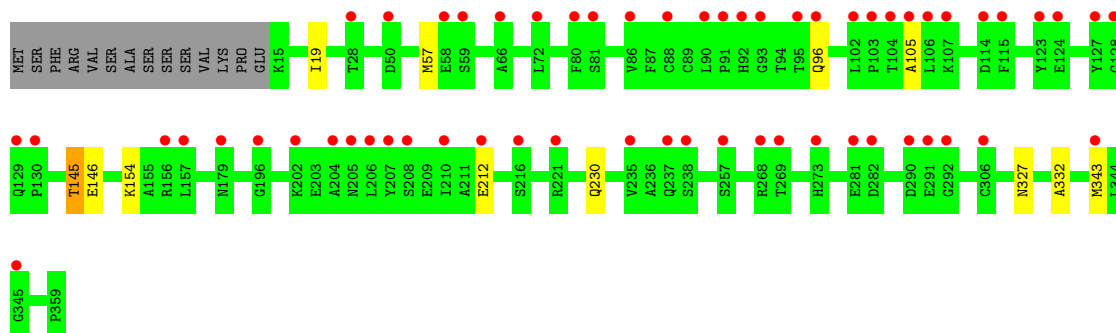


- Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase





- Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase



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- Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase



- Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase





- Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 3-B: 92%



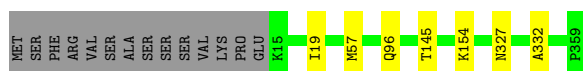
- Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 3-C: 92%



- Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 3-D: 94%



- Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 4-A: 93%



- Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 4-B: 92%



- Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 4-C: 91%



- Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 4-D: 94%



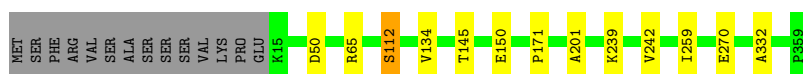
- Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 5-A: 93%



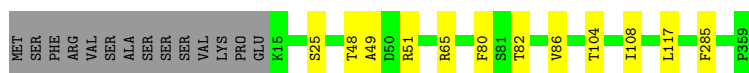
- Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 5-B: 92%



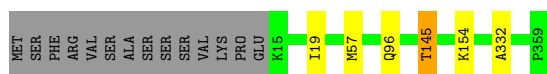
- Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 5-C: 93%



- Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 5-D: 94%



- Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 6-A: 93%



- Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 6-B: 92%



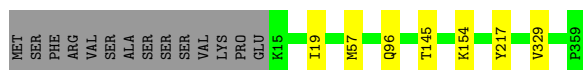
- Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 6-C: 91% 5%



- Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 6-D: 94%



- Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 7-A: 93%



- Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 7-B: 92%



- Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 7-C: 92%



- Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 7-D: 94%



- Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 8-A: 94%



- Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

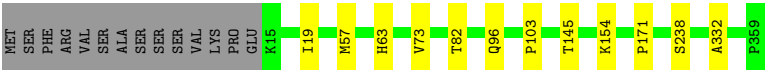
Chain 8-B: 92%



● Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase



● Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.60Å 107.07Å 85.75Å 90.00° 118.88° 90.00°	Depositor
Resolution (Å)	27.31 – 2.19 27.31 – 2.19	Depositor EDS
% Data completeness (in resolution range)	92.9 (27.31-2.19) 92.9 (27.31-2.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.61 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.152 , 0.212 0.153 , 0.209	Depositor DCC
R_{free} test set	3240 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.860	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.04 , 66.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.002 for -h-l,k,h 0.002 for l,k,-h-l 0.018 for h,-k,-h-l 0.017 for -h-l,-k,l 0.016 for l,-k,h	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	93408	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% 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	0.37	0/2734	0.65	3/3709 (0.1%)
1	1-B	0.31	0/2734	0.54	1/3709 (0.0%)
1	1-C	0.32	0/2734	0.55	2/3709 (0.1%)
1	1-D	0.35	0/2734	0.57	1/3709 (0.0%)
1	2-A	0.37	0/2734	0.65	3/3709 (0.1%)
1	2-B	0.31	0/2734	0.54	1/3709 (0.0%)
1	2-C	0.32	0/2734	0.55	2/3709 (0.1%)
1	2-D	0.35	0/2734	0.57	1/3709 (0.0%)
1	3-A	0.37	0/2734	0.65	3/3709 (0.1%)
1	3-B	0.31	0/2734	0.54	1/3709 (0.0%)
1	3-C	0.32	0/2734	0.55	2/3709 (0.1%)
1	3-D	0.35	0/2734	0.57	1/3709 (0.0%)
1	4-A	0.37	0/2734	0.65	3/3709 (0.1%)
1	4-B	0.31	0/2734	0.54	1/3709 (0.0%)
1	4-C	0.32	0/2734	0.55	2/3709 (0.1%)
1	4-D	0.35	0/2734	0.57	1/3709 (0.0%)
1	5-A	0.37	0/2734	0.65	3/3709 (0.1%)
1	5-B	0.31	0/2734	0.54	1/3709 (0.0%)
1	5-C	0.32	0/2734	0.55	2/3709 (0.1%)
1	5-D	0.35	0/2734	0.57	1/3709 (0.0%)
1	6-A	0.37	0/2734	0.65	3/3709 (0.1%)
1	6-B	0.31	0/2734	0.54	1/3709 (0.0%)
1	6-C	0.32	0/2734	0.55	2/3709 (0.1%)
1	6-D	0.35	0/2734	0.57	1/3709 (0.0%)
1	7-A	0.37	0/2734	0.65	3/3709 (0.1%)
1	7-B	0.31	0/2734	0.54	1/3709 (0.0%)
1	7-C	0.32	0/2734	0.55	2/3709 (0.1%)
1	7-D	0.35	0/2734	0.57	1/3709 (0.0%)
1	8-A	0.37	0/2734	0.65	3/3709 (0.1%)
1	8-B	0.31	0/2734	0.54	1/3709 (0.0%)
1	8-C	0.32	0/2734	0.55	2/3709 (0.1%)
1	8-D	0.35	0/2734	0.57	1/3709 (0.0%)
All	All	0.34	0/87488	0.58	56/118688 (0.0%)

There are no bond length outliers.

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-A	285	PHE	N-CA-C	6.71	121.63	113.38
1	2-A	285	PHE	N-CA-C	6.71	121.63	113.38
1	3-A	285	PHE	N-CA-C	6.71	121.63	113.38
1	4-A	285	PHE	N-CA-C	6.71	121.63	113.38
1	5-A	285	PHE	N-CA-C	6.71	121.63	113.38
1	6-A	285	PHE	N-CA-C	6.71	121.63	113.38
1	7-A	285	PHE	N-CA-C	6.71	121.63	113.38
1	8-A	285	PHE	N-CA-C	6.71	121.63	113.38
1	1-C	285	PHE	N-CA-C	5.93	120.67	112.90
1	2-C	285	PHE	N-CA-C	5.93	120.67	112.90
1	3-C	285	PHE	N-CA-C	5.93	120.67	112.90
1	4-C	285	PHE	N-CA-C	5.93	120.67	112.90
1	5-C	285	PHE	N-CA-C	5.93	120.67	112.90
1	6-C	285	PHE	N-CA-C	5.93	120.67	112.90
1	7-C	285	PHE	N-CA-C	5.93	120.67	112.90
1	8-C	285	PHE	N-CA-C	5.93	120.67	112.90
1	1-B	259	ILE	N-CA-C	5.67	116.28	107.99
1	2-B	259	ILE	N-CA-C	5.67	116.28	107.99
1	3-B	259	ILE	N-CA-C	5.67	116.28	107.99
1	4-B	259	ILE	N-CA-C	5.67	116.28	107.99
1	5-B	259	ILE	N-CA-C	5.67	116.28	107.99
1	6-B	259	ILE	N-CA-C	5.67	116.28	107.99
1	7-B	259	ILE	N-CA-C	5.67	116.28	107.99
1	8-B	259	ILE	N-CA-C	5.67	116.28	107.99
1	1-A	81	SER	N-CA-C	-5.63	106.17	113.16
1	2-A	81	SER	N-CA-C	-5.63	106.17	113.16
1	3-A	81	SER	N-CA-C	-5.63	106.17	113.16
1	4-A	81	SER	N-CA-C	-5.63	106.17	113.16
1	5-A	81	SER	N-CA-C	-5.63	106.17	113.16
1	6-A	81	SER	N-CA-C	-5.63	106.17	113.16
1	7-A	81	SER	N-CA-C	-5.63	106.17	113.16
1	8-A	81	SER	N-CA-C	-5.63	106.17	113.16
1	1-C	108	ILE	N-CA-C	5.29	116.35	108.46
1	2-C	108	ILE	N-CA-C	5.29	116.35	108.46
1	3-C	108	ILE	N-CA-C	5.29	116.35	108.46
1	4-C	108	ILE	N-CA-C	5.29	116.35	108.46
1	5-C	108	ILE	N-CA-C	5.29	116.35	108.46
1	6-C	108	ILE	N-CA-C	5.29	116.35	108.46
1	7-C	108	ILE	N-CA-C	5.29	116.35	108.46
1	8-C	108	ILE	N-CA-C	5.29	116.35	108.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-D	19	ILE	N-CA-C	5.21	116.80	108.89
1	2-D	19	ILE	N-CA-C	5.21	116.80	108.89
1	3-D	19	ILE	N-CA-C	5.21	116.80	108.89
1	4-D	19	ILE	N-CA-C	5.21	116.80	108.89
1	5-D	19	ILE	N-CA-C	5.21	116.80	108.89
1	6-D	19	ILE	N-CA-C	5.21	116.80	108.89
1	7-D	19	ILE	N-CA-C	5.21	116.80	108.89
1	8-D	19	ILE	N-CA-C	5.21	116.80	108.89
1	1-A	107	LYS	N-CA-C	-5.12	102.28	109.96
1	2-A	107	LYS	N-CA-C	-5.12	102.28	109.96
1	3-A	107	LYS	N-CA-C	-5.12	102.28	109.96
1	4-A	107	LYS	N-CA-C	-5.12	102.28	109.96
1	5-A	107	LYS	N-CA-C	-5.12	102.28	109.96
1	6-A	107	LYS	N-CA-C	-5.12	102.28	109.96
1	7-A	107	LYS	N-CA-C	-5.12	102.28	109.96
1	8-A	107	LYS	N-CA-C	-5.12	102.28	109.96

There are no chirality outliers.

There are no planarity outliers.

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	2680	0	2718	0	0
1	1-B	2680	0	2718	0	0
1	1-C	2680	0	2718	0	0
1	1-D	2680	0	2718	0	0
1	2-A	2680	0	2718	0	0
1	2-B	2680	0	2718	0	0
1	2-C	2680	0	2718	0	0
1	2-D	2680	0	2718	0	0
1	3-A	2680	0	2718	0	0
1	3-B	2680	0	2718	0	0
1	3-C	2680	0	2718	0	0
1	3-D	2680	0	2718	0	0
1	4-A	2680	0	2718	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	4-B	2680	0	2718	0	0
1	4-C	2680	0	2718	0	0
1	4-D	2680	0	2718	0	0
1	5-A	2680	0	2718	0	0
1	5-B	2680	0	2718	0	0
1	5-C	2680	0	2718	0	0
1	5-D	2680	0	2718	0	0
1	6-A	2680	0	2718	0	0
1	6-B	2680	0	2718	0	0
1	6-C	2680	0	2718	0	0
1	6-D	2680	0	2718	0	0
1	7-A	2680	0	2718	0	0
1	7-B	2680	0	2718	0	0
1	7-C	2680	0	2718	0	0
1	7-D	2680	0	2718	0	0
1	8-A	2680	0	2718	0	0
1	8-B	2680	0	2718	0	0
1	8-C	2680	0	2718	0	0
1	8-D	2680	0	2718	0	0
2	1-A	270	0	0	0	0
2	1-B	225	0	0	0	0
2	1-C	220	0	0	0	0
2	1-D	241	0	0	0	0
2	2-A	263	0	0	0	0
2	2-B	227	0	0	0	0
2	2-C	231	0	0	0	0
2	2-D	235	0	0	0	0
2	3-A	268	0	0	0	0
2	3-B	216	0	0	0	0
2	3-C	228	0	0	0	0
2	3-D	244	0	0	0	0
2	4-A	267	0	0	0	0
2	4-B	224	0	0	0	0
2	4-C	223	0	0	0	0
2	4-D	242	0	0	0	0
2	5-A	262	0	0	0	0
2	5-B	223	0	0	0	0
2	5-C	229	0	0	0	0
2	5-D	242	0	0	0	0
2	6-A	267	0	0	0	0
2	6-B	225	0	0	0	0
2	6-C	224	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	6-D	240	0	0	0	0
2	7-A	269	0	0	0	0
2	7-B	223	0	0	0	0
2	7-C	224	0	0	0	0
2	7-D	240	0	0	0	0
2	8-A	267	0	0	0	0
2	8-B	222	0	0	0	0
2	8-C	231	0	0	0	0
2	8-D	236	0	0	0	0
All	All	93408	0	86976	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 [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	1-A	343/359 (96%)	318 (93%)	22 (6%)	3 (1%)	14	14
1	1-B	343/359 (96%)	311 (91%)	25 (7%)	7 (2%)	6	4
1	1-C	343/359 (96%)	317 (92%)	24 (7%)	2 (1%)	21	23
1	1-D	343/359 (96%)	316 (92%)	19 (6%)	8 (2%)	5	3
1	2-A	343/359 (96%)	316 (92%)	24 (7%)	3 (1%)	14	14
1	2-B	343/359 (96%)	318 (93%)	16 (5%)	9 (3%)	4	2
1	2-C	343/359 (96%)	305 (89%)	30 (9%)	8 (2%)	5	3
1	2-D	343/359 (96%)	315 (92%)	21 (6%)	7 (2%)	6	4
1	3-A	343/359 (96%)	310 (90%)	29 (8%)	4 (1%)	10	8
1	3-B	343/359 (96%)	308 (90%)	26 (8%)	9 (3%)	4	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3-C	343/359 (96%)	304 (89%)	33 (10%)	6 (2%)	7	5
1	3-D	343/359 (96%)	316 (92%)	25 (7%)	2 (1%)	21	23
1	4-A	343/359 (96%)	317 (92%)	22 (6%)	4 (1%)	10	8
1	4-B	343/359 (96%)	299 (87%)	34 (10%)	10 (3%)	3	2
1	4-C	343/359 (96%)	310 (90%)	24 (7%)	9 (3%)	4	2
1	4-D	343/359 (96%)	312 (91%)	28 (8%)	3 (1%)	14	14
1	5-A	343/359 (96%)	318 (93%)	21 (6%)	4 (1%)	10	8
1	5-B	343/359 (96%)	313 (91%)	22 (6%)	8 (2%)	5	3
1	5-C	343/359 (96%)	311 (91%)	29 (8%)	3 (1%)	14	14
1	5-D	343/359 (96%)	310 (90%)	31 (9%)	2 (1%)	21	23
1	6-A	343/359 (96%)	320 (93%)	18 (5%)	5 (2%)	8	6
1	6-B	343/359 (96%)	301 (88%)	32 (9%)	10 (3%)	3	2
1	6-C	343/359 (96%)	310 (90%)	25 (7%)	8 (2%)	5	3
1	6-D	343/359 (96%)	312 (91%)	29 (8%)	2 (1%)	21	23
1	7-A	343/359 (96%)	316 (92%)	24 (7%)	3 (1%)	14	14
1	7-B	343/359 (96%)	304 (89%)	31 (9%)	8 (2%)	5	3
1	7-C	343/359 (96%)	311 (91%)	28 (8%)	4 (1%)	10	8
1	7-D	343/359 (96%)	309 (90%)	30 (9%)	4 (1%)	10	8
1	8-A	343/359 (96%)	317 (92%)	24 (7%)	2 (1%)	21	23
1	8-B	343/359 (96%)	310 (90%)	25 (7%)	8 (2%)	5	3
1	8-C	343/359 (96%)	308 (90%)	28 (8%)	7 (2%)	6	4
1	8-D	343/359 (96%)	309 (90%)	27 (8%)	7 (2%)	6	4
All	All	10976/11488 (96%)	9971 (91%)	826 (8%)	179 (2%)	7	6

All (179) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-C	332	ALA
1	1-D	105	ALA
1	1-D	212	GLU
1	2-A	161	PRO
1	2-C	145	THR
1	2-D	197	ALA
1	3-A	327	ASN

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Mol	Chain	Res	Type
1	3-D	332	ALA
1	4-A	145	THR
1	4-B	238	SER
1	4-B	329	VAL
1	4-C	128	GLY
1	4-C	263	MET
1	4-D	172	LEU
1	4-D	173	VAL
1	5-A	332	ALA
1	5-B	50	ASP
1	6-B	223	ARG
1	7-A	303	SER
1	7-D	115	PHE
1	7-D	145	THR
1	8-A	103	PRO
1	8-B	142	TYR
1	1-B	145	THR
1	1-B	146	GLU
1	1-D	332	ALA
1	2-C	49	ALA
1	2-D	25	SER
1	2-D	133	ALA
1	2-D	194	VAL
1	2-D	220	THR
1	3-A	145	THR
1	3-B	194	VAL
1	3-B	332	ALA
1	3-C	115	PHE
1	3-C	119	ASN
1	3-C	120	ILE
1	3-D	327	ASN
1	4-B	285	PHE
1	4-C	125	GLU
1	4-C	332	ALA
1	4-D	332	ALA
1	5-B	112	SER
1	5-C	104	THR
1	6-A	222	HIS
1	6-B	49	ALA
1	6-C	46	LEU
1	6-C	104	THR
1	7-B	145	THR

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Mol	Chain	Res	Type
1	7-B	201	ALA
1	7-C	104	THR
1	8-B	144	LEU
1	8-C	41	HIS
1	8-D	82	THR
1	1-A	332	ALA
1	1-B	106	LEU
1	1-D	145	THR
1	1-D	327	ASN
1	2-B	49	ALA
1	2-B	106	LEU
1	2-B	145	THR
1	2-B	146	GLU
1	2-C	104	THR
1	2-C	133	ALA
1	2-C	146	GLU
1	2-D	211	ALA
1	3-A	114	ASP
1	3-B	76	LYS
1	4-B	75	VAL
1	5-A	114	ASP
1	5-B	145	THR
1	5-B	201	ALA
1	6-B	115	PHE
1	6-C	16	ASP
1	6-C	161	PRO
1	6-C	179	ASN
1	6-D	217	TYR
1	7-A	114	ASP
1	7-A	332	ALA
1	7-B	49	ALA
1	8-B	50	ASP
1	8-B	146	GLU
1	8-B	258	THR
1	8-D	63	HIS
1	1-C	134	VAL
1	1-D	146	GLU
1	1-D	230	GLN
1	1-D	343	MET
1	2-B	300	VAL
1	2-C	183	HIS
1	3-A	216	SER

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Mol	Chain	Res	Type
1	3-B	51	ARG
1	3-B	52	LYS
1	3-C	329	VAL
1	3-C	332	ALA
1	4-A	80	PHE
1	4-A	133	ALA
1	4-B	119	ASN
1	4-B	301	ARG
1	4-C	103	PRO
1	4-C	329	VAL
1	5-B	332	ALA
1	5-D	145	THR
1	6-A	133	ALA
1	6-A	332	ALA
1	6-B	50	ASP
1	6-B	51	ARG
1	6-B	96	GLN
1	6-C	313	ASP
1	7-B	119	ASN
1	7-B	313	ASP
1	7-C	281	GLU
1	7-D	238	SER
1	8-C	104	THR
1	8-D	332	ALA
1	1-A	220	THR
1	1-B	49	ALA
1	1-B	80	PHE
1	1-B	332	ALA
1	2-A	112	SER
1	2-B	104	THR
1	2-C	332	ALA
1	3-B	49	ALA
1	3-B	50	ASP
1	3-C	104	THR
1	4-B	76	LYS
1	4-B	332	ALA
1	4-C	173	VAL
1	5-A	133	ALA
1	5-D	332	ALA
1	6-A	134	VAL
1	6-C	49	ALA
1	7-B	50	ASP

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Mol	Chain	Res	Type
1	7-B	332	ALA
1	7-B	348	GLU
1	7-C	49	ALA
1	7-C	332	ALA
1	7-D	290	ASP
1	8-A	133	ALA
1	8-B	332	ALA
1	8-C	49	ALA
1	8-C	124	GLU
1	8-D	103	PRO
1	8-D	171	PRO
1	8-D	238	SER
1	1-A	210	ILE
1	2-D	252	ILE
1	3-B	252	ILE
1	4-C	126	TRP
1	5-B	171	PRO
1	5-C	49	ALA
1	5-C	80	PHE
1	6-B	37	ALA
1	6-B	332	ALA
1	8-B	51	ARG
1	8-C	134	VAL
1	8-C	318	ARG
1	4-A	329	VAL
1	6-A	171	PRO
1	6-D	329	VAL
1	8-B	143	GLY
1	1-B	103	PRO
1	2-A	325	ILE
1	2-B	252	ILE
1	2-B	356	PRO
1	2-C	300	VAL
1	4-B	171	PRO
1	5-A	329	VAL
1	6-B	171	PRO
1	8-D	73	VAL
1	4-C	252	ILE
1	5-B	134	VAL
1	5-B	242	VAL
1	6-C	171	PRO
1	2-B	171	PRO

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Mol	Chain	Res	Type
1	3-B	171	PRO
1	4-B	40	PRO
1	6-B	342	ILE
1	8-C	40	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	295/308 (96%)	291 (99%)	4 (1%)	59	75
1	1-B	295/308 (96%)	290 (98%)	5 (2%)	53	69
1	1-C	295/308 (96%)	288 (98%)	7 (2%)	43	58
1	1-D	295/308 (96%)	291 (99%)	4 (1%)	59	75
1	2-A	295/308 (96%)	291 (99%)	4 (1%)	59	75
1	2-B	295/308 (96%)	290 (98%)	5 (2%)	53	69
1	2-C	295/308 (96%)	288 (98%)	7 (2%)	43	58
1	2-D	295/308 (96%)	291 (99%)	4 (1%)	59	75
1	3-A	295/308 (96%)	291 (99%)	4 (1%)	59	75
1	3-B	295/308 (96%)	290 (98%)	5 (2%)	53	69
1	3-C	295/308 (96%)	288 (98%)	7 (2%)	43	58
1	3-D	295/308 (96%)	291 (99%)	4 (1%)	59	75
1	4-A	295/308 (96%)	291 (99%)	4 (1%)	59	75
1	4-B	295/308 (96%)	290 (98%)	5 (2%)	53	69
1	4-C	295/308 (96%)	288 (98%)	7 (2%)	43	58
1	4-D	295/308 (96%)	291 (99%)	4 (1%)	59	75
1	5-A	295/308 (96%)	291 (99%)	4 (1%)	59	75
1	5-B	295/308 (96%)	290 (98%)	5 (2%)	53	69
1	5-C	295/308 (96%)	288 (98%)	7 (2%)	43	58
1	5-D	295/308 (96%)	291 (99%)	4 (1%)	59	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	6-A	295/308 (96%)	291 (99%)	4 (1%)	59	75
1	6-B	295/308 (96%)	290 (98%)	5 (2%)	53	69
1	6-C	295/308 (96%)	288 (98%)	7 (2%)	43	58
1	6-D	295/308 (96%)	291 (99%)	4 (1%)	59	75
1	7-A	295/308 (96%)	291 (99%)	4 (1%)	59	75
1	7-B	295/308 (96%)	290 (98%)	5 (2%)	53	69
1	7-C	295/308 (96%)	288 (98%)	7 (2%)	43	58
1	7-D	295/308 (96%)	291 (99%)	4 (1%)	59	75
1	8-A	295/308 (96%)	291 (99%)	4 (1%)	59	75
1	8-B	295/308 (96%)	290 (98%)	5 (2%)	53	69
1	8-C	295/308 (96%)	288 (98%)	7 (2%)	43	58
1	8-D	295/308 (96%)	291 (99%)	4 (1%)	59	75
All	All	9440/9856 (96%)	9280 (98%)	160 (2%)	53	69

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	48	THR
1	1-A	145	THR
1	1-A	184	GLU
1	1-A	191	LYS
1	1-B	65	ARG
1	1-B	112	SER
1	1-B	150	GLU
1	1-B	239	LYS
1	1-B	270	GLU
1	1-C	25	SER
1	1-C	48	THR
1	1-C	51	ARG
1	1-C	65	ARG
1	1-C	82	THR
1	1-C	86	VAL
1	1-C	117	LEU
1	1-D	57	MET
1	1-D	96	GLN
1	1-D	145	THR
1	1-D	154	LYS
1	2-A	48	THR

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Mol	Chain	Res	Type
1	2-A	145	THR
1	2-A	184	GLU
1	2-A	191	LYS
1	2-B	65	ARG
1	2-B	112	SER
1	2-B	150	GLU
1	2-B	239	LYS
1	2-B	270	GLU
1	2-C	25	SER
1	2-C	48	THR
1	2-C	51	ARG
1	2-C	65	ARG
1	2-C	82	THR
1	2-C	86	VAL
1	2-C	117	LEU
1	2-D	57	MET
1	2-D	96	GLN
1	2-D	145	THR
1	2-D	154	LYS
1	3-A	48	THR
1	3-A	145	THR
1	3-A	184	GLU
1	3-A	191	LYS
1	3-B	65	ARG
1	3-B	112	SER
1	3-B	150	GLU
1	3-B	239	LYS
1	3-B	270	GLU
1	3-C	25	SER
1	3-C	48	THR
1	3-C	51	ARG
1	3-C	65	ARG
1	3-C	82	THR
1	3-C	86	VAL
1	3-C	117	LEU
1	3-D	57	MET
1	3-D	96	GLN
1	3-D	145	THR
1	3-D	154	LYS
1	4-A	48	THR
1	4-A	145	THR
1	4-A	184	GLU

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Mol	Chain	Res	Type
1	4-A	191	LYS
1	4-B	65	ARG
1	4-B	112	SER
1	4-B	150	GLU
1	4-B	239	LYS
1	4-B	270	GLU
1	4-C	25	SER
1	4-C	48	THR
1	4-C	51	ARG
1	4-C	65	ARG
1	4-C	82	THR
1	4-C	86	VAL
1	4-C	117	LEU
1	4-D	57	MET
1	4-D	96	GLN
1	4-D	145	THR
1	4-D	154	LYS
1	5-A	48	THR
1	5-A	145	THR
1	5-A	184	GLU
1	5-A	191	LYS
1	5-B	65	ARG
1	5-B	112	SER
1	5-B	150	GLU
1	5-B	239	LYS
1	5-B	270	GLU
1	5-C	25	SER
1	5-C	48	THR
1	5-C	51	ARG
1	5-C	65	ARG
1	5-C	82	THR
1	5-C	86	VAL
1	5-C	117	LEU
1	5-D	57	MET
1	5-D	96	GLN
1	5-D	145	THR
1	5-D	154	LYS
1	6-A	48	THR
1	6-A	145	THR
1	6-A	184	GLU
1	6-A	191	LYS
1	6-B	65	ARG

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Mol	Chain	Res	Type
1	6-B	112	SER
1	6-B	150	GLU
1	6-B	239	LYS
1	6-B	270	GLU
1	6-C	25	SER
1	6-C	48	THR
1	6-C	51	ARG
1	6-C	65	ARG
1	6-C	82	THR
1	6-C	86	VAL
1	6-C	117	LEU
1	6-D	57	MET
1	6-D	96	GLN
1	6-D	145	THR
1	6-D	154	LYS
1	7-A	48	THR
1	7-A	145	THR
1	7-A	184	GLU
1	7-A	191	LYS
1	7-B	65	ARG
1	7-B	112	SER
1	7-B	150	GLU
1	7-B	239	LYS
1	7-B	270	GLU
1	7-C	25	SER
1	7-C	48	THR
1	7-C	51	ARG
1	7-C	65	ARG
1	7-C	82	THR
1	7-C	86	VAL
1	7-C	117	LEU
1	7-D	57	MET
1	7-D	96	GLN
1	7-D	145	THR
1	7-D	154	LYS
1	8-A	48	THR
1	8-A	145	THR
1	8-A	184	GLU
1	8-A	191	LYS
1	8-B	65	ARG
1	8-B	112	SER
1	8-B	150	GLU

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Mol	Chain	Res	Type
1	8-B	239	LYS
1	8-B	270	GLU
1	8-C	25	SER
1	8-C	48	THR
1	8-C	51	ARG
1	8-C	65	ARG
1	8-C	82	THR
1	8-C	86	VAL
1	8-C	117	LEU
1	8-D	57	MET
1	8-D	96	GLN
1	8-D	145	THR
1	8-D	154	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (214) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	55	GLN
1	1-A	63	HIS
1	1-A	67	GLN
1	1-A	129	GLN
1	1-A	185	ASN
1	1-A	237	GLN
1	1-A	273	HIS
1	1-A	274	GLN
1	1-B	41	HIS
1	1-B	55	GLN
1	1-B	129	GLN
1	1-B	237	GLN
1	1-B	275	GLN
1	1-B	299	ASN
1	1-B	338	GLN
1	1-B	355	GLN
1	1-C	43	GLN
1	1-C	63	HIS
1	1-C	129	GLN
1	1-C	205	ASN
1	1-C	275	GLN
1	1-D	63	HIS
1	1-D	96	GLN
1	1-D	179	ASN
1	1-D	205	ASN

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Mol	Chain	Res	Type
1	1-D	256	GLN
1	1-D	275	GLN
1	2-A	41	HIS
1	2-A	67	GLN
1	2-A	129	GLN
1	2-A	185	ASN
1	2-A	237	GLN
1	2-A	275	GLN
1	2-B	38	ASN
1	2-B	55	GLN
1	2-B	237	GLN
1	2-B	273	HIS
1	2-B	275	GLN
1	2-B	335	GLN
1	2-B	338	GLN
1	2-C	67	GLN
1	2-C	129	GLN
1	2-C	274	GLN
1	2-C	275	GLN
1	2-C	339	ASN
1	2-C	341	ASN
1	2-C	354	HIS
1	2-D	43	GLN
1	2-D	129	GLN
1	2-D	205	ASN
1	3-A	67	GLN
1	3-A	129	GLN
1	3-A	169	GLN
1	3-A	237	GLN
1	3-A	273	HIS
1	3-A	274	GLN
1	3-A	275	GLN
1	3-A	299	ASN
1	3-A	335	GLN
1	3-B	38	ASN
1	3-B	55	GLN
1	3-B	179	ASN
1	3-B	205	ASN
1	3-B	237	GLN
1	3-B	256	GLN
1	3-B	275	GLN
1	3-B	299	ASN

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Mol	Chain	Res	Type
1	3-C	63	HIS
1	3-C	92	HIS
1	3-C	96	GLN
1	3-C	205	ASN
1	3-C	230	GLN
1	3-C	273	HIS
1	3-C	275	GLN
1	3-D	43	GLN
1	3-D	55	GLN
1	3-D	63	HIS
1	3-D	92	HIS
1	3-D	205	ASN
1	3-D	256	GLN
1	3-D	274	GLN
1	4-A	38	ASN
1	4-A	41	HIS
1	4-A	67	GLN
1	4-A	185	ASN
1	4-A	237	GLN
1	4-A	273	HIS
1	4-A	274	GLN
1	4-A	275	GLN
1	4-A	299	ASN
1	4-B	38	ASN
1	4-B	55	GLN
1	4-B	160	ASN
1	4-B	222	HIS
1	4-B	224	HIS
1	4-B	237	GLN
1	4-B	273	HIS
1	4-B	274	GLN
1	4-B	275	GLN
1	4-B	299	ASN
1	4-B	339	ASN
1	4-B	354	HIS
1	4-C	38	ASN
1	4-C	43	GLN
1	4-C	63	HIS
1	4-C	67	GLN
1	4-C	169	GLN
1	4-C	183	HIS
1	4-C	185	ASN

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Mol	Chain	Res	Type
1	4-C	205	ASN
1	4-C	273	HIS
1	4-C	274	GLN
1	4-C	299	ASN
1	4-D	129	GLN
1	4-D	205	ASN
1	4-D	274	GLN
1	5-A	63	HIS
1	5-A	169	GLN
1	5-A	237	GLN
1	5-A	256	GLN
1	5-A	273	HIS
1	5-A	274	GLN
1	5-B	169	GLN
1	5-B	237	GLN
1	5-B	256	GLN
1	5-B	274	GLN
1	5-B	275	GLN
1	5-C	129	GLN
1	5-C	185	ASN
1	5-C	256	GLN
1	5-C	275	GLN
1	5-C	354	HIS
1	5-D	41	HIS
1	5-D	183	HIS
1	5-D	299	ASN
1	6-A	38	ASN
1	6-A	55	GLN
1	6-A	67	GLN
1	6-A	160	ASN
1	6-A	169	GLN
1	6-A	183	HIS
1	6-A	185	ASN
1	6-A	237	GLN
1	6-A	273	HIS
1	6-A	354	HIS
1	6-B	55	GLN
1	6-B	237	GLN
1	6-B	256	GLN
1	6-B	273	HIS
1	6-B	275	GLN
1	6-C	43	GLN

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Mol	Chain	Res	Type
1	6-C	63	HIS
1	6-C	129	GLN
1	6-C	256	GLN
1	6-C	354	HIS
1	6-C	355	GLN
1	6-D	129	GLN
1	6-D	205	ASN
1	6-D	274	GLN
1	6-D	354	HIS
1	7-A	41	HIS
1	7-A	63	HIS
1	7-A	67	GLN
1	7-A	185	ASN
1	7-A	237	GLN
1	7-A	273	HIS
1	7-A	274	GLN
1	7-A	275	GLN
1	7-B	67	GLN
1	7-B	237	GLN
1	7-B	256	GLN
1	7-B	275	GLN
1	7-B	299	ASN
1	7-B	307	HIS
1	7-B	354	HIS
1	7-C	63	HIS
1	7-C	92	HIS
1	7-C	129	GLN
1	7-C	273	HIS
1	7-C	307	HIS
1	7-C	354	HIS
1	7-D	92	HIS
1	7-D	183	HIS
1	7-D	224	HIS
1	7-D	274	GLN
1	7-D	307	HIS
1	8-A	38	ASN
1	8-A	41	HIS
1	8-A	63	HIS
1	8-A	67	GLN
1	8-A	183	HIS
1	8-A	237	GLN
1	8-A	273	HIS

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Mol	Chain	Res	Type
1	8-A	299	ASN
1	8-B	67	GLN
1	8-B	185	ASN
1	8-B	237	GLN
1	8-B	274	GLN
1	8-B	275	GLN
1	8-B	307	HIS
1	8-C	43	GLN
1	8-C	63	HIS
1	8-C	67	GLN
1	8-C	205	ASN
1	8-C	274	GLN
1	8-C	354	HIS
1	8-D	63	HIS
1	8-D	129	GLN
1	8-D	169	GLN
1	8-D	256	GLN
1	8-D	274	GLN
1	8-D	275	GLN
1	8-D	307	HIS
1	8-D	335	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](#)

There are no ligands in this entry.

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	1-A	345/359 (96%)	0.90	46 (13%) 7 5	2, 4, 7, 8	345 (100%)
1	1-B	345/359 (96%)	1.11	57 (16%) 4 3	2, 4, 7, 12	345 (100%)
1	1-C	345/359 (96%)	1.55	109 (31%) 1 1	2, 4, 8, 10	345 (100%)
1	1-D	345/359 (96%)	1.03	59 (17%) 4 3	2, 4, 7, 11	345 (100%)
1	2-A	0/359	-	-	-	-
1	2-B	0/359	-	-	-	-
1	2-C	0/359	-	-	-	-
1	2-D	0/359	-	-	-	-
1	3-A	0/359	-	-	-	-
1	3-B	0/359	-	-	-	-
1	3-C	0/359	-	-	-	-
1	3-D	0/359	-	-	-	-
1	4-A	0/359	-	-	-	-
1	4-B	0/359	-	-	-	-
1	4-C	0/359	-	-	-	-
1	4-D	0/359	-	-	-	-
1	5-A	0/359	-	-	-	-
1	5-B	0/359	-	-	-	-
1	5-C	0/359	-	-	-	-
1	5-D	0/359	-	-	-	-
1	6-A	0/359	-	-	-	-
1	6-B	0/359	-	-	-	-
1	6-C	0/359	-	-	-	-
1	6-D	0/359	-	-	-	-
1	7-A	0/359	-	-	-	-
1	7-B	0/359	-	-	-	-
1	7-C	0/359	-	-	-	-
1	7-D	0/359	-	-	-	-
1	8-A	0/359	-	-	-	-
1	8-B	0/359	-	-	-	-
1	8-C	0/359	-	-	-	-

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	8-D	0/359	-	-	-	-
All	All	1380/11488 (12%)	1.15	271 (19%) 3 2	2, 4, 7, 12	1380 (100%)

All (271) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-D	106	LEU	9.0
1	1-C	331	GLY	8.6
1	1-C	309	SER	8.2
1	1-D	205	ASN	7.1
1	1-B	306	CYS	6.5
1	1-C	82	THR	6.1
1	1-A	209	GLU	5.9
1	1-C	308	MET	5.8
1	1-B	104	THR	5.8
1	1-C	73	VAL	5.6
1	1-C	134	VAL	5.6
1	1-C	316	PRO	5.5
1	1-D	306	CYS	5.5
1	1-C	104	THR	5.1
1	1-D	128	GLY	5.0
1	1-A	79	ASP	5.0
1	1-C	306	CYS	4.9
1	1-C	310	VAL	4.7
1	1-C	25	SER	4.6
1	1-D	257	SER	4.6
1	1-C	22	LEU	4.5
1	1-D	92	HIS	4.5
1	1-C	83	VAL	4.4
1	1-C	78	ALA	4.3
1	1-A	54	GLY	4.3
1	1-C	323	SER	4.3
1	1-C	157	LEU	4.3
1	1-A	80	PHE	4.2
1	1-C	42	PHE	4.2
1	1-B	127	TYR	4.1
1	1-C	24	ALA	4.1
1	1-D	281	GLU	4.1
1	1-C	102	LEU	4.1
1	1-D	216	SER	4.1
1	1-B	105	ALA	4.0
1	1-D	88	CYS	4.0

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Mol	Chain	Res	Type	RSRZ
1	1-C	106	LEU	3.9
1	1-C	305	TYR	3.9
1	1-A	38	ASN	3.9
1	1-C	359	PRO	3.8
1	1-C	235	VAL	3.8
1	1-C	15	LYS	3.8
1	1-C	44	VAL	3.8
1	1-C	17	ILE	3.7
1	1-C	72	LEU	3.7
1	1-C	75	VAL	3.7
1	1-C	257	SER	3.7
1	1-C	278	THR	3.7
1	1-B	88	CYS	3.7
1	1-C	26	GLY	3.7
1	1-B	90	LEU	3.6
1	1-D	59	SER	3.6
1	1-B	305	TYR	3.6
1	1-C	88	CYS	3.6
1	1-C	46	LEU	3.6
1	1-C	49	ALA	3.6
1	1-C	53	ALA	3.6
1	1-A	210	ILE	3.5
1	1-C	115	PHE	3.5
1	1-C	215	SER	3.5
1	1-B	329	VAL	3.5
1	1-C	18	ARG	3.4
1	1-D	123	TYR	3.4
1	1-D	127	TYR	3.4
1	1-A	303	SER	3.4
1	1-A	53	ALA	3.4
1	1-D	104	THR	3.4
1	1-C	33	VAL	3.4
1	1-C	84	ASP	3.4
1	1-C	92	HIS	3.3
1	1-B	223	ARG	3.3
1	1-A	104	THR	3.3
1	1-A	115	PHE	3.3
1	1-A	316	PRO	3.2
1	1-D	345	GLY	3.2
1	1-C	117	LEU	3.2
1	1-C	50	ASP	3.2
1	1-C	90	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	1-A	83	VAL	3.2
1	1-D	206	LEU	3.2
1	1-B	85	ALA	3.1
1	1-A	358	PHE	3.1
1	1-C	20	GLY	3.1
1	1-C	114	ASP	3.1
1	1-A	246	PRO	3.1
1	1-D	86	VAL	3.1
1	1-D	208	SER	3.1
1	1-C	23	GLY	3.1
1	1-C	311	PHE	3.1
1	1-B	73	VAL	3.1
1	1-B	355	GLN	3.1
1	1-A	213	GLY	3.0
1	1-B	292	GLY	3.0
1	1-D	156	ARG	3.0
1	1-A	133	ALA	3.0
1	1-B	78	ALA	3.0
1	1-C	281	GLU	3.0
1	1-C	80	PHE	3.0
1	1-C	140	VAL	3.0
1	1-D	212	GLU	3.0
1	1-A	94	THR	3.0
1	1-D	292	GLY	3.0
1	1-A	110	ASP	3.0
1	1-A	222	HIS	3.0
1	1-C	358	PHE	3.0
1	1-C	51	ARG	2.9
1	1-C	103	PRO	2.9
1	1-B	92	HIS	2.9
1	1-C	108	ILE	2.9
1	1-C	315	ILE	2.9
1	1-D	91	PRO	2.9
1	1-A	317	GLY	2.9
1	1-C	303	SER	2.9
1	1-D	179	ASN	2.9
1	1-C	105	ALA	2.9
1	1-D	105	ALA	2.9
1	1-A	92	HIS	2.9
1	1-C	16	ASP	2.8
1	1-C	79	ASP	2.8
1	1-D	221	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	1-B	220	THR	2.8
1	1-D	58	GLU	2.8
1	1-B	347	PRO	2.8
1	1-C	130	PRO	2.8
1	1-D	115	PHE	2.8
1	1-D	157	LEU	2.8
1	1-B	118	ARG	2.7
1	1-C	74	SER	2.7
1	1-C	317	GLY	2.7
1	1-C	280	TYR	2.7
1	1-C	346	TYR	2.7
1	1-B	304	ASN	2.7
1	1-D	107	LYS	2.7
1	1-D	273	HIS	2.7
1	1-B	132	LYS	2.7
1	1-D	96	GLN	2.7
1	1-A	82	THR	2.7
1	1-A	106	LEU	2.7
1	1-D	269	THR	2.6
1	1-A	359	PRO	2.6
1	1-C	70	PRO	2.6
1	1-B	97	GLU	2.6
1	1-B	91	PRO	2.6
1	1-C	136	LEU	2.6
1	1-C	155	ALA	2.6
1	1-A	109	VAL	2.6
1	1-D	343	MET	2.6
1	1-C	156	ARG	2.6
1	1-B	46	LEU	2.6
1	1-B	43	GLN	2.5
1	1-B	54	GLY	2.5
1	1-C	127	TYR	2.5
1	1-A	16	ASP	2.5
1	1-A	57	MET	2.5
1	1-A	355	GLN	2.5
1	1-C	139	GLU	2.5
1	1-D	268	ARG	2.5
1	1-C	299	ASN	2.5
1	1-D	207	TYR	2.5
1	1-B	192	SER	2.5
1	1-B	171	PRO	2.4
1	1-A	102	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	1-B	177	LYS	2.4
1	1-C	107	LYS	2.4
1	1-D	237	GLN	2.4
1	1-B	75	VAL	2.4
1	1-A	130	PRO	2.4
1	1-C	91	PRO	2.4
1	1-A	211	ALA	2.4
1	1-D	93	GLY	2.4
1	1-C	327	ASN	2.4
1	1-A	58	GLU	2.4
1	1-C	101	GLU	2.4
1	1-D	114	ASP	2.4
1	1-C	342	ILE	2.4
1	1-B	28	THR	2.4
1	1-C	65	ARG	2.4
1	1-C	40	PRO	2.4
1	1-A	78	ALA	2.4
1	1-B	102	LEU	2.4
1	1-B	300	VAL	2.4
1	1-D	81	SER	2.4
1	1-C	71	THR	2.4
1	1-A	129	GLN	2.3
1	1-C	69	LEU	2.3
1	1-B	77	ASP	2.3
1	1-B	80	PHE	2.3
1	1-A	56	SER	2.3
1	1-B	257	SER	2.3
1	1-C	158	VAL	2.3
1	1-B	51	ARG	2.3
1	1-A	132	LYS	2.3
1	1-A	59	SER	2.3
1	1-C	45	THR	2.3
1	1-D	130	PRO	2.3
1	1-D	66	ALA	2.3
1	1-B	234	ASP	2.3
1	1-D	102	LEU	2.3
1	1-D	124	GLU	2.3
1	1-C	43	GLN	2.3
1	1-B	178	ALA	2.3
1	1-B	336	ALA	2.3
1	1-A	128	GLY	2.3
1	1-C	76	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	1-D	90	LEU	2.3
1	1-B	184	GLU	2.2
1	1-D	103	PRO	2.2
1	1-C	57	MET	2.2
1	1-C	89	CYS	2.2
1	1-A	183	HIS	2.2
1	1-C	129	GLN	2.2
1	1-D	129	GLN	2.2
1	1-C	246	PRO	2.2
1	1-C	350	THR	2.2
1	1-A	282	ASP	2.2
1	1-A	208	SER	2.2
1	1-D	238	SER	2.2
1	1-B	68	LYS	2.2
1	1-B	76	LYS	2.2
1	1-B	82	THR	2.2
1	1-C	159	ALA	2.2
1	1-C	332	ALA	2.2
1	1-C	123	TYR	2.2
1	1-C	277	LYS	2.2
1	1-B	45	THR	2.2
1	1-B	103	PRO	2.1
1	1-D	282	ASP	2.2
1	1-D	291	GLU	2.1
1	1-A	134	VAL	2.1
1	1-B	128	GLY	2.1
1	1-C	236	ALA	2.1
1	1-B	89	CYS	2.1
1	1-C	172	LEU	2.1
1	1-C	81	SER	2.1
1	1-C	52	LYS	2.1
1	1-B	339	ASN	2.1
1	1-B	284	GLU	2.1
1	1-D	28	THR	2.1
1	1-D	95	THR	2.1
1	1-A	98	ILE	2.1
1	1-B	252	ILE	2.1
1	1-C	302	GLY	2.1
1	1-D	196	GLY	2.1
1	1-C	133	ALA	2.1
1	1-D	204	ALA	2.1
1	1-B	101	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	1-C	304	ASN	2.1
1	1-B	120	ILE	2.1
1	1-B	181	ILE	2.1
1	1-D	80	PHE	2.1
1	1-B	83	VAL	2.1
1	1-D	235	VAL	2.1
1	1-C	36	LEU	2.1
1	1-D	72	LEU	2.1
1	1-A	77	ASP	2.1
1	1-D	290	ASP	2.1
1	1-C	143	GLY	2.1
1	1-C	154	LYS	2.1
1	1-D	202	LYS	2.1
1	1-D	210	ILE	2.1
1	1-B	165	PRO	2.0
1	1-C	128	GLY	2.0
1	1-A	120	ILE	2.0
1	1-C	58	GLU	2.0
1	1-C	86	VAL	2.0
1	1-B	66	ALA	2.0
1	1-C	77	ASP	2.0
1	1-D	50	ASP	2.0
1	1-B	183	HIS	2.0
1	1-A	93	GLY	2.0
1	1-C	345	GLY	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.