



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:40 AM UTC

PDB ID : 2Q50 / pdb_00002q50
Title : Ensemble refinement of the protein crystal structure of a glyoxylate/hydroxy pyruvate reductase from Homo sapiens
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 : 2.45 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:

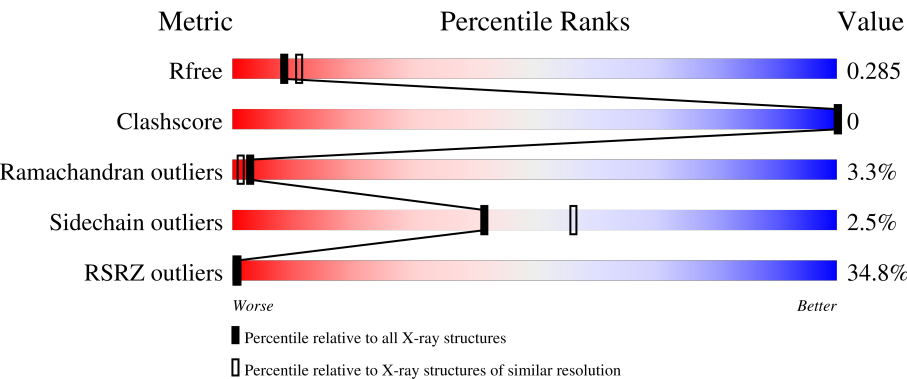
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.45 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



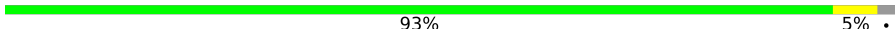
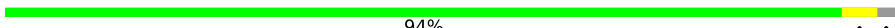
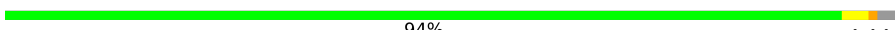
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1-A	328	32% 92%6%
1	1-B	328	30% 96%..
1	1-C	328	31% 92%6%
1	1-D	328	41% 90%8%
1	2-A	328	91%7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	2-B	328	 93% 5% .
1	2-C	328	 92% 5% .
1	2-D	328	 93% 5% .
1	3-A	328	 92% 5% .
1	3-B	328	 92% 5% .
1	3-C	328	 92% 6% .
1	3-D	328	 94% . .
1	4-A	328	 91% 6% .
1	4-B	328	 94% . .
1	4-C	328	 90% 7% .
1	4-D	328	 93% 5% .
1	5-A	328	 93% 5% .
1	5-B	328	 94% . . .
1	5-C	328	 92% 6% .
1	5-D	328	 94% . .
1	6-A	328	 88% 10% .
1	6-B	328	 92% 6% .
1	6-C	328	 90% 8% .
1	6-D	328	 92% 6% .
1	7-A	328	 89% 9% .
1	7-B	328	 90% 8% .
1	7-C	328	 91% 7% .
1	7-D	328	 93% 5% .
1	8-A	328	 92% 6% .
1	8-B	328	 94% . .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	8-C	328	91% 6% .
1	8-D	328	94% . .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 81744 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 Glyoxylate reductase/hydroxypyruvate reductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-A	321	Total	C	N	O	S	Se	0	0	0
			2442	1542	431	457	7	5			
1	2-A	321	Total	C	N	O	S	Se	0	0	0
			2442	1542	431	457	7	5			
1	3-A	321	Total	C	N	O	S	Se	0	0	0
			2442	1542	431	457	7	5			
1	4-A	321	Total	C	N	O	S	Se	0	0	0
			2442	1542	431	457	7	5			
1	5-A	321	Total	C	N	O	S	Se	0	0	0
			2442	1542	431	457	7	5			
1	6-A	321	Total	C	N	O	S	Se	0	0	0
			2442	1542	431	457	7	5			
1	7-A	321	Total	C	N	O	S	Se	0	0	0
			2442	1542	431	457	7	5			
1	8-A	321	Total	C	N	O	S	Se	0	0	0
			2442	1542	431	457	7	5			
1	1-B	321	Total	C	N	O	S	Se	0	0	0
			2442	1542	431	457	7	5			
1	2-B	321	Total	C	N	O	S	Se	0	0	0
			2442	1542	431	457	7	5			
1	3-B	321	Total	C	N	O	S	Se	0	0	0
			2442	1542	431	457	7	5			
1	4-B	321	Total	C	N	O	S	Se	0	0	0
			2442	1542	431	457	7	5			
1	5-B	321	Total	C	N	O	S	Se	0	0	0
			2442	1542	431	457	7	5			
1	6-B	321	Total	C	N	O	S	Se	0	0	0
			2442	1542	431	457	7	5			
1	7-B	321	Total	C	N	O	S	Se	0	0	0
			2442	1542	431	457	7	5			
1	8-B	321	Total	C	N	O	S	Se	0	0	0
			2442	1542	431	457	7	5			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-C	321	Total	C	N	O	S	Se	0	0	0
			2442	1542	431	457	7	5			
1	2-C	321	Total	C	N	O	S	Se	0	0	0
			2442	1542	431	457	7	5			
1	3-C	321	Total	C	N	O	S	Se	0	0	0
			2442	1542	431	457	7	5			
1	4-C	321	Total	C	N	O	S	Se	0	0	0
			2442	1542	431	457	7	5			
1	5-C	321	Total	C	N	O	S	Se	0	0	0
			2442	1542	431	457	7	5			
1	6-C	321	Total	C	N	O	S	Se	0	0	0
			2442	1542	431	457	7	5			
1	7-C	321	Total	C	N	O	S	Se	0	0	0
			2442	1542	431	457	7	5			
1	8-C	321	Total	C	N	O	S	Se	0	0	0
			2442	1542	431	457	7	5			
1	1-D	321	Total	C	N	O	S	Se	0	0	0
			2442	1542	431	457	7	5			
1	2-D	321	Total	C	N	O	S	Se	0	0	0
			2442	1542	431	457	7	5			
1	3-D	321	Total	C	N	O	S	Se	0	0	0
			2442	1542	431	457	7	5			
1	4-D	321	Total	C	N	O	S	Se	0	0	0
			2442	1542	431	457	7	5			
1	5-D	321	Total	C	N	O	S	Se	0	0	0
			2442	1542	431	457	7	5			
1	6-D	321	Total	C	N	O	S	Se	0	0	0
			2442	1542	431	457	7	5			
1	7-D	321	Total	C	N	O	S	Se	0	0	0
			2442	1542	431	457	7	5			
1	8-D	321	Total	C	N	O	S	Se	0	0	0
			2442	1542	431	457	7	5			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP Q9UBQ7
A	7	MSE	MET	modified residue	UNP Q9UBQ7
A	81	MSE	MET	modified residue	UNP Q9UBQ7
A	234	MSE	MET	modified residue	UNP Q9UBQ7
A	305	MSE	MET	modified residue	UNP Q9UBQ7
A	322	MSE	MET	modified residue	UNP Q9UBQ7
B	1	SER	-	expression tag	UNP Q9UBQ7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	7	MSE	MET	modified residue	UNP Q9UBQ7
B	81	MSE	MET	modified residue	UNP Q9UBQ7
B	234	MSE	MET	modified residue	UNP Q9UBQ7
B	305	MSE	MET	modified residue	UNP Q9UBQ7
B	322	MSE	MET	modified residue	UNP Q9UBQ7
C	1	SER	-	expression tag	UNP Q9UBQ7
C	7	MSE	MET	modified residue	UNP Q9UBQ7
C	81	MSE	MET	modified residue	UNP Q9UBQ7
C	234	MSE	MET	modified residue	UNP Q9UBQ7
C	305	MSE	MET	modified residue	UNP Q9UBQ7
C	322	MSE	MET	modified residue	UNP Q9UBQ7
D	1	SER	-	expression tag	UNP Q9UBQ7
D	7	MSE	MET	modified residue	UNP Q9UBQ7
D	81	MSE	MET	modified residue	UNP Q9UBQ7
D	234	MSE	MET	modified residue	UNP Q9UBQ7
D	305	MSE	MET	modified residue	UNP Q9UBQ7
D	322	MSE	MET	modified residue	UNP Q9UBQ7

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	1-A	103	Total O 103 103	0	0
2	2-A	104	Total O 104 104	0	0
2	3-A	104	Total O 104 104	0	0
2	4-A	104	Total O 104 104	0	0
2	5-A	111	Total O 111 111	0	0
2	6-A	107	Total O 107 107	0	0
2	7-A	106	Total O 106 106	0	0
2	8-A	108	Total O 108 108	0	0
2	1-B	130	Total O 130 130	0	0
2	2-B	128	Total O 128 128	0	0
2	3-B	128	Total O 128 128	0	0

Continued on next page...

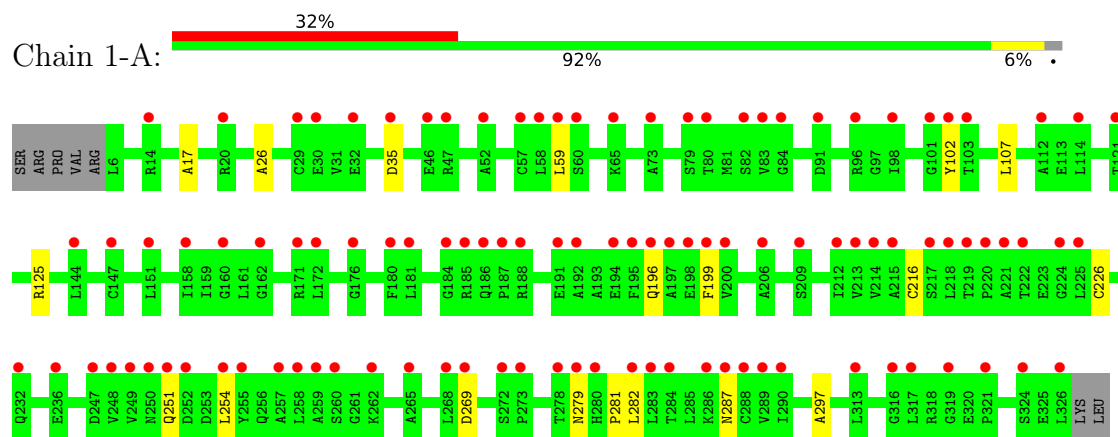
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	4-B	128	Total 128	O 128	0	0
2	5-B	121	Total 121	O 121	0	0
2	6-B	125	Total 125	O 125	0	0
2	7-B	126	Total 126	O 126	0	0
2	8-B	124	Total 124	O 124	0	0
2	1-C	122	Total 122	O 122	0	0
2	2-C	122	Total 122	O 122	0	0
2	3-C	121	Total 121	O 121	0	0
2	4-C	122	Total 122	O 122	0	0
2	5-C	121	Total 121	O 121	0	0
2	6-C	120	Total 120	O 120	0	0
2	7-C	119	Total 119	O 119	0	0
2	8-C	119	Total 119	O 119	0	0
2	1-D	95	Total 95	O 95	0	0
2	2-D	96	Total 96	O 96	0	0
2	3-D	97	Total 97	O 97	0	0
2	4-D	96	Total 96	O 96	0	0
2	5-D	97	Total 97	O 97	0	0
2	6-D	98	Total 98	O 98	0	0
2	7-D	99	Total 99	O 99	0	0
2	8-D	99	Total 99	O 99	0	0

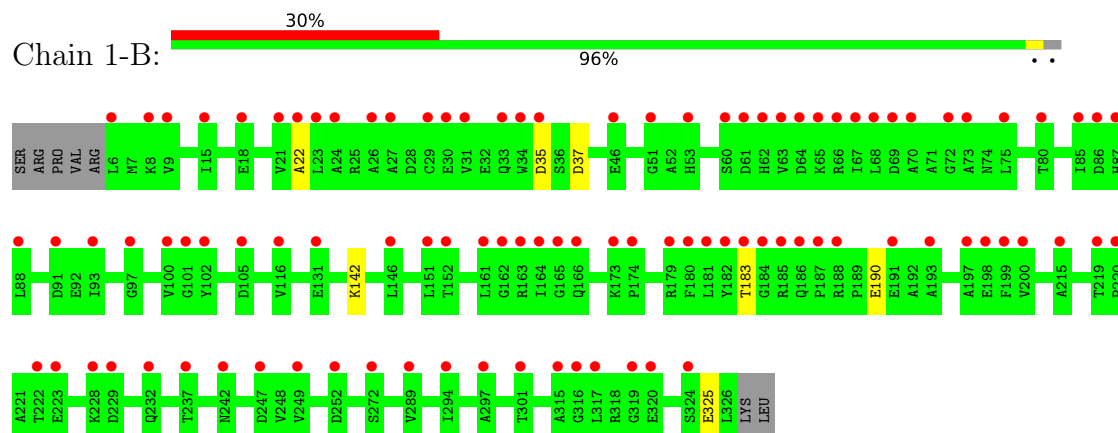
3 Residue-property plots [i](#)

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.

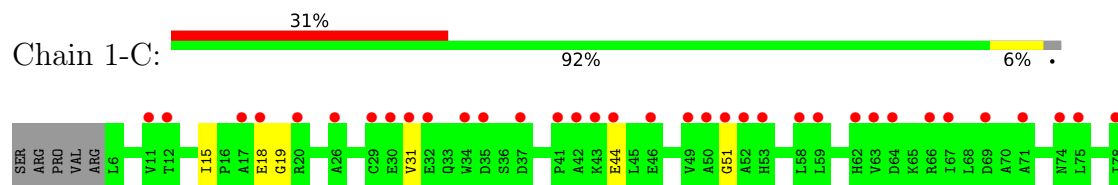
- Molecule 1: Glyoxylate reductase/hydroxypyruvate reductase

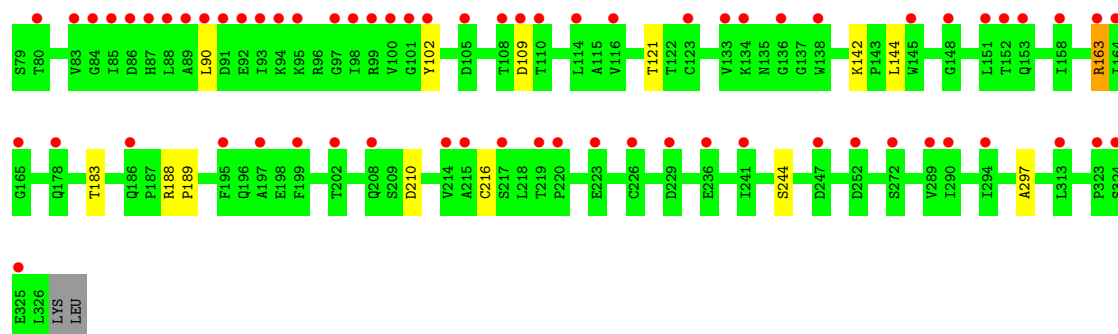


- Molecule 1: Glyoxylate reductase/hydroxypyruvate reductase

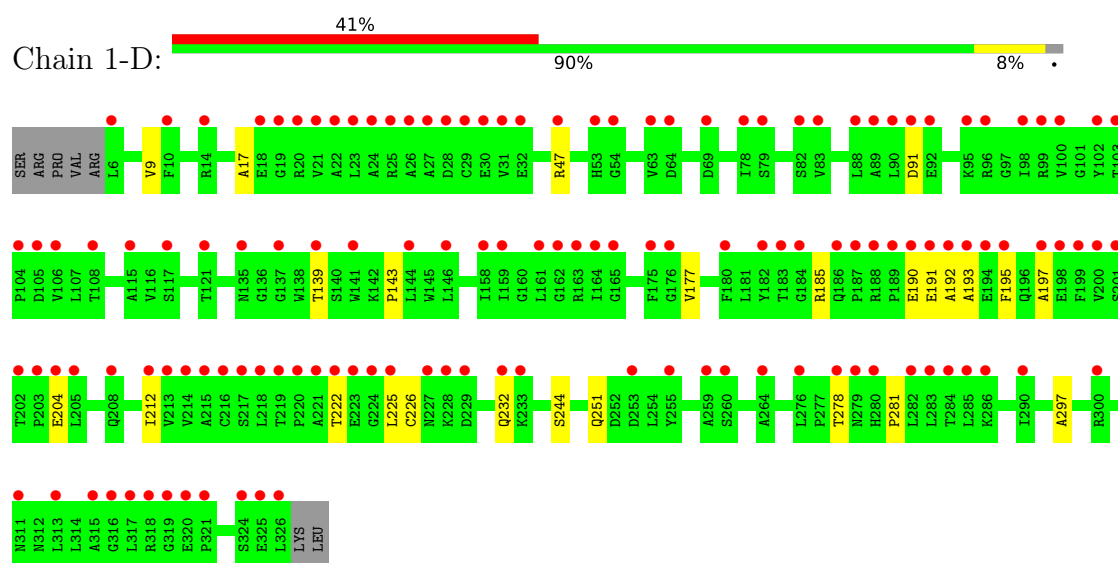


- Molecule 1: Glyoxylate reductase/hydroxypyruvate reductase

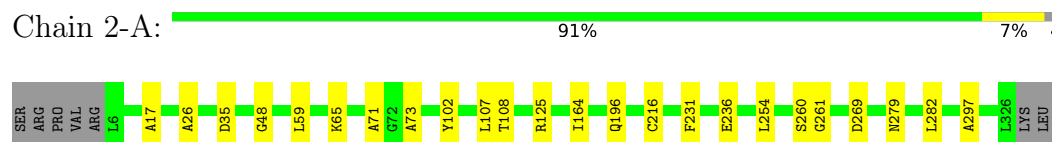




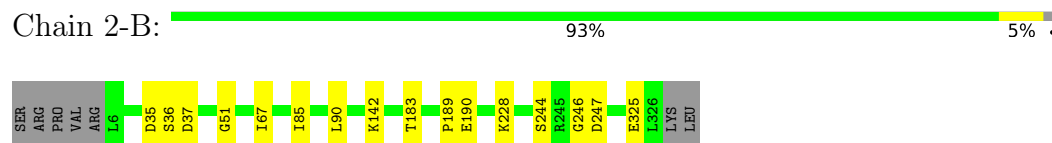
- Molecule 1: Glyoxylate reductase/hydroxypyruvate reductase



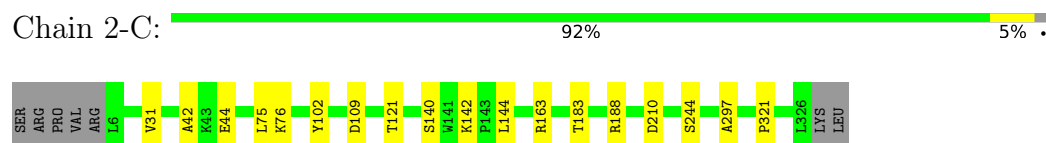
- Molecule 1: Glyoxylate reductase/hydroxypyruvate reductase



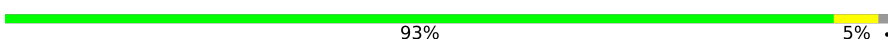
- Molecule 1: Glyoxylate reductase/hydroxypyruvate reductase

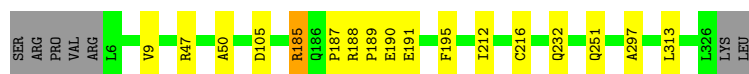


- Molecule 1: Glyoxylate reductase/hydroxypyruvate reductase

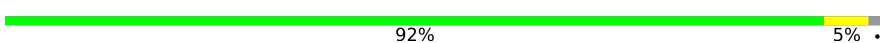


- Molecule 1: Glyoxylate reductase/hydroxypyruvate reductase

Chain 2-D:  93% 5% .



- Molecule 1: Glyoxylate reductase/hydroxypyruvate reductase

Chain 3-A:  92% 5% .



- Molecule 1: Glyoxylate reductase/hydroxypyruvate reductase

Chain 3-B:  92% 5% .

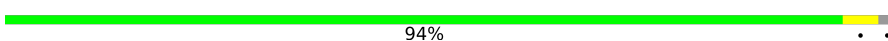


- Molecule 1: Glyoxylate reductase/hydroxypyruvate reductase

Chain 3-C:  92% 6% .

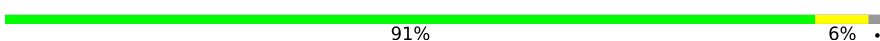


- Molecule 1: Glyoxylate reductase/hydroxypyruvate reductase

Chain 3-D:  94% 5% .

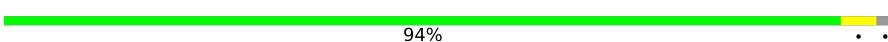


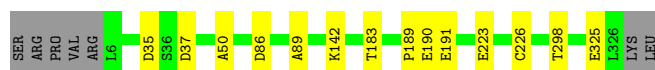
- Molecule 1: Glyoxylate reductase/hydroxypyruvate reductase

Chain 4-A:  91% 6% .

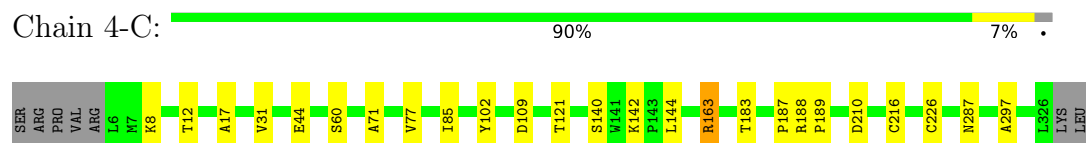


- Molecule 1: Glyoxylate reductase/hydroxypyruvate reductase

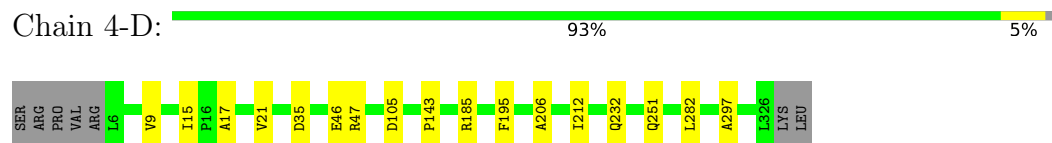
Chain 4-B:  94% 5% .



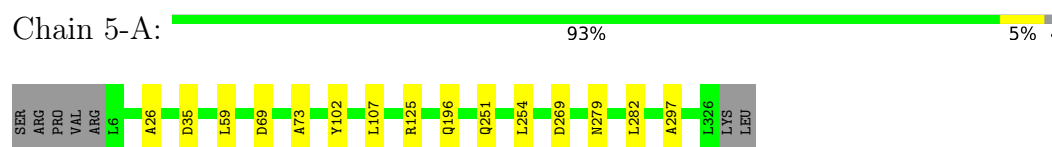
- Molecule 1: Glyoxylate reductase/hydroxypyruvate reductase



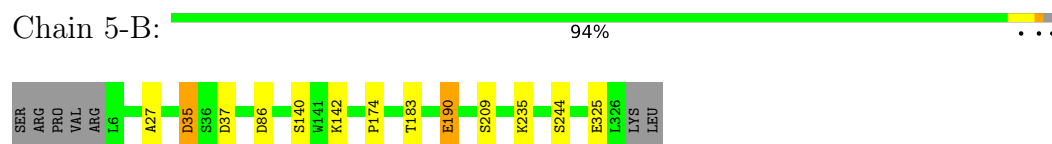
- Molecule 1: Glyoxylate reductase/hydroxypyruvate reductase



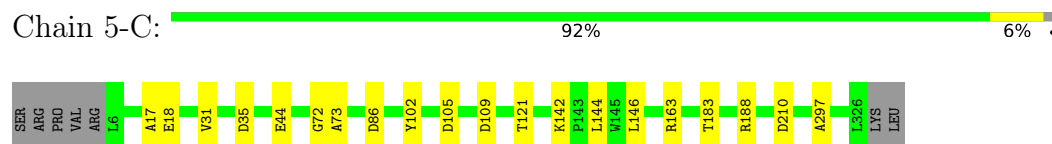
- Molecule 1: Glyoxylate reductase/hydroxypyruvate reductase



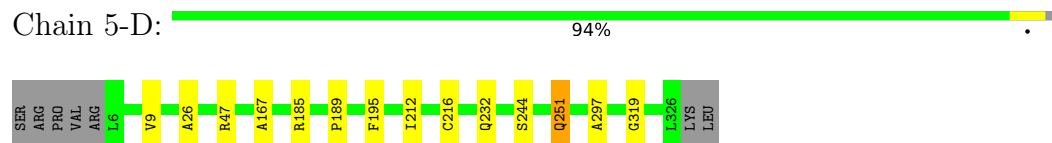
- Molecule 1: Glyoxylate reductase/hydroxypyruvate reductase



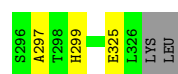
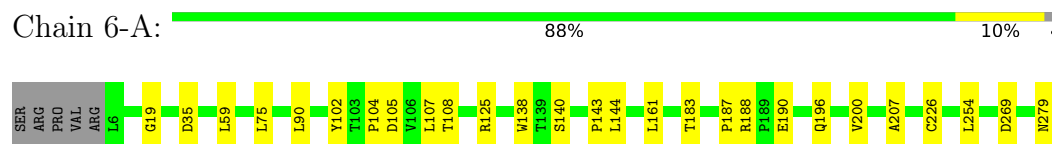
- Molecule 1: Glyoxylate reductase/hydroxypyruvate reductase



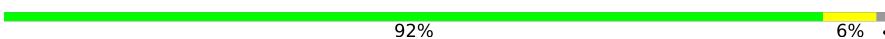
- Molecule 1: Glyoxylate reductase/hydroxypyruvate reductase



- Molecule 1: Glyoxylate reductase/hydroxypyruvate reductase



- Molecule 1: Glyoxylate reductase/hydroxypyruvate reductase

Chain 6-B:  92% 6% .

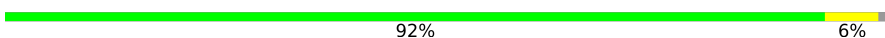


- Molecule 1: Glyoxylate reductase/hydroxypyruvate reductase

Chain 6-C:  90% 8% .



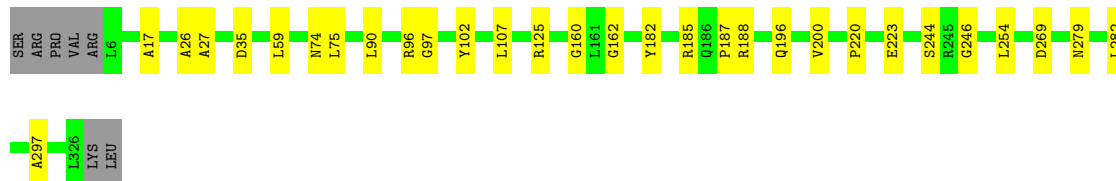
- Molecule 1: Glyoxylate reductase/hydroxypyruvate reductase

Chain 6-D:  92% 6% .



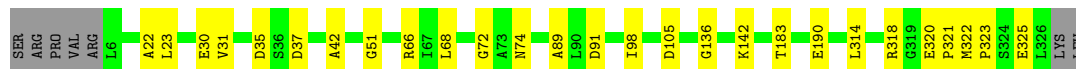
- Molecule 1: Glyoxylate reductase/hydroxypyruvate reductase

Chain 7-A:  89% 9% .

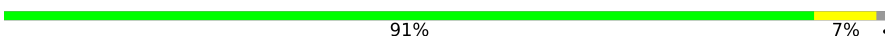


- Molecule 1: Glyoxylate reductase/hydroxypyruvate reductase

Chain 7-B:  90% 8% .

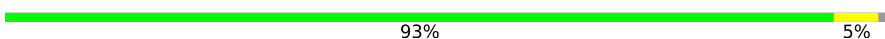


- Molecule 1: Glyoxylate reductase/hydroxypyruvate reductase

Chain 7-C:  91% 7% .



- Molecule 1: Glyoxylate reductase/hydroxypyruvate reductase

Chain 7-D:  93% 5% .



- Molecule 1: Glyoxylate reductase/hydroxypyruvate reductase

Chain 8-A: 92% 6% .



- Molecule 1: Glyoxylate reductase/hydroxypyruvate reductase

Chain 8-B: 94% . .



- Molecule 1: Glyoxylate reductase/hydroxypyruvate reductase

Chain 8-C: 91% 6% .



- Molecule 1: Glyoxylate reductase/hydroxypyruvate reductase

Chain 8-D: 94% . .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.00Å 66.44Å 148.77Å 90.00° 98.59° 90.00°	Depositor
Resolution (Å)	49.33 – 2.45 49.33 – 2.46	Depositor EDS
% Data completeness (in resolution range)	93.0 (49.33-2.45) 93.1 (49.33-2.46)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 2.45Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.200 , 0.286 0.204 , 0.285	Depositor DCC
R_{free} test set	2551 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	31.6	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.04 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	81744	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.90% 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	0.22	0/2481	0.48	3/3363 (0.1%)
1	1-B	0.24	0/2481	0.53	3/3363 (0.1%)
1	1-C	0.24	0/2481	0.56	7/3363 (0.2%)
1	1-D	0.24	0/2481	0.48	1/3363 (0.0%)
1	2-A	0.22	0/2481	0.48	3/3363 (0.1%)
1	2-B	0.24	0/2481	0.53	3/3363 (0.1%)
1	2-C	0.24	0/2481	0.56	7/3363 (0.2%)
1	2-D	0.24	0/2481	0.48	1/3363 (0.0%)
1	3-A	0.22	0/2481	0.48	3/3363 (0.1%)
1	3-B	0.24	0/2481	0.53	3/3363 (0.1%)
1	3-C	0.24	0/2481	0.56	7/3363 (0.2%)
1	3-D	0.24	0/2481	0.48	1/3363 (0.0%)
1	4-A	0.22	0/2481	0.48	3/3363 (0.1%)
1	4-B	0.24	0/2481	0.53	3/3363 (0.1%)
1	4-C	0.24	0/2481	0.56	7/3363 (0.2%)
1	4-D	0.24	0/2481	0.48	1/3363 (0.0%)
1	5-A	0.22	0/2481	0.48	3/3363 (0.1%)
1	5-B	0.24	0/2481	0.53	3/3363 (0.1%)
1	5-C	0.24	0/2481	0.56	7/3363 (0.2%)
1	5-D	0.24	0/2481	0.48	1/3363 (0.0%)
1	6-A	0.22	0/2481	0.48	3/3363 (0.1%)
1	6-B	0.24	0/2481	0.53	3/3363 (0.1%)
1	6-C	0.24	0/2481	0.56	7/3363 (0.2%)
1	6-D	0.24	0/2481	0.48	1/3363 (0.0%)
1	7-A	0.22	0/2481	0.48	3/3363 (0.1%)
1	7-B	0.24	0/2481	0.53	3/3363 (0.1%)
1	7-C	0.24	0/2481	0.56	7/3363 (0.2%)
1	7-D	0.24	0/2481	0.48	1/3363 (0.0%)
1	8-A	0.22	0/2481	0.48	3/3363 (0.1%)
1	8-B	0.24	0/2481	0.53	3/3363 (0.1%)
1	8-C	0.24	0/2481	0.56	7/3363 (0.2%)
1	8-D	0.24	0/2481	0.48	1/3363 (0.0%)
All	All	0.24	0/79392	0.51	112/107616 (0.1%)

There are no bond length outliers.

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-B	142	LYS	CA-C-N	6.00	125.62	119.56
1	1-B	142	LYS	C-N-CA	6.00	125.62	119.56
1	2-B	142	LYS	CA-C-N	6.00	125.62	119.56
1	2-B	142	LYS	C-N-CA	6.00	125.62	119.56
1	3-B	142	LYS	CA-C-N	6.00	125.62	119.56
1	3-B	142	LYS	C-N-CA	6.00	125.62	119.56
1	4-B	142	LYS	CA-C-N	6.00	125.62	119.56
1	4-B	142	LYS	C-N-CA	6.00	125.62	119.56
1	5-B	142	LYS	CA-C-N	6.00	125.62	119.56
1	5-B	142	LYS	C-N-CA	6.00	125.62	119.56
1	6-B	142	LYS	CA-C-N	6.00	125.62	119.56
1	6-B	142	LYS	C-N-CA	6.00	125.62	119.56
1	7-B	142	LYS	CA-C-N	6.00	125.62	119.56
1	7-B	142	LYS	C-N-CA	6.00	125.62	119.56
1	8-B	142	LYS	CA-C-N	6.00	125.62	119.56
1	8-B	142	LYS	C-N-CA	6.00	125.62	119.56
1	1-C	210	ASP	N-CA-C	-5.96	105.84	113.23
1	2-C	210	ASP	N-CA-C	-5.96	105.84	113.23
1	3-C	210	ASP	N-CA-C	-5.96	105.84	113.23
1	4-C	210	ASP	N-CA-C	-5.96	105.84	113.23
1	5-C	210	ASP	N-CA-C	-5.96	105.84	113.23
1	6-C	210	ASP	N-CA-C	-5.96	105.84	113.23
1	7-C	210	ASP	N-CA-C	-5.96	105.84	113.23
1	8-C	210	ASP	N-CA-C	-5.96	105.84	113.23
1	1-C	297	ALA	N-CA-C	5.82	119.53	111.55
1	2-C	297	ALA	N-CA-C	5.82	119.53	111.55
1	3-C	297	ALA	N-CA-C	5.82	119.53	111.55
1	4-C	297	ALA	N-CA-C	5.82	119.53	111.55
1	5-C	297	ALA	N-CA-C	5.82	119.53	111.55
1	6-C	297	ALA	N-CA-C	5.82	119.53	111.55
1	7-C	297	ALA	N-CA-C	5.82	119.53	111.55
1	8-C	297	ALA	N-CA-C	5.82	119.53	111.55
1	1-B	37	ASP	N-CA-C	-5.74	106.89	112.97
1	2-B	37	ASP	N-CA-C	-5.74	106.89	112.97
1	3-B	37	ASP	N-CA-C	-5.74	106.89	112.97
1	4-B	37	ASP	N-CA-C	-5.74	106.89	112.97
1	5-B	37	ASP	N-CA-C	-5.74	106.89	112.97
1	6-B	37	ASP	N-CA-C	-5.74	106.89	112.97
1	7-B	37	ASP	N-CA-C	-5.74	106.89	112.97
1	8-B	37	ASP	N-CA-C	-5.74	106.89	112.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-D	297	ALA	N-CA-C	5.67	122.87	110.80
1	2-D	297	ALA	N-CA-C	5.67	122.87	110.80
1	3-D	297	ALA	N-CA-C	5.67	122.87	110.80
1	4-D	297	ALA	N-CA-C	5.67	122.87	110.80
1	5-D	297	ALA	N-CA-C	5.67	122.87	110.80
1	6-D	297	ALA	N-CA-C	5.67	122.87	110.80
1	7-D	297	ALA	N-CA-C	5.67	122.87	110.80
1	8-D	297	ALA	N-CA-C	5.67	122.87	110.80
1	1-C	188	ARG	CA-C-N	5.53	126.75	119.84
1	1-C	188	ARG	C-N-CA	5.53	126.75	119.84
1	2-C	188	ARG	CA-C-N	5.53	126.75	119.84
1	2-C	188	ARG	C-N-CA	5.53	126.75	119.84
1	3-C	188	ARG	CA-C-N	5.53	126.75	119.84
1	3-C	188	ARG	C-N-CA	5.53	126.75	119.84
1	4-C	188	ARG	CA-C-N	5.53	126.75	119.84
1	4-C	188	ARG	C-N-CA	5.53	126.75	119.84
1	5-C	188	ARG	CA-C-N	5.53	126.75	119.84
1	5-C	188	ARG	C-N-CA	5.53	126.75	119.84
1	6-C	188	ARG	CA-C-N	5.53	126.75	119.84
1	6-C	188	ARG	C-N-CA	5.53	126.75	119.84
1	7-C	188	ARG	CA-C-N	5.53	126.75	119.84
1	7-C	188	ARG	C-N-CA	5.53	126.75	119.84
1	8-C	188	ARG	CA-C-N	5.53	126.75	119.84
1	8-C	188	ARG	C-N-CA	5.53	126.75	119.84
1	1-C	142	LYS	CA-C-N	5.49	125.84	119.47
1	1-C	142	LYS	C-N-CA	5.49	125.84	119.47
1	2-C	142	LYS	CA-C-N	5.49	125.84	119.47
1	2-C	142	LYS	C-N-CA	5.49	125.84	119.47
1	3-C	142	LYS	CA-C-N	5.49	125.84	119.47
1	3-C	142	LYS	C-N-CA	5.49	125.84	119.47
1	4-C	142	LYS	CA-C-N	5.49	125.84	119.47
1	4-C	142	LYS	C-N-CA	5.49	125.84	119.47
1	5-C	142	LYS	CA-C-N	5.49	125.84	119.47
1	5-C	142	LYS	C-N-CA	5.49	125.84	119.47
1	6-C	142	LYS	CA-C-N	5.49	125.84	119.47
1	6-C	142	LYS	C-N-CA	5.49	125.84	119.47
1	7-C	142	LYS	CA-C-N	5.49	125.84	119.47
1	7-C	142	LYS	C-N-CA	5.49	125.84	119.47
1	8-C	142	LYS	CA-C-N	5.49	125.84	119.47
1	8-C	142	LYS	C-N-CA	5.49	125.84	119.47
1	1-A	125	ARG	N-CA-C	5.25	118.69	111.54
1	2-A	125	ARG	N-CA-C	5.25	118.69	111.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3-A	125	ARG	N-CA-C	5.25	118.69	111.54
1	4-A	125	ARG	N-CA-C	5.25	118.69	111.54
1	5-A	125	ARG	N-CA-C	5.25	118.69	111.54
1	6-A	125	ARG	N-CA-C	5.25	118.69	111.54
1	7-A	125	ARG	N-CA-C	5.25	118.69	111.54
1	8-A	125	ARG	N-CA-C	5.25	118.69	111.54
1	1-A	297	ALA	N-CA-C	5.21	121.89	110.80
1	2-A	297	ALA	N-CA-C	5.21	121.89	110.80
1	3-A	297	ALA	N-CA-C	5.21	121.89	110.80
1	4-A	297	ALA	N-CA-C	5.21	121.89	110.80
1	5-A	297	ALA	N-CA-C	5.21	121.89	110.80
1	6-A	297	ALA	N-CA-C	5.21	121.89	110.80
1	7-A	297	ALA	N-CA-C	5.21	121.89	110.80
1	8-A	297	ALA	N-CA-C	5.21	121.89	110.80
1	1-A	269	ASP	N-CA-C	-5.11	107.08	113.72
1	2-A	269	ASP	N-CA-C	-5.11	107.08	113.72
1	3-A	269	ASP	N-CA-C	-5.11	107.08	113.72
1	4-A	269	ASP	N-CA-C	-5.11	107.08	113.72
1	5-A	269	ASP	N-CA-C	-5.11	107.08	113.72
1	6-A	269	ASP	N-CA-C	-5.11	107.08	113.72
1	7-A	269	ASP	N-CA-C	-5.11	107.08	113.72
1	8-A	269	ASP	N-CA-C	-5.11	107.08	113.72
1	1-C	31	VAL	N-CA-C	5.00	116.50	108.89
1	2-C	31	VAL	N-CA-C	5.00	116.50	108.89
1	3-C	31	VAL	N-CA-C	5.00	116.50	108.89
1	4-C	31	VAL	N-CA-C	5.00	116.50	108.89
1	5-C	31	VAL	N-CA-C	5.00	116.50	108.89
1	6-C	31	VAL	N-CA-C	5.00	116.50	108.89
1	7-C	31	VAL	N-CA-C	5.00	116.50	108.89
1	8-C	31	VAL	N-CA-C	5.00	116.50	108.89

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	2442	0	2491	0	0
1	1-B	2442	0	2491	0	0
1	1-C	2442	0	2491	0	0
1	1-D	2442	0	2491	0	0
1	2-A	2442	0	2491	0	0
1	2-B	2442	0	2491	0	0
1	2-C	2442	0	2491	0	0
1	2-D	2442	0	2491	0	0
1	3-A	2442	0	2491	0	0
1	3-B	2442	0	2491	0	0
1	3-C	2442	0	2491	0	0
1	3-D	2442	0	2491	0	0
1	4-A	2442	0	2491	0	0
1	4-B	2442	0	2491	0	0
1	4-C	2442	0	2491	0	0
1	4-D	2442	0	2491	0	0
1	5-A	2442	0	2491	0	0
1	5-B	2442	0	2491	0	0
1	5-C	2442	0	2491	0	0
1	5-D	2442	0	2491	0	0
1	6-A	2442	0	2491	0	0
1	6-B	2442	0	2491	0	0
1	6-C	2442	0	2491	0	0
1	6-D	2442	0	2491	0	0
1	7-A	2442	0	2491	0	0
1	7-B	2442	0	2491	0	0
1	7-C	2442	0	2491	0	0
1	7-D	2442	0	2491	0	0
1	8-A	2442	0	2491	0	0
1	8-B	2442	0	2491	0	0
1	8-C	2442	0	2491	0	0
1	8-D	2442	0	2491	0	0
2	1-A	103	0	0	0	0
2	1-B	130	0	0	0	0
2	1-C	122	0	0	0	0
2	1-D	95	0	0	0	0
2	2-A	104	0	0	0	0
2	2-B	128	0	0	0	0
2	2-C	122	0	0	0	0
2	2-D	96	0	0	0	0
2	3-A	104	0	0	0	0
2	3-B	128	0	0	0	0
2	3-C	121	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	3-D	97	0	0	0	0
2	4-A	104	0	0	0	0
2	4-B	128	0	0	0	0
2	4-C	122	0	0	0	0
2	4-D	96	0	0	0	0
2	5-A	111	0	0	0	0
2	5-B	121	0	0	0	0
2	5-C	121	0	0	0	0
2	5-D	97	0	0	0	0
2	6-A	107	0	0	0	0
2	6-B	125	0	0	0	0
2	6-C	120	0	0	0	0
2	6-D	98	0	0	0	0
2	7-A	106	0	0	0	0
2	7-B	126	0	0	0	0
2	7-C	119	0	0	0	0
2	7-D	99	0	0	0	0
2	8-A	108	0	0	0	0
2	8-B	124	0	0	0	0
2	8-C	119	0	0	0	0
2	8-D	99	0	0	0	0
All	All	81744	0	79712	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	319/328 (97%)	263 (82%)	48 (15%)	8 (2%)	4 3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-B	319/328 (97%)	276 (86%)	42 (13%)	1 (0%)	36	45
1	1-C	319/328 (97%)	269 (84%)	41 (13%)	9 (3%)	4	2
1	1-D	319/328 (97%)	258 (81%)	44 (14%)	17 (5%)	1	0
1	2-A	319/328 (97%)	253 (79%)	53 (17%)	13 (4%)	2	1
1	2-B	319/328 (97%)	269 (84%)	40 (12%)	10 (3%)	3	1
1	2-C	319/328 (97%)	272 (85%)	41 (13%)	6 (2%)	6	5
1	2-D	319/328 (97%)	276 (86%)	33 (10%)	10 (3%)	3	1
1	3-A	319/328 (97%)	263 (82%)	48 (15%)	8 (2%)	4	3
1	3-B	319/328 (97%)	275 (86%)	31 (10%)	13 (4%)	2	1
1	3-C	319/328 (97%)	276 (86%)	35 (11%)	8 (2%)	4	3
1	3-D	319/328 (97%)	266 (83%)	47 (15%)	6 (2%)	6	5
1	4-A	319/328 (97%)	253 (79%)	55 (17%)	11 (3%)	3	1
1	4-B	319/328 (97%)	267 (84%)	44 (14%)	8 (2%)	4	3
1	4-C	319/328 (97%)	266 (83%)	39 (12%)	14 (4%)	2	0
1	4-D	319/328 (97%)	275 (86%)	35 (11%)	9 (3%)	4	2
1	5-A	319/328 (97%)	276 (86%)	39 (12%)	4 (1%)	9	9
1	5-B	319/328 (97%)	272 (85%)	38 (12%)	9 (3%)	4	2
1	5-C	319/328 (97%)	274 (86%)	37 (12%)	8 (2%)	4	3
1	5-D	319/328 (97%)	278 (87%)	34 (11%)	7 (2%)	5	3
1	6-A	319/328 (97%)	247 (77%)	51 (16%)	21 (7%)	1	0
1	6-B	319/328 (97%)	268 (84%)	37 (12%)	14 (4%)	2	0
1	6-C	319/328 (97%)	263 (82%)	42 (13%)	14 (4%)	2	0
1	6-D	319/328 (97%)	268 (84%)	40 (12%)	11 (3%)	3	1
1	7-A	319/328 (97%)	255 (80%)	45 (14%)	19 (6%)	1	0
1	7-B	319/328 (97%)	239 (75%)	59 (18%)	21 (7%)	1	0
1	7-C	319/328 (97%)	273 (86%)	35 (11%)	11 (3%)	3	1
1	7-D	319/328 (97%)	270 (85%)	41 (13%)	8 (2%)	4	3
1	8-A	319/328 (97%)	264 (83%)	45 (14%)	10 (3%)	3	1
1	8-B	319/328 (97%)	275 (86%)	35 (11%)	9 (3%)	4	2
1	8-C	319/328 (97%)	271 (85%)	39 (12%)	9 (3%)	4	2
1	8-D	319/328 (97%)	277 (87%)	36 (11%)	6 (2%)	6	5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	10208/10496 (97%)	8547 (84%)	1329 (13%)	332 (3%)	3 1

All (332) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	251	GLN
1	1-B	22	ALA
1	1-C	18	GLU
1	1-C	163	ARG
1	1-C	244	SER
1	1-D	91	ASP
1	1-D	177	VAL
1	1-D	197	ALA
1	1-D	225	LEU
1	2-A	260	SER
1	2-B	228	LYS
1	2-C	76	LYS
1	2-D	187	PRO
1	2-D	188	ARG
1	2-D	191	GLU
1	3-A	209	SER
1	3-A	315	ALA
1	3-B	64	ASP
1	3-B	244	SER
1	3-C	42	ALA
1	3-C	189	PRO
1	3-C	244	SER
1	4-A	98	ILE
1	4-A	262	LYS
1	4-A	320	GLU
1	4-B	89	ALA
1	4-B	223	GLU
1	4-B	298	THR
1	4-C	12	THR
1	4-C	60	SER
1	4-C	140	SER
1	4-C	163	ARG
1	5-B	140	SER
1	5-B	209	SER
1	5-B	244	SER
1	5-C	17	ALA
1	5-C	73	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-A	75	LEU
1	6-A	108	THR
1	6-A	138	TRP
1	6-A	161	LEU
1	6-A	183	THR
1	6-B	226	CYS
1	6-B	244	SER
1	6-B	297	ALA
1	6-C	35	ASP
1	6-C	95	LYS
1	6-C	105	ASP
1	6-C	189	PRO
1	6-D	36	SER
1	6-D	218	LEU
1	7-A	26	ALA
1	7-A	27	ALA
1	7-A	75	LEU
1	7-A	185	ARG
1	7-B	22	ALA
1	7-B	74	ASN
1	7-B	321	PRO
1	7-C	49	VAL
1	7-C	105	ASP
1	7-C	324	SER
1	8-A	216	CYS
1	8-A	251	GLN
1	8-B	106	VAL
1	8-B	136	GLY
1	8-B	324	SER
1	8-B	325	GLU
1	8-C	15	ILE
1	1-A	26	ALA
1	1-C	216	CYS
1	1-D	191	GLU
1	1-D	192	ALA
1	1-D	226	CYS
1	1-D	278	THR
1	2-A	17	ALA
1	2-A	26	ALA
1	2-A	231	PHE
1	2-B	36	SER
1	2-B	85	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-B	90	LEU
1	2-B	247	ASP
1	2-C	244	SER
1	2-D	185	ARG
1	2-D	313	LEU
1	3-A	278	THR
1	3-A	282	LEU
1	3-B	63	VAL
1	3-B	95	LYS
1	3-B	190	GLU
1	3-B	247	ASP
1	3-C	63	VAL
1	3-C	190	GLU
1	3-D	282	LEU
1	4-A	35	ASP
1	4-A	207	ALA
1	4-A	234	MSE
1	4-B	86	ASP
1	4-B	189	PRO
1	4-B	191	GLU
1	4-B	226	CYS
1	4-C	71	ALA
1	4-C	216	CYS
1	4-D	282	LEU
1	5-A	26	ALA
1	5-A	73	ALA
1	5-B	27	ALA
1	5-B	35	ASP
1	5-C	72	GLY
1	5-C	86	ASP
1	5-C	105	ASP
1	5-C	146	LEU
1	5-D	216	CYS
1	5-D	319	GLY
1	6-A	90	LEU
1	6-A	105	ASP
1	6-A	207	ALA
1	6-B	140	SER
1	6-B	185	ARG
1	6-B	225	LEU
1	6-C	77	VAL
1	6-C	190	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-C	191	GLU
1	6-D	50	ALA
1	7-A	96	ARG
1	7-A	182	TYR
1	7-A	223	GLU
1	7-A	244	SER
1	7-B	31	VAL
1	7-B	51	GLY
1	7-B	66	ARG
1	7-B	72	GLY
1	7-B	98	ILE
1	7-B	105	ASP
1	7-B	136	GLY
1	7-B	314	LEU
1	7-C	35	ASP
1	7-C	63	VAL
1	7-C	87	HIS
1	7-D	105	ASP
1	7-D	279	ASN
1	8-A	28	ASP
1	8-A	35	ASP
1	8-A	207	ALA
1	8-A	217	SER
1	8-B	105	ASP
1	8-B	140	SER
1	8-C	17	ALA
1	8-D	153	GLN
1	1-A	199	PHE
1	1-A	226	CYS
1	1-C	19	GLY
1	1-D	17	ALA
1	1-D	139	THR
1	1-D	190	GLU
1	1-D	193	ALA
1	2-A	71	ALA
1	2-A	73	ALA
1	2-A	216	CYS
1	2-B	244	SER
1	2-C	42	ALA
1	2-D	105	ASP
1	2-D	216	CYS
1	3-A	207	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3-B	50	ALA
1	3-B	73	ALA
1	3-B	185	ARG
1	3-D	27	ALA
1	3-D	190	GLU
1	4-A	278	THR
1	4-C	226	CYS
1	4-D	17	ALA
1	4-D	35	ASP
1	4-D	206	ALA
1	5-B	235	LYS
1	5-D	26	ALA
1	5-D	244	SER
1	6-A	104	PRO
1	6-A	143	PRO
1	6-A	144	LEU
1	6-A	226	CYS
1	6-B	86	ASP
1	6-C	96	ARG
1	6-D	190	GLU
1	6-D	203	PRO
1	6-D	264	ALA
1	7-A	97	GLY
1	7-A	160	GLY
1	7-A	220	PRO
1	7-B	89	ALA
1	7-B	323	PRO
1	7-C	52	ALA
1	7-C	75	LEU
1	7-C	190	GLU
1	7-D	226	CYS
1	7-D	306	SER
1	8-C	73	ALA
1	8-C	90	LEU
1	8-C	140	SER
1	8-D	190	GLU
1	8-D	244	SER
1	1-A	287	ASN
1	1-D	222	THR
1	1-D	244	SER
1	2-A	236	GLU
1	2-A	261	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-B	51	GLY
1	2-C	75	LEU
1	2-C	140	SER
1	2-D	190	GLU
1	3-A	41	PRO
1	3-B	36	SER
1	3-B	189	PRO
1	3-C	73	ALA
1	3-D	183	THR
1	4-A	324	SER
1	4-C	8	LYS
1	4-D	143	PRO
1	5-A	251	GLN
1	5-B	190	GLU
1	5-C	18	GLU
1	5-D	167	ALA
1	5-D	189	PRO
1	6-A	140	SER
1	6-A	299	HIS
1	6-B	87	HIS
1	6-B	174	PRO
1	6-B	311	ASN
1	6-D	189	PRO
1	6-D	191	GLU
1	6-D	262	LYS
1	6-D	295	GLY
1	7-A	90	LEU
1	7-A	187	PRO
1	7-B	23	LEU
1	7-B	30	GLU
1	7-B	42	ALA
1	7-B	320	GLU
1	7-C	85	ILE
1	7-C	96	ARG
1	7-D	229	ASP
1	8-A	25	ARG
1	8-A	232	GLN
1	8-B	86	ASP
1	8-D	26	ALA
1	8-D	264	ALA
1	1-A	17	ALA
1	1-A	216	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-C	15	ILE
1	1-C	90	LEU
1	1-C	189	PRO
1	1-D	204	GLU
1	1-D	281	PRO
1	2-A	48	GLY
1	2-A	65	LYS
1	2-A	108	THR
1	2-D	50	ALA
1	2-D	189	PRO
1	3-D	319	GLY
1	4-A	88	LEU
1	4-A	247	ASP
1	4-B	50	ALA
1	4-C	189	PRO
1	4-D	105	ASP
1	5-A	69	ASP
1	5-B	86	ASP
1	5-B	174	PRO
1	5-C	35	ASP
1	5-D	251	GLN
1	6-A	188	ARG
1	6-A	190	GLU
1	6-A	325	GLU
1	7-A	74	ASN
1	7-A	200	VAL
1	7-B	68	LEU
1	7-B	91	ASP
1	7-B	318	ARG
1	7-D	26	ALA
1	7-D	228	LYS
1	8-A	27	ALA
1	2-B	189	PRO
1	3-C	85	ILE
1	3-C	187	PRO
1	3-D	260	SER
1	4-C	17	ALA
1	4-C	187	PRO
1	4-C	287	ASN
1	4-D	46	GLU
1	6-A	200	VAL
1	6-C	34	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-C	50	ALA
1	6-C	98	ILE
1	6-D	228	LYS
1	7-A	17	ALA
1	7-A	246	GLY
1	7-D	206	ALA
1	8-B	93	ILE
1	8-C	18	GLU
1	1-A	281	PRO
1	1-D	143	PRO
1	6-A	19	GLY
1	6-A	295	GLY
1	6-B	202	THR
1	6-C	93	ILE
1	7-A	162	GLY
1	2-A	164	ILE
1	2-B	67	ILE
1	2-B	246	GLY
1	3-A	281	PRO
1	4-A	323	PRO
1	4-C	77	VAL
1	4-C	85	ILE
1	4-D	21	VAL
1	6-B	67	ILE
1	8-C	51	GLY
1	8-C	103	THR
1	1-C	51	GLY
1	2-C	321	PRO
1	3-A	321	PRO
1	6-B	85	ILE
1	6-C	295	GLY
1	8-A	224	GLY
1	8-B	77	VAL
1	8-C	93	ILE
1	6-A	187	PRO
1	6-B	184	GLY
1	6-C	49	VAL
1	7-B	322	MSE
1	3-B	93	ILE
1	3-B	220	PRO
1	4-D	15	ILE
1	7-A	188	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8-D	189	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	262/264 (99%)	254 (97%)	8 (3%)	35	50
1	1-B	262/264 (99%)	258 (98%)	4 (2%)	57	70
1	1-C	262/264 (99%)	255 (97%)	7 (3%)	39	54
1	1-D	262/264 (99%)	255 (97%)	7 (3%)	39	54
1	2-A	262/264 (99%)	254 (97%)	8 (3%)	35	50
1	2-B	262/264 (99%)	258 (98%)	4 (2%)	57	70
1	2-C	262/264 (99%)	255 (97%)	7 (3%)	39	54
1	2-D	262/264 (99%)	255 (97%)	7 (3%)	39	54
1	3-A	262/264 (99%)	254 (97%)	8 (3%)	35	50
1	3-B	262/264 (99%)	258 (98%)	4 (2%)	57	70
1	3-C	262/264 (99%)	255 (97%)	7 (3%)	39	54
1	3-D	262/264 (99%)	255 (97%)	7 (3%)	39	54
1	4-A	262/264 (99%)	254 (97%)	8 (3%)	35	50
1	4-B	262/264 (99%)	258 (98%)	4 (2%)	57	70
1	4-C	262/264 (99%)	255 (97%)	7 (3%)	39	54
1	4-D	262/264 (99%)	255 (97%)	7 (3%)	39	54
1	5-A	262/264 (99%)	254 (97%)	8 (3%)	35	50
1	5-B	262/264 (99%)	258 (98%)	4 (2%)	57	70
1	5-C	262/264 (99%)	255 (97%)	7 (3%)	39	54
1	5-D	262/264 (99%)	255 (97%)	7 (3%)	39	54
1	6-A	262/264 (99%)	254 (97%)	8 (3%)	35	50
1	6-B	262/264 (99%)	258 (98%)	4 (2%)	57	70
1	6-C	262/264 (99%)	255 (97%)	7 (3%)	39	54

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	6-D	262/264 (99%)	255 (97%)	7 (3%)	39	54
1	7-A	262/264 (99%)	254 (97%)	8 (3%)	35	50
1	7-B	262/264 (99%)	258 (98%)	4 (2%)	57	70
1	7-C	262/264 (99%)	255 (97%)	7 (3%)	39	54
1	7-D	262/264 (99%)	255 (97%)	7 (3%)	39	54
1	8-A	262/264 (99%)	254 (97%)	8 (3%)	35	50
1	8-B	262/264 (99%)	258 (98%)	4 (2%)	57	70
1	8-C	262/264 (99%)	255 (97%)	7 (3%)	39	54
1	8-D	262/264 (99%)	255 (97%)	7 (3%)	39	54
All	All	8384/8448 (99%)	8176 (98%)	208 (2%)	42	56

All (208) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	35	ASP
1	1-A	59	LEU
1	1-A	102	TYR
1	1-A	107	LEU
1	1-A	196	GLN
1	1-A	254	LEU
1	1-A	279	ASN
1	1-A	282	LEU
1	1-B	35	ASP
1	1-B	183	THR
1	1-B	190	GLU
1	1-B	325	GLU
1	1-C	44	GLU
1	1-C	102	TYR
1	1-C	109	ASP
1	1-C	121	THR
1	1-C	144	LEU
1	1-C	163	ARG
1	1-C	183	THR
1	1-D	9	VAL
1	1-D	47	ARG
1	1-D	185	ARG
1	1-D	195	PHE
1	1-D	212	ILE
1	1-D	232	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-D	251	GLN
1	2-A	35	ASP
1	2-A	59	LEU
1	2-A	102	TYR
1	2-A	107	LEU
1	2-A	196	GLN
1	2-A	254	LEU
1	2-A	279	ASN
1	2-A	282	LEU
1	2-B	35	ASP
1	2-B	183	THR
1	2-B	190	GLU
1	2-B	325	GLU
1	2-C	44	GLU
1	2-C	102	TYR
1	2-C	109	ASP
1	2-C	121	THR
1	2-C	144	LEU
1	2-C	163	ARG
1	2-C	183	THR
1	2-D	9	VAL
1	2-D	47	ARG
1	2-D	185	ARG
1	2-D	195	PHE
1	2-D	212	ILE
1	2-D	232	GLN
1	2-D	251	GLN
1	3-A	35	ASP
1	3-A	59	LEU
1	3-A	102	TYR
1	3-A	107	LEU
1	3-A	196	GLN
1	3-A	254	LEU
1	3-A	279	ASN
1	3-A	282	LEU
1	3-B	35	ASP
1	3-B	183	THR
1	3-B	190	GLU
1	3-B	325	GLU
1	3-C	44	GLU
1	3-C	102	TYR
1	3-C	109	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3-C	121	THR
1	3-C	144	LEU
1	3-C	163	ARG
1	3-C	183	THR
1	3-D	9	VAL
1	3-D	47	ARG
1	3-D	185	ARG
1	3-D	195	PHE
1	3-D	212	ILE
1	3-D	232	GLN
1	3-D	251	GLN
1	4-A	35	ASP
1	4-A	59	LEU
1	4-A	102	TYR
1	4-A	107	LEU
1	4-A	196	GLN
1	4-A	254	LEU
1	4-A	279	ASN
1	4-A	282	LEU
1	4-B	35	ASP
1	4-B	183	THR
1	4-B	190	GLU
1	4-B	325	GLU
1	4-C	44	GLU
1	4-C	102	TYR
1	4-C	109	ASP
1	4-C	121	THR
1	4-C	144	LEU
1	4-C	163	ARG
1	4-C	183	THR
1	4-D	9	VAL
1	4-D	47	ARG
1	4-D	185	ARG
1	4-D	195	PHE
1	4-D	212	ILE
1	4-D	232	GLN
1	4-D	251	GLN
1	5-A	35	ASP
1	5-A	59	LEU
1	5-A	102	TYR
1	5-A	107	LEU
1	5-A	196	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5-A	254	LEU
1	5-A	279	ASN
1	5-A	282	LEU
1	5-B	35	ASP
1	5-B	183	THR
1	5-B	190	GLU
1	5-B	325	GLU
1	5-C	44	GLU
1	5-C	102	TYR
1	5-C	109	ASP
1	5-C	121	THR
1	5-C	144	LEU
1	5-C	163	ARG
1	5-C	183	THR
1	5-D	9	VAL
1	5-D	47	ARG
1	5-D	185	ARG
1	5-D	195	PHE
1	5-D	212	ILE
1	5-D	232	GLN
1	5-D	251	GLN
1	6-A	35	ASP
1	6-A	59	LEU
1	6-A	102	TYR
1	6-A	107	LEU
1	6-A	196	GLN
1	6-A	254	LEU
1	6-A	279	ASN
1	6-A	282	LEU
1	6-B	35	ASP
1	6-B	183	THR
1	6-B	190	GLU
1	6-B	325	GLU
1	6-C	44	GLU
1	6-C	102	TYR
1	6-C	109	ASP
1	6-C	121	THR
1	6-C	144	LEU
1	6-C	163	ARG
1	6-C	183	THR
1	6-D	9	VAL
1	6-D	47	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-D	185	ARG
1	6-D	195	PHE
1	6-D	212	ILE
1	6-D	232	GLN
1	6-D	251	GLN
1	7-A	35	ASP
1	7-A	59	LEU
1	7-A	102	TYR
1	7-A	107	LEU
1	7-A	196	GLN
1	7-A	254	LEU
1	7-A	279	ASN
1	7-A	282	LEU
1	7-B	35	ASP
1	7-B	183	THR
1	7-B	190	GLU
1	7-B	325	GLU
1	7-C	44	GLU
1	7-C	102	TYR
1	7-C	109	ASP
1	7-C	121	THR
1	7-C	144	LEU
1	7-C	163	ARG
1	7-C	183	THR
1	7-D	9	VAL
1	7-D	47	ARG
1	7-D	185	ARG
1	7-D	195	PHE
1	7-D	212	ILE
1	7-D	232	GLN
1	7-D	251	GLN
1	8-A	35	ASP
1	8-A	59	LEU
1	8-A	102	TYR
1	8-A	107	LEU
1	8-A	196	GLN
1	8-A	254	LEU
1	8-A	279	ASN
1	8-A	282	LEU
1	8-B	35	ASP
1	8-B	183	THR
1	8-B	190	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8-B	325	GLU
1	8-C	44	GLU
1	8-C	102	TYR
1	8-C	109	ASP
1	8-C	121	THR
1	8-C	144	LEU
1	8-C	163	ARG
1	8-C	183	THR
1	8-D	9	VAL
1	8-D	47	ARG
1	8-D	185	ARG
1	8-D	195	PHE
1	8-D	212	ILE
1	8-D	232	GLN
1	8-D	251	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (162) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	279	ASN
1	1-B	33	GLN
1	1-B	87	HIS
1	1-B	166	GLN
1	1-B	178	GLN
1	1-B	232	GLN
1	1-B	293	HIS
1	1-B	303	ASN
1	1-C	53	HIS
1	1-C	178	GLN
1	1-D	33	GLN
1	1-D	166	GLN
1	1-D	178	GLN
1	1-D	251	GLN
1	2-A	53	HIS
1	2-A	62	HIS
1	2-A	74	ASN
1	2-A	186	GLN
1	2-A	251	GLN
1	2-A	256	GLN
1	2-A	299	HIS
1	2-B	33	GLN
1	2-B	62	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-B	87	HIS
1	2-B	178	GLN
1	2-B	232	GLN
1	2-B	303	ASN
1	2-C	178	GLN
1	2-C	293	HIS
1	2-D	33	GLN
1	2-D	153	GLN
1	2-D	166	GLN
1	2-D	208	GLN
1	2-D	279	ASN
1	2-D	303	ASN
1	2-D	311	ASN
1	3-A	208	GLN
1	3-A	280	HIS
1	3-A	312	ASN
1	3-B	33	GLN
1	3-B	87	HIS
1	3-B	166	GLN
1	3-B	186	GLN
1	3-B	208	GLN
1	3-B	232	GLN
1	3-B	256	GLN
1	3-B	299	HIS
1	3-B	303	ASN
1	3-B	311	ASN
1	3-C	33	GLN
1	3-C	74	ASN
1	3-C	166	GLN
1	3-C	178	GLN
1	3-C	293	HIS
1	3-D	33	GLN
1	3-D	166	GLN
1	3-D	196	GLN
1	3-D	312	ASN
1	4-A	53	HIS
1	4-A	74	ASN
1	4-A	153	GLN
1	4-A	178	GLN
1	4-A	232	GLN
1	4-A	250	ASN
1	4-B	33	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-B	87	HIS
1	4-B	153	GLN
1	4-B	232	GLN
1	4-B	256	GLN
1	4-B	303	ASN
1	4-C	33	GLN
1	4-C	87	HIS
1	4-C	178	GLN
1	4-C	293	HIS
1	4-D	153	GLN
1	4-D	208	GLN
1	4-D	311	ASN
1	5-A	33	GLN
1	5-A	208	GLN
1	5-A	232	GLN
1	5-A	251	GLN
1	5-A	256	GLN
1	5-A	293	HIS
1	5-A	299	HIS
1	5-B	53	HIS
1	5-B	74	ASN
1	5-B	178	GLN
1	5-B	186	GLN
1	5-B	208	GLN
1	5-B	232	GLN
1	5-B	251	GLN
1	5-B	256	GLN
1	5-B	303	ASN
1	5-C	33	GLN
1	5-C	74	ASN
1	5-C	250	ASN
1	5-C	299	HIS
1	5-D	33	GLN
1	5-D	279	ASN
1	6-A	33	GLN
1	6-A	53	HIS
1	6-A	166	GLN
1	6-A	232	GLN
1	6-A	299	HIS
1	6-B	166	GLN
1	6-B	186	GLN
1	6-B	251	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-B	303	ASN
1	6-B	312	ASN
1	6-C	53	HIS
1	6-C	178	GLN
1	6-C	186	GLN
1	6-C	251	GLN
1	6-C	299	HIS
1	6-D	166	GLN
1	6-D	196	GLN
1	6-D	208	GLN
1	6-D	227	ASN
1	6-D	232	GLN
1	6-D	311	ASN
1	7-A	53	HIS
1	7-A	62	HIS
1	7-A	74	ASN
1	7-A	186	GLN
1	7-A	227	ASN
1	7-A	256	GLN
1	7-B	166	GLN
1	7-B	178	GLN
1	7-B	208	GLN
1	7-B	232	GLN
1	7-B	251	GLN
1	7-B	256	GLN
1	7-B	303	ASN
1	7-B	311	ASN
1	7-C	74	ASN
1	7-C	299	HIS
1	7-D	153	GLN
1	7-D	178	GLN
1	7-D	232	GLN
1	7-D	242	ASN
1	7-D	250	ASN
1	7-D	280	HIS
1	8-A	53	HIS
1	8-A	62	HIS
1	8-A	74	ASN
1	8-A	166	GLN
1	8-A	196	GLN
1	8-A	208	GLN
1	8-A	242	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8-A	299	HIS
1	8-B	178	GLN
1	8-B	232	GLN
1	8-B	256	GLN
1	8-B	311	ASN
1	8-C	33	GLN
1	8-C	178	GLN
1	8-C	227	ASN
1	8-C	232	GLN
1	8-C	293	HIS
1	8-C	299	HIS
1	8-D	33	GLN
1	8-D	166	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 [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 ⓘ

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	316/328 (96%)	1.78	106 (33%) 1 1	2, 3, 4, 5	316 (100%)
1	1-B	316/328 (96%)	1.70	99 (31%) 1 1	2, 3, 4, 5	316 (100%)
1	1-C	316/328 (96%)	1.78	102 (32%) 1 1	2, 3, 4, 5	316 (100%)
1	1-D	316/328 (96%)	2.17	133 (42%) 0 0	2, 3, 4, 5	316 (100%)
1	2-A	0/328	-	-	-	-
1	2-B	0/328	-	-	-	-
1	2-C	0/328	-	-	-	-
1	2-D	0/328	-	-	-	-
1	3-A	0/328	-	-	-	-
1	3-B	0/328	-	-	-	-
1	3-C	0/328	-	-	-	-
1	3-D	0/328	-	-	-	-
1	4-A	0/328	-	-	-	-
1	4-B	0/328	-	-	-	-
1	4-C	0/328	-	-	-	-
1	4-D	0/328	-	-	-	-
1	5-A	0/328	-	-	-	-
1	5-B	0/328	-	-	-	-
1	5-C	0/328	-	-	-	-
1	5-D	0/328	-	-	-	-
1	6-A	0/328	-	-	-	-
1	6-B	0/328	-	-	-	-
1	6-C	0/328	-	-	-	-
1	6-D	0/328	-	-	-	-
1	7-A	0/328	-	-	-	-
1	7-B	0/328	-	-	-	-
1	7-C	0/328	-	-	-	-
1	7-D	0/328	-	-	-	-
1	8-A	0/328	-	-	-	-
1	8-B	0/328	-	-	-	-
1	8-C	0/328	-	-	-	-

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	8-D	0/328	-	-	-	-
All	All	1264/10496 (12%)	1.86	440 (34%) 1 1	2, 3, 4, 5	1264 (100%)

All (440) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-B	63	VAL	9.5
1	1-D	201	SER	8.5
1	1-D	319	GLY	8.1
1	1-A	218	LEU	8.0
1	1-D	218	LEU	7.2
1	1-D	102	TYR	7.2
1	1-D	200	VAL	7.1
1	1-D	222	THR	6.5
1	1-A	288	CYS	6.4
1	1-B	101	GLY	6.3
1	1-D	186	GLN	6.1
1	1-C	91	ASP	6.1
1	1-B	162	GLY	5.9
1	1-B	64	ASP	5.9
1	1-D	219	THR	5.9
1	1-D	193	ALA	5.8
1	1-D	203	PRO	5.7
1	1-C	69	ASP	5.6
1	1-D	184	GLY	5.5
1	1-D	221	ALA	5.4
1	1-A	215	ALA	5.4
1	1-C	74	ASN	5.3
1	1-D	320	GLU	5.3
1	1-C	98	ILE	5.2
1	1-B	319	GLY	5.2
1	1-D	29	CYS	5.2
1	1-D	321	PRO	5.1
1	1-D	188	ARG	5.1
1	1-C	97	GLY	5.1
1	1-C	52	ALA	5.1
1	1-D	161	LEU	5.0
1	1-A	257	ALA	4.9
1	1-D	194	GLU	4.9
1	1-D	280	HIS	4.9
1	1-D	202	THR	4.8
1	1-D	106	VAL	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-C	89	ALA	4.8
1	1-B	29	CYS	4.8
1	1-D	205	LEU	4.8
1	1-B	186	GLN	4.7
1	1-B	182	TYR	4.7
1	1-A	47	ARG	4.6
1	1-C	109	ASP	4.6
1	1-D	282	LEU	4.6
1	1-B	68	LEU	4.5
1	1-C	51	GLY	4.5
1	1-B	73	ALA	4.5
1	1-C	67	ILE	4.5
1	1-D	204	GLU	4.5
1	1-A	273	PRO	4.4
1	1-C	50	ALA	4.4
1	1-A	221	ALA	4.4
1	1-A	279	ASN	4.4
1	1-D	279	ASN	4.4
1	1-B	184	GLY	4.3
1	1-D	220	PRO	4.3
1	1-A	195	PHE	4.3
1	1-D	182	TYR	4.3
1	1-C	88	LEU	4.3
1	1-D	317	LEU	4.3
1	1-C	63	VAL	4.3
1	1-D	103	THR	4.3
1	1-C	95	LYS	4.3
1	1-C	44	GLU	4.3
1	1-A	324	SER	4.3
1	1-B	62	HIS	4.2
1	1-A	194	GLU	4.2
1	1-D	180	PHE	4.2
1	1-D	199	PHE	4.2
1	1-B	161	LEU	4.2
1	1-B	102	TYR	4.2
1	1-C	17	ALA	4.2
1	1-D	26	ALA	4.2
1	1-D	195	PHE	4.2
1	1-D	187	PRO	4.2
1	1-C	93	ILE	4.2
1	1-A	102	TYR	4.1
1	1-D	31	VAL	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-C	59	LEU	4.1
1	1-D	192	ALA	4.1
1	1-C	229	ASP	4.0
1	1-B	220	PRO	4.0
1	1-A	35	ASP	4.0
1	1-C	86	ASP	4.0
1	1-A	101	GLY	4.0
1	1-A	247	ASP	4.0
1	1-D	215	ALA	3.9
1	1-C	90	LEU	3.9
1	1-A	222	THR	3.9
1	1-C	197	ALA	3.9
1	1-B	67	ILE	3.9
1	1-C	75	LEU	3.9
1	1-D	25	ARG	3.9
1	1-D	183	THR	3.9
1	1-B	26	ALA	3.8
1	1-D	208	GLN	3.8
1	1-A	219	THR	3.8
1	1-B	70	ALA	3.8
1	1-C	30	GLU	3.8
1	1-B	166	GLN	3.8
1	1-B	219	THR	3.8
1	1-A	265	ALA	3.8
1	1-A	186	GLN	3.8
1	1-B	183	THR	3.7
1	1-C	11	VAL	3.7
1	1-A	278	THR	3.7
1	1-D	217	SER	3.7
1	1-D	22	ALA	3.7
1	1-D	216	CYS	3.7
1	1-B	18	GLU	3.7
1	1-C	101	GLY	3.7
1	1-C	153	GLN	3.7
1	1-B	320	GLU	3.7
1	1-D	32	GLU	3.7
1	1-C	252	ASP	3.7
1	1-D	315	ALA	3.7
1	1-D	229	ASP	3.7
1	1-A	103	THR	3.6
1	1-B	51	GLY	3.6
1	1-D	19	GLY	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-C	62	HIS	3.6
1	1-C	49	VAL	3.6
1	1-D	21	VAL	3.6
1	1-D	139	THR	3.6
1	1-B	315	ALA	3.6
1	1-A	220	PRO	3.6
1	1-D	189	PRO	3.6
1	1-C	108	THR	3.6
1	1-D	18	GLU	3.6
1	1-C	94	LYS	3.6
1	1-B	164	ILE	3.6
1	1-A	280	HIS	3.5
1	1-A	258	LEU	3.5
1	1-B	316	GLY	3.5
1	1-D	91	ASP	3.5
1	1-B	46	GLU	3.5
1	1-B	185	ARG	3.5
1	1-B	222	THR	3.5
1	1-B	229	ASP	3.5
1	1-D	191	GLU	3.5
1	1-A	251	GLN	3.5
1	1-A	187	PRO	3.5
1	1-D	316	GLY	3.5
1	1-D	98	ILE	3.5
1	1-A	287	ASN	3.4
1	1-B	9	VAL	3.4
1	1-D	162	GLY	3.4
1	1-D	165	GLY	3.4
1	1-D	78	ILE	3.4
1	1-D	190	GLU	3.4
1	1-C	105	ASP	3.4
1	1-D	144	LEU	3.4
1	1-A	286	LYS	3.4
1	1-A	32	GLU	3.4
1	1-C	20	ARG	3.4
1	1-D	23	LEU	3.4
1	1-A	29	CYS	3.4
1	1-C	202	THR	3.4
1	1-D	224	GLY	3.4
1	1-A	20	ARG	3.4
1	1-D	158	ILE	3.3
1	1-D	100	VAL	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-C	53	HIS	3.3
1	1-C	34	TRP	3.3
1	1-C	43	LYS	3.3
1	1-A	217	SER	3.3
1	1-A	319	GLY	3.3
1	1-C	152	THR	3.3
1	1-B	85	ILE	3.3
1	1-D	99	ARG	3.2
1	1-C	100	VAL	3.2
1	1-D	176	GLY	3.2
1	1-C	164	ILE	3.2
1	1-A	254	LEU	3.2
1	1-C	66	ARG	3.2
1	1-D	6	LEU	3.2
1	1-B	27	ALA	3.2
1	1-C	31	VAL	3.2
1	1-C	313	LEU	3.1
1	1-D	198	GLU	3.1
1	1-C	110	THR	3.1
1	1-D	163	ARG	3.1
1	1-A	236	GLU	3.1
1	1-B	91	ASP	3.1
1	1-C	83	VAL	3.1
1	1-B	131	GLU	3.1
1	1-B	223	GLU	3.1
1	1-D	104	PRO	3.1
1	1-A	188	ARG	3.0
1	1-B	66	ARG	3.0
1	1-C	78	ILE	3.0
1	1-D	108	THR	3.0
1	1-B	30	GLU	3.0
1	1-D	159	ILE	3.0
1	1-D	214	VAL	3.0
1	1-D	228	LYS	3.0
1	1-C	84	GLY	3.0
1	1-C	223	GLU	3.0
1	1-D	284	THR	3.0
1	1-C	29	CYS	3.0
1	1-A	206	ALA	2.9
1	1-C	71	ALA	2.9
1	1-A	199	PHE	2.9
1	1-D	64	ASP	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-C	186	GLN	2.9
1	1-D	14	ARG	2.9
1	1-B	21	VAL	2.9
1	1-A	224	GLY	2.9
1	1-D	20	ARG	2.9
1	1-D	259	ALA	2.9
1	1-A	151	LEU	2.9
1	1-A	91	ASP	2.9
1	1-A	84	GLY	2.9
1	1-A	162	GLY	2.9
1	1-A	260	SER	2.8
1	1-C	324	SER	2.8
1	1-C	85	ILE	2.8
1	1-D	311	ASN	2.8
1	1-C	133	VAL	2.8
1	1-A	321	PRO	2.8
1	1-C	41	PRO	2.8
1	1-B	151	LEU	2.8
1	1-D	90	LEU	2.8
1	1-A	79	SER	2.8
1	1-D	30	GLU	2.8
1	1-A	158	ILE	2.8
1	1-A	212	ILE	2.8
1	1-A	200	VAL	2.8
1	1-C	165	GLY	2.8
1	1-A	248	VAL	2.8
1	1-D	212	ILE	2.7
1	1-A	73	ALA	2.7
1	1-C	12	THR	2.7
1	1-B	324	SER	2.7
1	1-B	193	ALA	2.7
1	1-D	27	ALA	2.7
1	1-A	171	ARG	2.7
1	1-D	223	GLU	2.7
1	1-C	35	ASP	2.7
1	1-B	100	VAL	2.7
1	1-A	283	LEU	2.7
1	1-D	141	TRP	2.7
1	1-D	121	THR	2.7
1	1-C	236	GLU	2.7
1	1-C	323	PRO	2.7
1	1-A	272	SER	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-B	23	LEU	2.7
1	1-C	289	VAL	2.7
1	1-D	225	LEU	2.7
1	1-A	30	GLU	2.7
1	1-A	52	ALA	2.7
1	1-C	87	HIS	2.7
1	1-B	105	ASP	2.6
1	1-A	289	VAL	2.6
1	1-D	28	ASP	2.6
1	1-B	163	ARG	2.6
1	1-A	214	VAL	2.6
1	1-A	259	ALA	2.6
1	1-A	185	ARG	2.6
1	1-C	46	GLU	2.6
1	1-D	92	GLU	2.6
1	1-D	117	SER	2.6
1	1-B	301	THR	2.6
1	1-D	95	LYS	2.6
1	1-A	282	LEU	2.6
1	1-D	326	LEU	2.6
1	1-B	87	HIS	2.6
1	1-B	215	ALA	2.6
1	1-A	269	ASP	2.5
1	1-D	105	ASP	2.5
1	1-C	290	ILE	2.5
1	1-A	147	CYS	2.5
1	1-A	284	THR	2.5
1	1-D	278	THR	2.5
1	1-D	324	SER	2.5
1	1-D	47	ARG	2.5
1	1-B	97	GLY	2.5
1	1-A	58	LEU	2.5
1	1-B	199	PHE	2.5
1	1-B	8	LYS	2.5
1	1-B	31	VAL	2.5
1	1-A	192	ALA	2.5
1	1-A	196	GLN	2.5
1	1-B	289	VAL	2.5
1	1-D	213	VAL	2.5
1	1-B	188	ARG	2.5
1	1-D	115	ALA	2.5
1	1-D	79	SER	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-B	191	GLU	2.5
1	1-D	137	GLY	2.5
1	1-A	98	ILE	2.5
1	1-B	317	LEU	2.5
1	1-D	286	LYS	2.5
1	1-D	83	VAL	2.5
1	1-C	220	PRO	2.4
1	1-B	65	LYS	2.4
1	1-C	102	TYR	2.4
1	1-B	34	TRP	2.4
1	1-B	22	ALA	2.4
1	1-C	42	ALA	2.4
1	1-A	252	ASP	2.4
1	1-A	317	LEU	2.4
1	1-D	313	LEU	2.4
1	1-A	191	GLU	2.4
1	1-B	174	PRO	2.4
1	1-D	260	SER	2.4
1	1-A	316	GLY	2.4
1	1-B	72	GLY	2.4
1	1-D	54	GLY	2.4
1	1-D	290	ILE	2.4
1	1-D	96	ARG	2.4
1	1-A	180	PHE	2.4
1	1-A	249	VAL	2.4
1	1-D	227	ASN	2.4
1	1-A	197	ALA	2.4
1	1-C	26	ALA	2.4
1	1-A	46	GLU	2.4
1	1-B	60	SER	2.4
1	1-B	53	HIS	2.4
1	1-B	75	LEU	2.4
1	1-B	179	ARG	2.4
1	1-C	114	LEU	2.4
1	1-B	197	ALA	2.4
1	1-A	80	THR	2.3
1	1-A	290	ILE	2.3
1	1-C	163	ARG	2.3
1	1-D	53	HIS	2.3
1	1-D	285	LEU	2.3
1	1-B	173	LYS	2.3
1	1-A	96	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-A	59	LEU	2.3
1	1-D	88	LEU	2.3
1	1-D	283	LEU	2.3
1	1-B	69	ASP	2.3
1	1-C	214	VAL	2.3
1	1-A	250	ASN	2.3
1	1-B	242	ASN	2.3
1	1-B	152	THR	2.3
1	1-A	144	LEU	2.3
1	1-A	313	LEU	2.3
1	1-B	88	LEU	2.3
1	1-D	146	LEU	2.3
1	1-B	86	ASP	2.3
1	1-C	64	ASP	2.3
1	1-C	247	ASP	2.3
1	1-A	65	LYS	2.3
1	1-A	83	VAL	2.3
1	1-B	116	VAL	2.3
1	1-A	112	ALA	2.3
1	1-A	14	ARG	2.3
1	1-C	272	SER	2.3
1	1-B	93	ILE	2.3
1	1-B	181	LEU	2.3
1	1-D	164	ILE	2.3
1	1-B	198	GLU	2.3
1	1-A	57	CYS	2.3
1	1-D	24	ALA	2.2
1	1-D	264	ALA	2.2
1	1-B	165	GLY	2.2
1	1-A	209	SER	2.2
1	1-B	294	ILE	2.2
1	1-B	61	ASP	2.2
1	1-D	69	ASP	2.2
1	1-C	325	GLU	2.2
1	1-C	199	PHE	2.2
1	1-D	318	ARG	2.2
1	1-C	208	GLN	2.2
1	1-C	219	THR	2.2
1	1-A	262	LYS	2.2
1	1-C	148	GLY	2.2
1	1-A	114	LEU	2.2
1	1-B	247	ASP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-C	138	TRP	2.2
1	1-B	187	PRO	2.2
1	1-A	121	THR	2.2
1	1-A	232	GLN	2.2
1	1-D	232	GLN	2.2
1	1-A	268	LEU	2.2
1	1-B	35	ASP	2.2
1	1-A	198	GLU	2.2
1	1-D	325	GLU	2.2
1	1-A	213	VAL	2.2
1	1-B	249	VAL	2.2
1	1-D	89	ALA	2.2
1	1-D	135	ASN	2.2
1	1-B	33	GLN	2.2
1	1-B	80	THR	2.2
1	1-C	151	LEU	2.2
1	1-D	276	LEU	2.2
1	1-C	158	ILE	2.2
1	1-A	82	SER	2.2
1	1-D	82	SER	2.2
1	1-B	252	ASP	2.2
1	1-D	253	ASP	2.2
1	1-C	134	LYS	2.2
1	1-D	10	PHE	2.2
1	1-B	297	ALA	2.1
1	1-C	178	GLN	2.1
1	1-C	215	ALA	2.1
1	1-A	225	LEU	2.1
1	1-A	255	TYR	2.1
1	1-C	241	ILE	2.1
1	1-D	255	TYR	2.1
1	1-D	175	PHE	2.1
1	1-B	24	ALA	2.1
1	1-A	160	GLY	2.1
1	1-B	6	LEU	2.1
1	1-B	146	LEU	2.1
1	1-C	18	GLU	2.1
1	1-B	228	LYS	2.1
1	1-C	195	PHE	2.1
1	1-B	232	GLN	2.1
1	1-D	63	VAL	2.1
1	1-A	172	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-C	136	GLY	2.1
1	1-C	226	CYS	2.1
1	1-B	180	PHE	2.1
1	1-C	116	VAL	2.1
1	1-C	58	LEU	2.1
1	1-C	145	TRP	2.1
1	1-C	99	ARG	2.1
1	1-D	300	ARG	2.1
1	1-B	237	THR	2.1
1	1-C	32	GLU	2.1
1	1-D	233	LYS	2.1
1	1-C	123	CYS	2.1
1	1-B	200	VAL	2.0
1	1-A	326	LEU	2.0
1	1-A	176	GLY	2.0
1	1-A	184	GLY	2.0
1	1-A	60	SER	2.0
1	1-B	272	SER	2.0
1	1-C	217	SER	2.0
1	1-A	181	LEU	2.0
1	1-D	197	ALA	2.0
1	1-C	92	GLU	2.0
1	1-B	15	ILE	2.0
1	1-C	80	THR	2.0
1	1-C	294	ILE	2.0
1	1-C	37	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.