



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 7, 2020 – 03:40 PM BST

PDB ID : 7CE1
Title : Complex STRUCTURE OF TRANSCRIPTION FACTOR SghR with its COGNATE DNA
Authors : Ye, F.Z.; Wang, C.; Yan, X.F.; Zhang, L.H.; Gao, Y.G.
Deposited on : 2020-06-21
Resolution : 3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.14.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.2

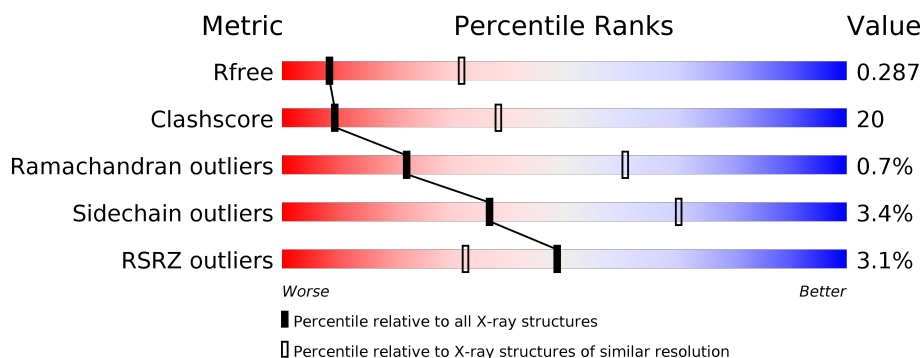
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	341	<div> <div>3%</div> <div> <div></div> <div>67%</div> <div>28%</div> <div>..</div> </div> </div>
1	B	341	<div> <div>2%</div> <div> <div></div> <div>67%</div> <div>28%</div> <div>..</div> </div> </div>
1	C	341	<div> <div></div> <div> <div>72%</div> <div>24%</div> <div>..</div> </div> </div>
1	D	341	<div> <div>2%</div> <div> <div></div> <div>64%</div> <div>31%</div> <div>..</div> </div> </div>
1	G	341	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>24%</div> <div>..</div> </div> </div>
1	H	341	<div> <div></div> <div> <div>72%</div> <div>24%</div> <div>..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	K	341	
1	L	341	
1	O	341	
1	P	341	
1	S	341	
1	T	341	
2	a	18	
2	b	18	
2	c	18	
2	d	18	
2	g	18	
2	h	18	
2	k	18	
2	l	18	
2	o	18	
2	p	18	
2	s	18	
2	t	18	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 32340 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 LacI-type transcription factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2505	1576	443	476	10			
1	B	328	Total	C	N	O	S	0	0	0
			2431	1535	425	462	9			
1	C	332	Total	C	N	O	S	0	0	0
			2534	1602	445	477	10			
1	D	327	Total	C	N	O	S	0	0	0
			2424	1534	424	459	7			
1	G	331	Total	C	N	O	S	0	0	0
			2456	1554	423	469	10			
1	H	331	Total	C	N	O	S	0	0	0
			2525	1593	448	474	10			
1	K	333	Total	C	N	O	S	0	0	0
			2460	1560	426	465	9			
1	L	329	Total	C	N	O	S	0	0	0
			2435	1537	428	462	8			
1	O	320	Total	C	N	O	S	0	0	0
			2250	1420	381	441	8			
1	P	324	Total	C	N	O	S	0	0	0
			2369	1509	404	449	7			
1	S	259	Total	C	N	O	S	0	0	0
			1770	1123	303	339	5			
1	T	292	Total	C	N	O	S	0	0	0
			1997	1254	348	388	7			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	351	LEU	-	expression tag	UNP A0A2I4PGE9
A	352	GLU	-	expression tag	UNP A0A2I4PGE9
A	353	HIS	-	expression tag	UNP A0A2I4PGE9
A	354	HIS	-	expression tag	UNP A0A2I4PGE9
A	355	HIS	-	expression tag	UNP A0A2I4PGE9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	356	HIS	-	expression tag	UNP A0A2I4PGE9
A	357	HIS	-	expression tag	UNP A0A2I4PGE9
A	358	HIS	-	expression tag	UNP A0A2I4PGE9
B	351	LEU	-	expression tag	UNP A0A2I4PGE9
B	352	GLU	-	expression tag	UNP A0A2I4PGE9
B	353	HIS	-	expression tag	UNP A0A2I4PGE9
B	354	HIS	-	expression tag	UNP A0A2I4PGE9
B	355	HIS	-	expression tag	UNP A0A2I4PGE9
B	356	HIS	-	expression tag	UNP A0A2I4PGE9
B	357	HIS	-	expression tag	UNP A0A2I4PGE9
B	358	HIS	-	expression tag	UNP A0A2I4PGE9
C	351	LEU	-	expression tag	UNP A0A2I4PGE9
C	352	GLU	-	expression tag	UNP A0A2I4PGE9
C	353	HIS	-	expression tag	UNP A0A2I4PGE9
C	354	HIS	-	expression tag	UNP A0A2I4PGE9
C	355	HIS	-	expression tag	UNP A0A2I4PGE9
C	356	HIS	-	expression tag	UNP A0A2I4PGE9
C	357	HIS	-	expression tag	UNP A0A2I4PGE9
C	358	HIS	-	expression tag	UNP A0A2I4PGE9
D	351	LEU	-	expression tag	UNP A0A2I4PGE9
D	352	GLU	-	expression tag	UNP A0A2I4PGE9
D	353	HIS	-	expression tag	UNP A0A2I4PGE9
D	354	HIS	-	expression tag	UNP A0A2I4PGE9
D	355	HIS	-	expression tag	UNP A0A2I4PGE9
D	356	HIS	-	expression tag	UNP A0A2I4PGE9
D	357	HIS	-	expression tag	UNP A0A2I4PGE9
D	358	HIS	-	expression tag	UNP A0A2I4PGE9
G	351	LEU	-	expression tag	UNP A0A2I4PGE9
G	352	GLU	-	expression tag	UNP A0A2I4PGE9
G	353	HIS	-	expression tag	UNP A0A2I4PGE9
G	354	HIS	-	expression tag	UNP A0A2I4PGE9
G	355	HIS	-	expression tag	UNP A0A2I4PGE9
G	356	HIS	-	expression tag	UNP A0A2I4PGE9
G	357	HIS	-	expression tag	UNP A0A2I4PGE9
G	358	HIS	-	expression tag	UNP A0A2I4PGE9
H	351	LEU	-	expression tag	UNP A0A2I4PGE9
H	352	GLU	-	expression tag	UNP A0A2I4PGE9
H	353	HIS	-	expression tag	UNP A0A2I4PGE9
H	354	HIS	-	expression tag	UNP A0A2I4PGE9
H	355	HIS	-	expression tag	UNP A0A2I4PGE9
H	356	HIS	-	expression tag	UNP A0A2I4PGE9
H	357	HIS	-	expression tag	UNP A0A2I4PGE9

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Chain	Residue	Modelled	Actual	Comment	Reference
H	358	HIS	-	expression tag	UNP A0A2I4PGE9
K	351	LEU	-	expression tag	UNP A0A2I4PGE9
K	352	GLU	-	expression tag	UNP A0A2I4PGE9
K	353	HIS	-	expression tag	UNP A0A2I4PGE9
K	354	HIS	-	expression tag	UNP A0A2I4PGE9
K	355	HIS	-	expression tag	UNP A0A2I4PGE9
K	356	HIS	-	expression tag	UNP A0A2I4PGE9
K	357	HIS	-	expression tag	UNP A0A2I4PGE9
K	358	HIS	-	expression tag	UNP A0A2I4PGE9
L	351	LEU	-	expression tag	UNP A0A2I4PGE9
L	352	GLU	-	expression tag	UNP A0A2I4PGE9
L	353	HIS	-	expression tag	UNP A0A2I4PGE9
L	354	HIS	-	expression tag	UNP A0A2I4PGE9
L	355	HIS	-	expression tag	UNP A0A2I4PGE9
L	356	HIS	-	expression tag	UNP A0A2I4PGE9
L	357	HIS	-	expression tag	UNP A0A2I4PGE9
L	358	HIS	-	expression tag	UNP A0A2I4PGE9
O	351	LEU	-	expression tag	UNP A0A2I4PGE9
O	352	GLU	-	expression tag	UNP A0A2I4PGE9
O	353	HIS	-	expression tag	UNP A0A2I4PGE9
O	354	HIS	-	expression tag	UNP A0A2I4PGE9
O	355	HIS	-	expression tag	UNP A0A2I4PGE9
O	356	HIS	-	expression tag	UNP A0A2I4PGE9
O	357	HIS	-	expression tag	UNP A0A2I4PGE9
O	358	HIS	-	expression tag	UNP A0A2I4PGE9
P	351	LEU	-	expression tag	UNP A0A2I4PGE9
P	352	GLU	-	expression tag	UNP A0A2I4PGE9
P	353	HIS	-	expression tag	UNP A0A2I4PGE9
P	354	HIS	-	expression tag	UNP A0A2I4PGE9
P	355	HIS	-	expression tag	UNP A0A2I4PGE9
P	356	HIS	-	expression tag	UNP A0A2I4PGE9
P	357	HIS	-	expression tag	UNP A0A2I4PGE9
P	358	HIS	-	expression tag	UNP A0A2I4PGE9
S	351	LEU	-	expression tag	UNP A0A2I4PGE9
S	352	GLU	-	expression tag	UNP A0A2I4PGE9
S	353	HIS	-	expression tag	UNP A0A2I4PGE9
S	354	HIS	-	expression tag	UNP A0A2I4PGE9
S	355	HIS	-	expression tag	UNP A0A2I4PGE9
S	356	HIS	-	expression tag	UNP A0A2I4PGE9
S	357	HIS	-	expression tag	UNP A0A2I4PGE9
S	358	HIS	-	expression tag	UNP A0A2I4PGE9
T	351	LEU	-	expression tag	UNP A0A2I4PGE9

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Chain	Residue	Modelled	Actual	Comment	Reference
T	352	GLU	-	expression tag	UNP A0A2I4PGE9
T	353	HIS	-	expression tag	UNP A0A2I4PGE9
T	354	HIS	-	expression tag	UNP A0A2I4PGE9
T	355	HIS	-	expression tag	UNP A0A2I4PGE9
T	356	HIS	-	expression tag	UNP A0A2I4PGE9
T	357	HIS	-	expression tag	UNP A0A2I4PGE9
T	358	HIS	-	expression tag	UNP A0A2I4PGE9

- Molecule 2 is a DNA chain called promoter DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	a	18	Total	C	N	O	P	0	0	0
			369	176	67	108	18			
2	b	18	Total	C	N	O	P	0	0	0
			369	176	67	108	18			
2	c	18	Total	C	N	O	P	0	0	0
			369	176	67	108	18			
2	d	18	Total	C	N	O	P	0	0	0
			369	176	67	108	18			
2	g	17	Total	C	N	O	P	0	0	0
			349	166	65	101	17			
2	h	17	Total	C	N	O	P	0	0	0
			349	166	65	101	17			
2	k	17	Total	C	N	O	P	0	0	0
			349	166	65	101	17			
2	l	17	Total	C	N	O	P	0	0	0
			349	166	65	101	17			
2	o	18	Total	C	N	O	P	0	0	0
			369	176	67	108	18			
2	p	17	Total	C	N	O	P	0	0	0
			349	166	65	101	17			
2	s	14	Total	C	N	O	P	0	0	0
			284	136	50	84	14			
2	t	14	Total	C	N	O	P	0	0	0
			285	136	50	85	14			

- Molecule 3 is water.

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

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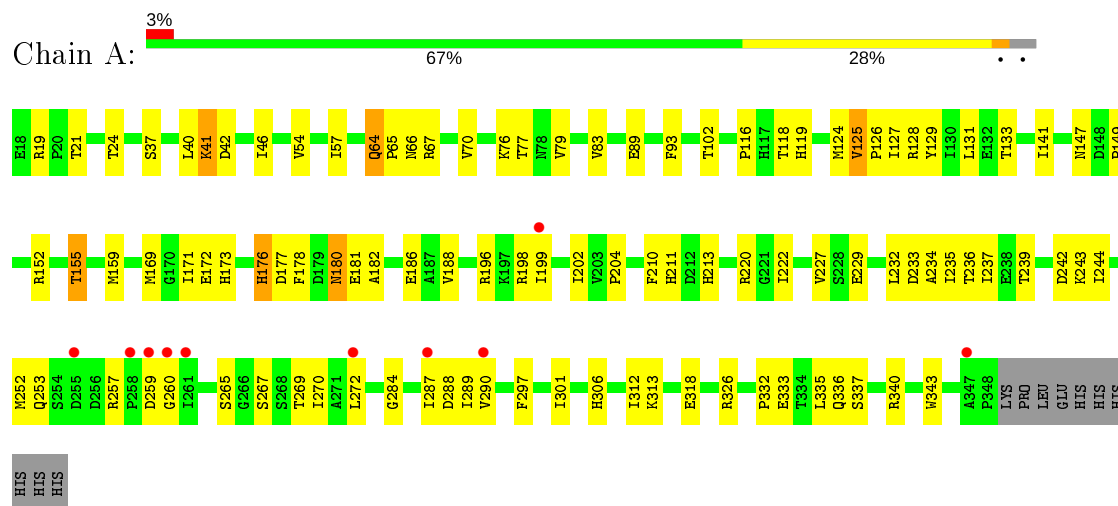
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	6	Total 6	O 6	0	0
3	D	2	Total 2	O 2	0	0
3	c	1	Total 1	O 1	0	0
3	d	1	Total 1	O 1	0	0
3	G	2	Total 2	O 2	0	0
3	H	1	Total 1	O 1	0	0
3	K	2	Total 2	O 2	0	0
3	L	2	Total 2	O 2	0	0
3	O	1	Total 1	O 1	0	0
3	P	1	Total 1	O 1	0	0
3	S	1	Total 1	O 1	0	0
3	T	1	Total 1	O 1	0	0

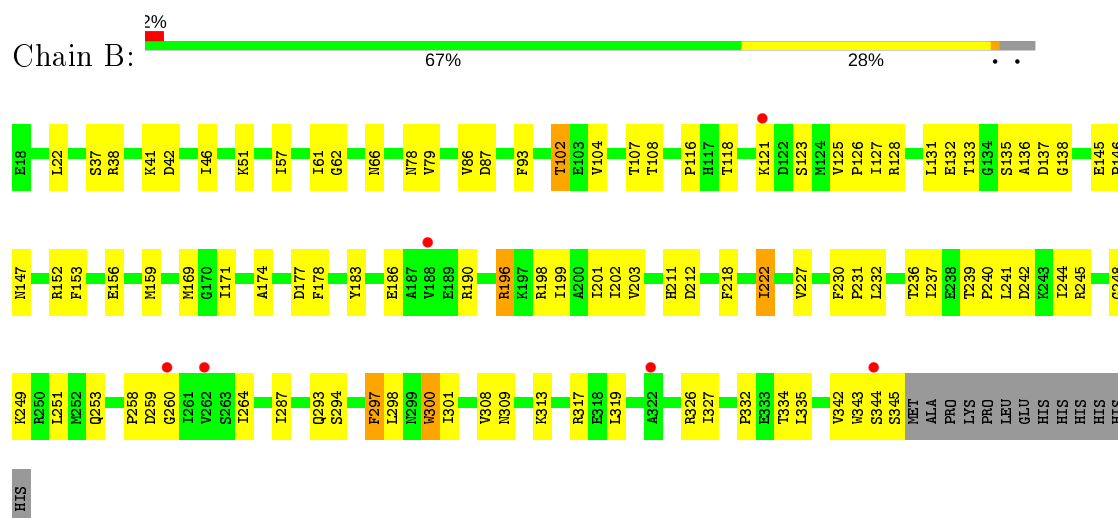
3 Residue-property plots [i](#)

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: LacI-type transcription factor

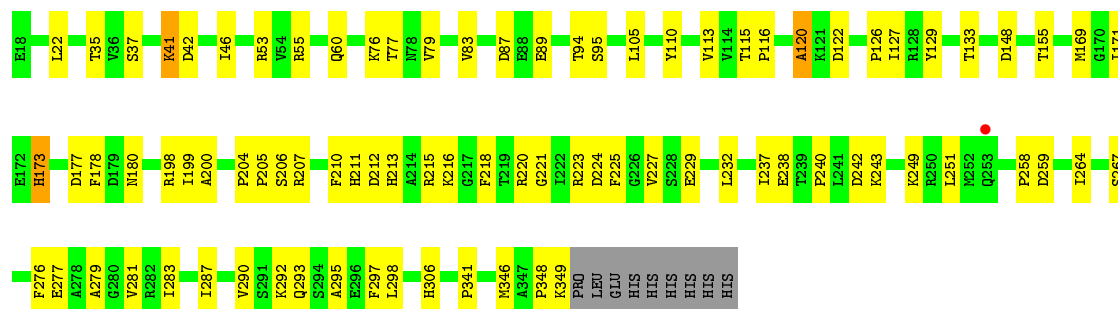


• Molecule 1: LacI-type transcription factor

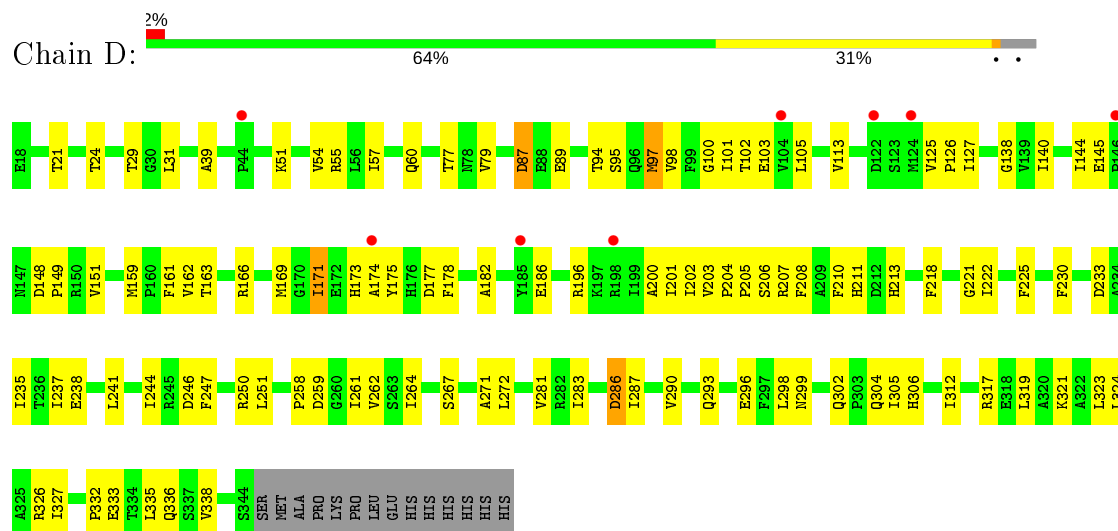


• Molecule 1: LacI-type transcription factor

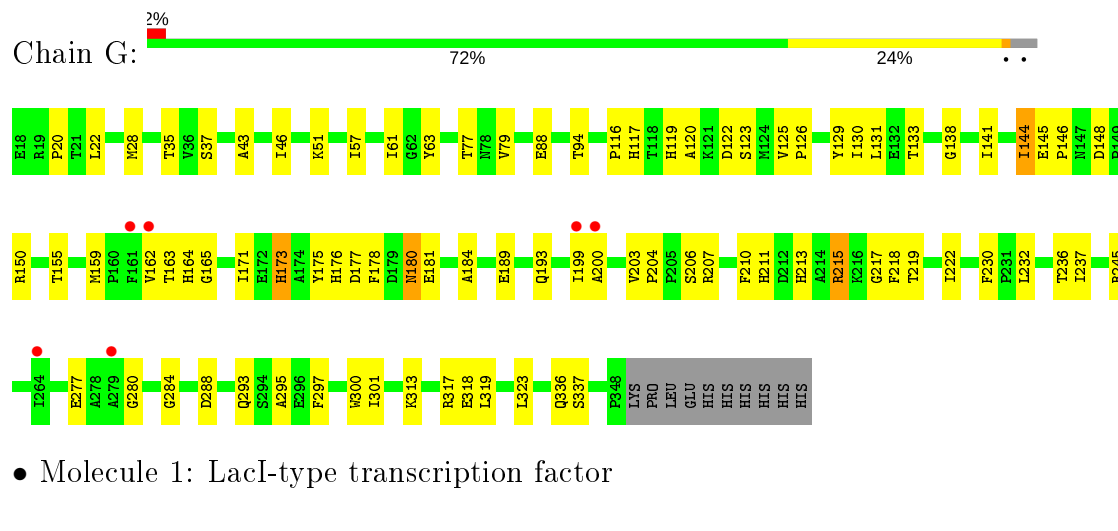




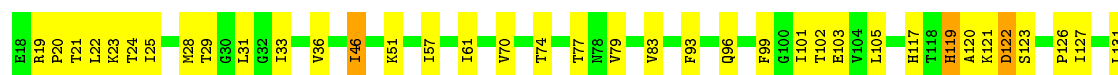
• Molecule 1: LacI-type transcription factor

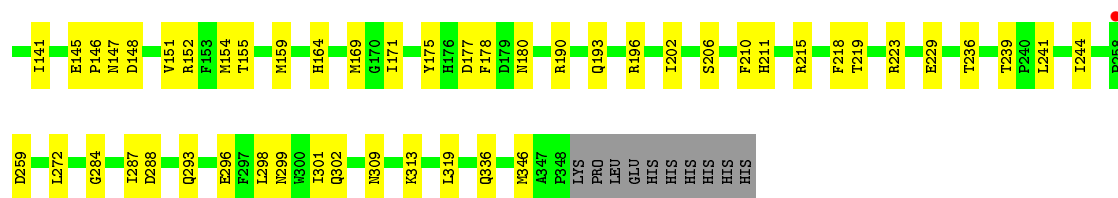


• Molecule 1: LacI-type transcription factor

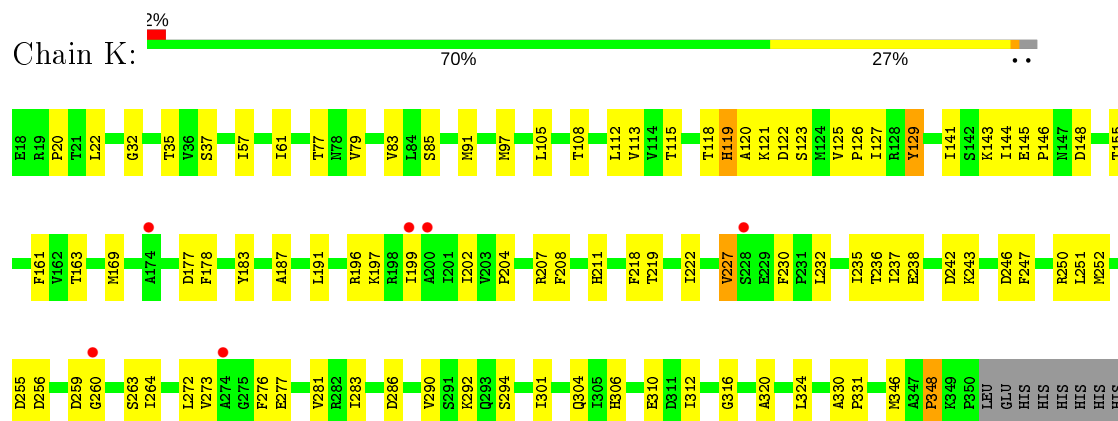


Chain H: 72%, 24%

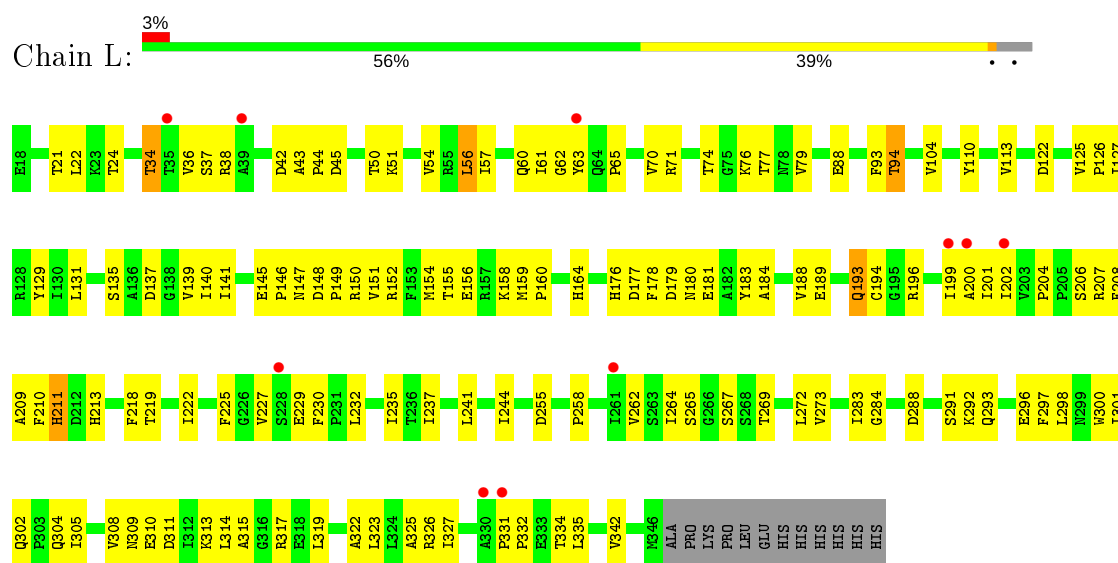




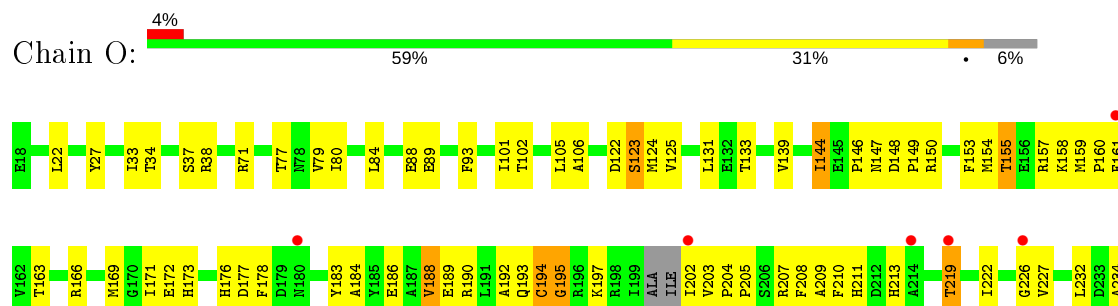
• Molecule 1: LacI-type transcription factor

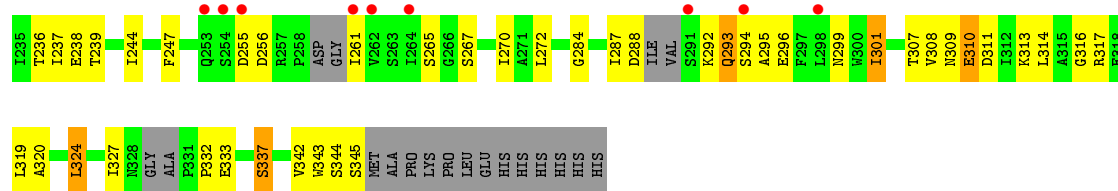


• Molecule 1: LacI-type transcription factor

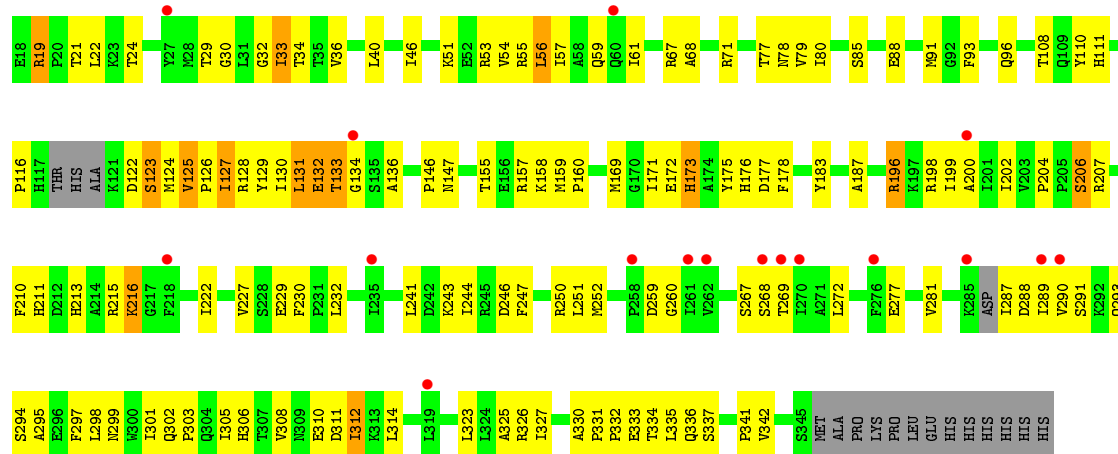


• Molecule 1: LacI-type transcription factor

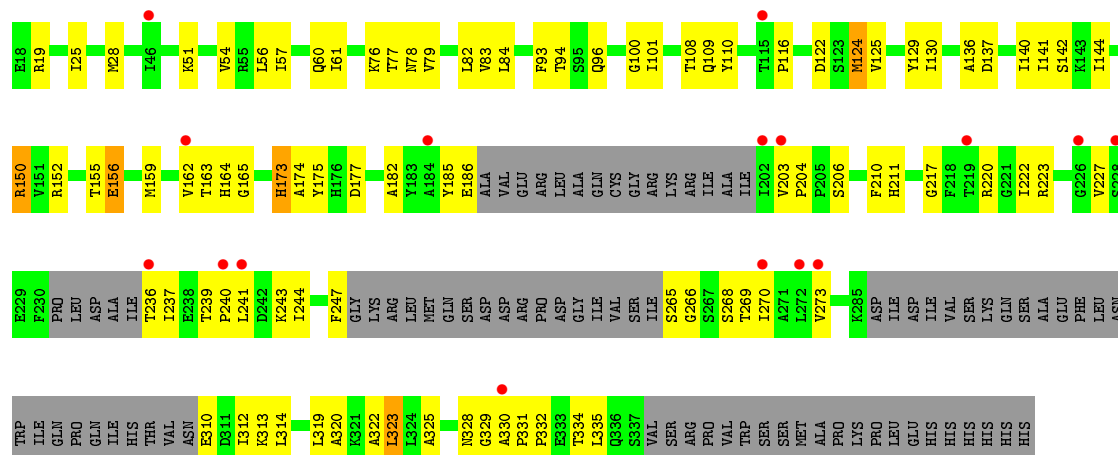




• Molecule 1: LacI-type transcription factor

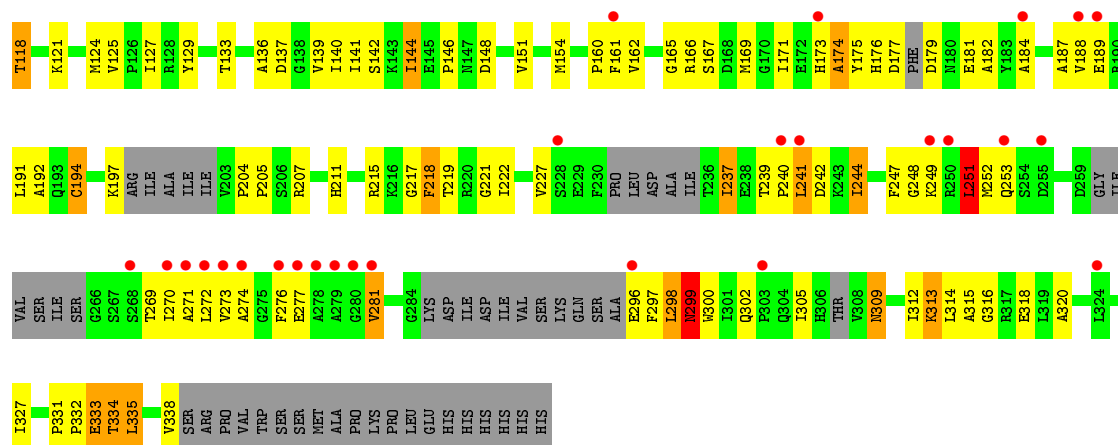


• Molecule 1: LacI-type transcription factor



• Molecule 1: LacI-type transcription factor





- Molecule 2: promoter DNA

Chain a: 72% 28%



- Molecule 2: promoter DNA

Chain b: 89% 11%



- Molecule 2: promoter DNA

Chain c: 94% 6%



- Molecule 2: promoter DNA

Chain d: 6% 94% 6%




- Molecule 2: promoter DNA

Chain g: 94% 6%




- Molecule 2: promoter DNA

Chain h:  89% 6% 6%



- Molecule 2: promoter DNA

Chain k:  83% 11% 6%



- Molecule 2: promoter DNA

Chain l:  94% 6%




- Molecule 2: promoter DNA

Chain o:  94% 6%



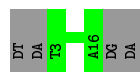
- Molecule 2: promoter DNA

Chain p:  89% 6% 6%



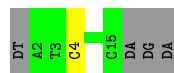
- Molecule 2: promoter DNA

Chain s:  78% 22%



- Molecule 2: promoter DNA

Chain t:  72% 6% 22%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	107.90Å 218.96Å 284.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.15 – 3.20 49.15 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.15-3.20) 100.0 (49.15-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.233 , 0.281 0.241 , 0.287	Depositor DCC
R_{free} test set	5591 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	98.6	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 90.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	32340	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.75% 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	A	0.41	0/2552	0.74	0/3471
1	B	0.41	0/2476	0.77	2/3374 (0.1%)
1	C	0.34	0/2584	0.69	0/3509
1	D	0.40	0/2471	0.75	2/3371 (0.1%)
1	G	0.36	0/2504	0.76	1/3412 (0.0%)
1	H	0.31	0/2574	0.67	0/3496
1	K	0.40	0/2510	0.76	1/3425 (0.0%)
1	L	0.38	0/2482	0.76	2/3385 (0.1%)
1	O	0.40	0/2285	0.77	3/3126 (0.1%)
1	P	0.44	0/2414	0.80	3/3293 (0.1%)
1	S	0.45	0/1796	0.86	2/2458 (0.1%)
1	T	0.50	0/2024	0.95	4/2770 (0.1%)
2	a	0.98	2/413 (0.5%)	1.03	4/635 (0.6%)
2	b	0.90	2/413 (0.5%)	0.94	0/635
2	c	0.77	0/413	1.06	1/635 (0.2%)
2	d	0.64	0/413	1.02	1/635 (0.2%)
2	g	0.74	0/391	1.05	0/601
2	h	0.70	0/391	1.04	1/601 (0.2%)
2	k	0.68	0/391	1.05	2/601 (0.3%)
2	l	0.75	0/391	1.03	0/601
2	o	0.80	1/413 (0.2%)	1.08	1/635 (0.2%)
2	p	0.73	0/391	0.98	1/601 (0.2%)
2	s	0.75	0/317	1.03	0/486
2	t	0.71	0/318	1.01	1/488 (0.2%)
All	All	0.47	5/33327 (0.0%)	0.82	32/46244 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	a	12	DT	O3'-P	-6.39	1.53	1.61
2	a	4	DC	O3'-P	-5.82	1.54	1.61
2	o	5	DT	O3'-P	5.19	1.67	1.61
2	b	4	DC	O3'-P	-5.18	1.54	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	12	DT	O3'-P	-5.17	1.54	1.61

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	56	LEU	CA-CB-CG	9.06	136.13	115.30
2	t	4	DC	O5'-P-OP2	-7.97	98.53	105.70
2	o	5	DT	P-O3'-C3'	7.66	128.89	119.70
2	a	3	DT	P-O3'-C3'	6.25	127.20	119.70
1	L	56	LEU	CA-CB-CG	-6.16	101.13	115.30

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	A	2505	0	2466	78	0
1	B	2431	0	2372	74	0
1	C	2534	0	2518	59	0
1	D	2424	0	2345	111	0
1	G	2456	0	2391	60	0
1	H	2525	0	2512	55	0
1	K	2460	0	2386	85	0
1	L	2435	0	2346	119	0
1	O	2250	0	2082	119	0
1	P	2369	0	2283	114	0
1	S	1770	0	1641	89	0
1	T	1997	0	1822	170	0
2	a	369	0	204	0	0
2	b	369	0	204	0	0
2	c	369	0	204	0	0
2	d	369	0	204	0	0
2	g	349	0	192	0	0
2	h	349	0	192	0	0
2	k	349	0	192	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	l	349	0	192	0	0
2	o	369	0	204	0	0
2	p	349	0	192	0	0
2	s	284	0	159	0	0
2	t	285	0	159	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	6	0	0	0	0
3	D	2	0	0	0	0
3	G	2	0	0	0	0
3	H	1	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
3	S	1	0	0	0	0
3	T	1	0	0	0	0
3	c	1	0	0	0	0
3	d	1	0	0	0	0
All	All	32340	0	29462	1091	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 20.

The worst 5 of 1091 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:83:VAL:CG2	1:T:141:ILE:HD13	1.48	1.39
1:D:148:ASP:HB3	1:D:151:VAL:CG2	1.64	1.25
1:T:241:LEU:CD1	1:T:271:ALA:HB3	1.71	1.20
1:T:83:VAL:HG23	1:T:141:ILE:CD1	1.79	1.11
1:O:202:ILE:HD11	1:O:272:LEU:HD11	1.24	1.10

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	329/341 (96%)	315 (96%)	12 (4%)	2 (1%)	25	64
1	B	326/341 (96%)	314 (96%)	11 (3%)	1 (0%)	41	74
1	C	330/341 (97%)	315 (96%)	11 (3%)	4 (1%)	13	49
1	D	325/341 (95%)	314 (97%)	10 (3%)	1 (0%)	41	74
1	G	329/341 (96%)	315 (96%)	14 (4%)	0	100	100
1	H	329/341 (96%)	319 (97%)	7 (2%)	3 (1%)	17	56
1	K	331/341 (97%)	315 (95%)	15 (4%)	1 (0%)	41	74
1	L	327/341 (96%)	318 (97%)	8 (2%)	1 (0%)	41	74
1	O	310/341 (91%)	295 (95%)	14 (4%)	1 (0%)	41	74
1	P	318/341 (93%)	302 (95%)	12 (4%)	4 (1%)	12	47
1	S	249/341 (73%)	241 (97%)	6 (2%)	2 (1%)	19	58
1	T	278/341 (82%)	258 (93%)	12 (4%)	8 (3%)	4	28
All	All	3781/4092 (92%)	3621 (96%)	132 (4%)	28 (1%)	22	61

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	120	ALA
1	C	122	ASP
1	H	122	ASP
1	P	123	SER
1	S	78	ASN

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	262/287 (91%)	250 (95%)	12 (5%)	27	63
1	B	249/287 (87%)	240 (96%)	9 (4%)	35	69
1	C	267/287 (93%)	261 (98%)	6 (2%)	52	79
1	D	245/287 (85%)	237 (97%)	8 (3%)	38	71
1	G	253/287 (88%)	249 (98%)	4 (2%)	62	84
1	H	266/287 (93%)	263 (99%)	3 (1%)	73	88
1	K	251/287 (88%)	248 (99%)	3 (1%)	71	88
1	L	246/287 (86%)	242 (98%)	4 (2%)	62	84
1	O	215/287 (75%)	205 (95%)	10 (5%)	26	62
1	P	238/287 (83%)	223 (94%)	15 (6%)	18	52
1	S	160/287 (56%)	154 (96%)	6 (4%)	33	67
1	T	183/287 (64%)	166 (91%)	17 (9%)	9	33
All	All	2835/3444 (82%)	2738 (97%)	97 (3%)	37	70

5 of 97 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	129	TYR
1	O	219	THR
1	T	244	ILE
1	L	45	ASP
1	O	84	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	299	ASN
1	O	293	GLN
1	T	109	GLN
1	D	211	HIS
1	D	293	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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	A	331/341 (97%)	0.12	10 (3%) 50 34	55, 99, 149, 231	0
1	B	328/341 (96%)	0.06	6 (1%) 68 55	49, 112, 181, 255	0
1	C	332/341 (97%)	-0.03	1 (0%) 94 92	45, 81, 125, 178	0
1	D	327/341 (95%)	0.09	8 (2%) 59 44	59, 109, 168, 236	0
1	G	331/341 (97%)	0.14	6 (1%) 68 55	46, 113, 175, 244	0
1	H	331/341 (97%)	-0.02	1 (0%) 94 92	41, 84, 139, 227	0
1	K	333/341 (97%)	0.10	6 (1%) 68 55	61, 110, 169, 238	0
1	L	329/341 (96%)	0.22	10 (3%) 50 34	66, 118, 178, 233	0
1	O	320/341 (93%)	0.28	15 (4%) 31 19	85, 143, 198, 244	0
1	P	324/341 (95%)	0.23	17 (5%) 27 15	79, 141, 191, 224	0
1	S	259/341 (75%)	0.32	16 (6%) 20 11	74, 145, 210, 255	0
1	T	292/341 (85%)	0.47	28 (9%) 8 4	84, 156, 216, 272	0
2	a	18/18 (100%)	-0.30	0 100 100	61, 77, 104, 107	0
2	b	18/18 (100%)	-0.32	0 100 100	58, 77, 102, 128	0
2	c	18/18 (100%)	-0.27	0 100 100	76, 104, 141, 159	0
2	d	18/18 (100%)	-0.11	1 (5%) 24 13	71, 105, 177, 220	0
2	g	17/18 (94%)	-0.38	0 100 100	54, 85, 118, 141	0
2	h	17/18 (94%)	-0.43	0 100 100	64, 78, 111, 119	0
2	k	17/18 (94%)	-0.21	0 100 100	96, 132, 196, 200	0
2	l	17/18 (94%)	-0.26	0 100 100	90, 121, 214, 226	0
2	o	18/18 (100%)	-0.30	0 100 100	111, 124, 168, 172	0
2	p	17/18 (94%)	-0.49	0 100 100	102, 123, 178, 190	0
2	s	14/18 (77%)	-0.33	0 100 100	110, 144, 153, 191	0
2	t	14/18 (77%)	-0.36	0 100 100	112, 128, 166, 185	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
All	All	4040/4308 (93%)	0.14	125 (3%)	49	32	41, 116, 188, 272	0

The worst 5 of 125 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	180	ASN	5.1
1	T	271	ALA	5.0
1	P	285	LYS	4.8
1	T	270	ILE	4.7
1	S	272	LEU	4.6

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 monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.