



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 05:45 PM UTC

PDB ID : 7CE1 / pdb_00007ce1
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 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

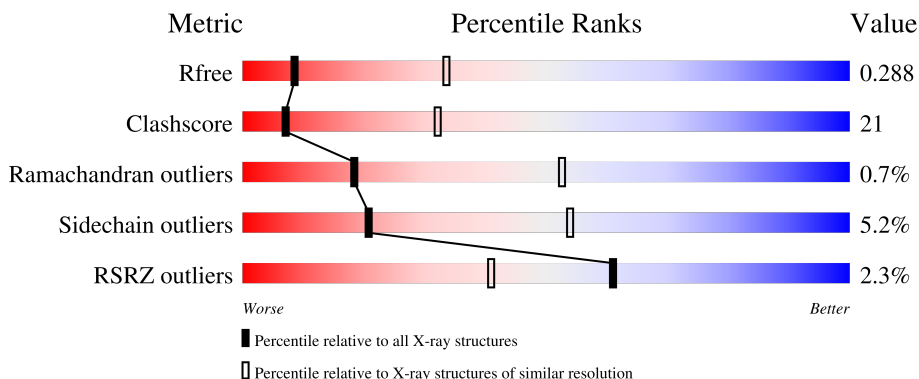
1 Overall quality at a glance

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.



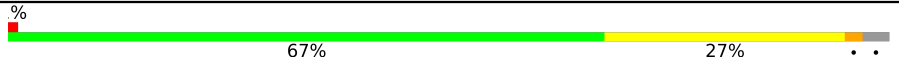

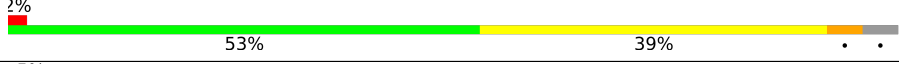

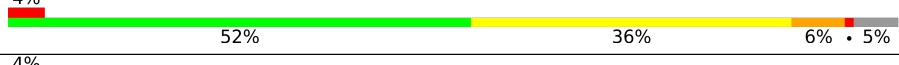
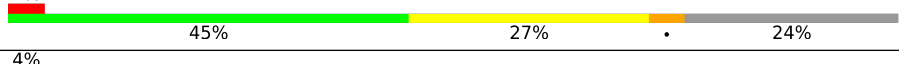
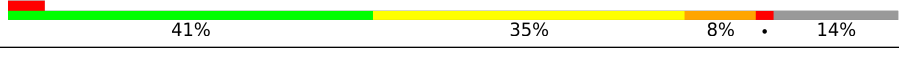


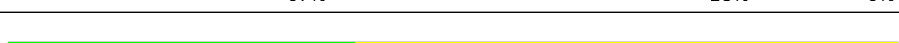
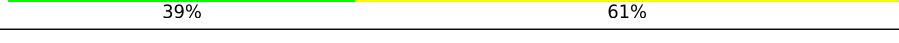
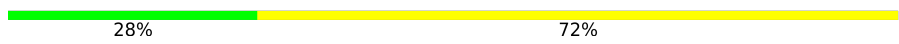
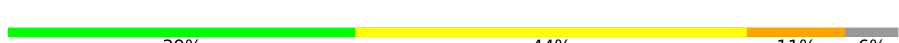
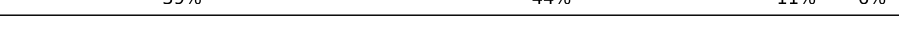
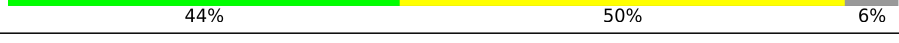

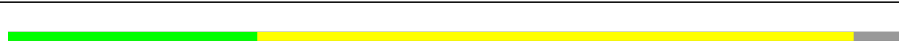
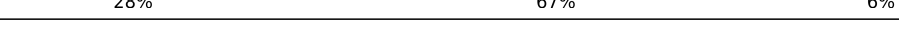

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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 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	A	341	 64% 30% 2% 2% 2%
1	B	341	 62% 32% 2% 2% 2%
1	C	341	 67% 29% 2% 2% 2%
1	D	341	 62% 30% 2% 2% 2%
1	G	341	 67% 26% 2% 2% 2%

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Mol	Chain	Length	Quality of chain
1	H	341	
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
			Total	C	N	O	S			
1	A	331	Total 2505	C 1576	N 443	O 476	S 10	0	0	0
1	B	328	Total 2431	C 1535	N 425	O 462	S 9	0	0	0
1	C	332	Total 2534	C 1602	N 445	O 477	S 10	0	0	0
1	D	327	Total 2424	C 1534	N 424	O 459	S 7	0	0	0
1	G	331	Total 2456	C 1554	N 423	O 469	S 10	0	0	0
1	H	331	Total 2525	C 1593	N 448	O 474	S 10	0	0	0
1	K	333	Total 2460	C 1560	N 426	O 465	S 9	0	0	0
1	L	329	Total 2435	C 1537	N 428	O 462	S 8	0	0	0
1	O	320	Total 2250	C 1420	N 381	O 441	S 8	0	0	0
1	P	324	Total 2369	C 1509	N 404	O 449	S 7	0	0	0
1	S	259	Total 1770	C 1123	N 303	O 339	S 5	0	0	0
1	T	292	Total 1997	C 1254	N 348	O 388	S 7	0	0	0

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

- Molecule 3 is water.

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

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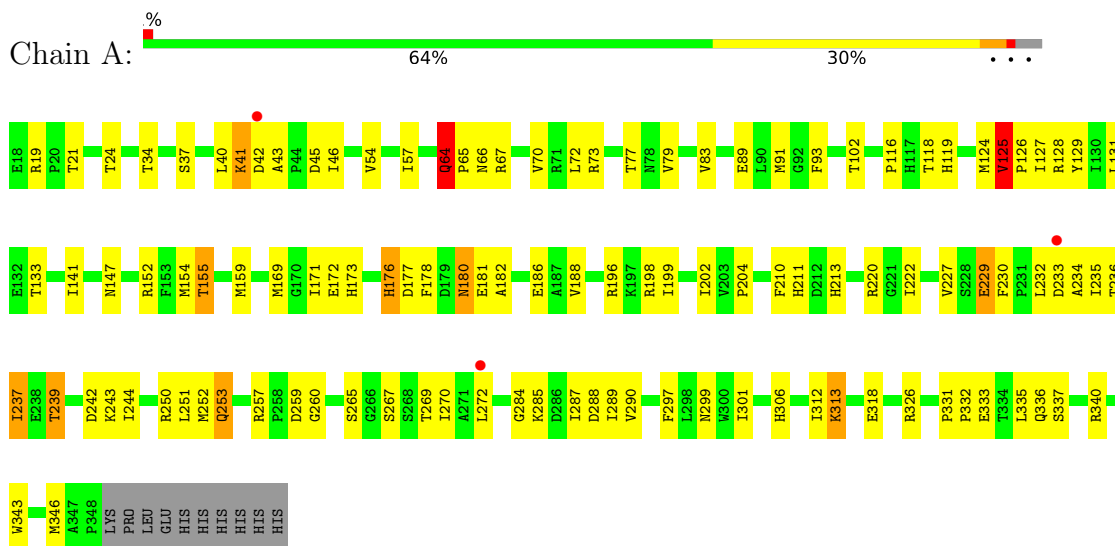
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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3	D	2	Total O 2 2	0	0
3	c	1	Total O 1 1	0	0
3	d	1	Total O 1 1	0	0
3	G	2	Total O 2 2	0	0
3	H	1	Total O 1 1	0	0
3	K	2	Total O 2 2	0	0
3	L	2	Total O 2 2	0	0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

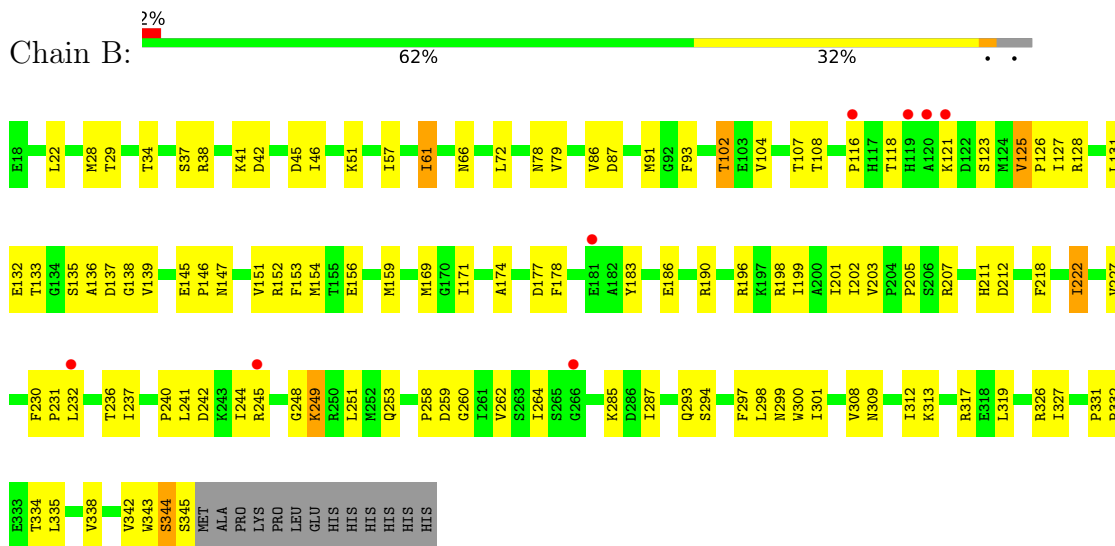
3 Residue-property plots i

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

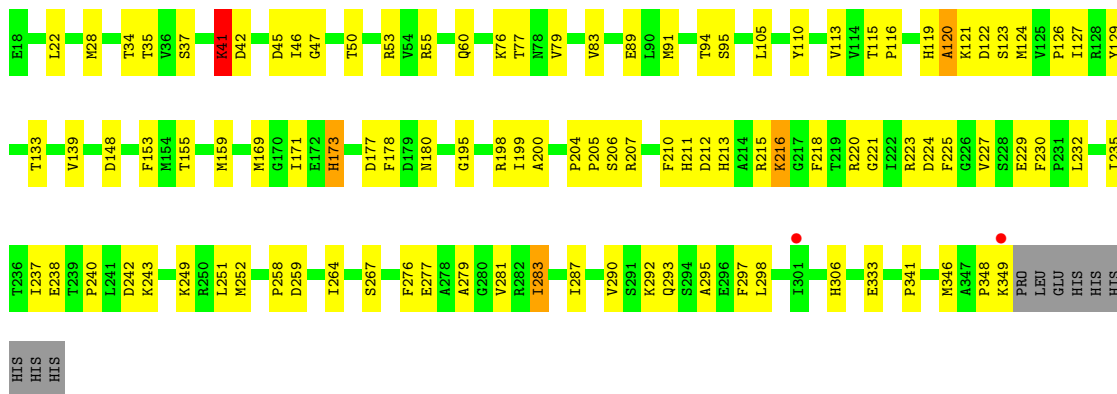


- Molecule 1: LacI-type transcription factor

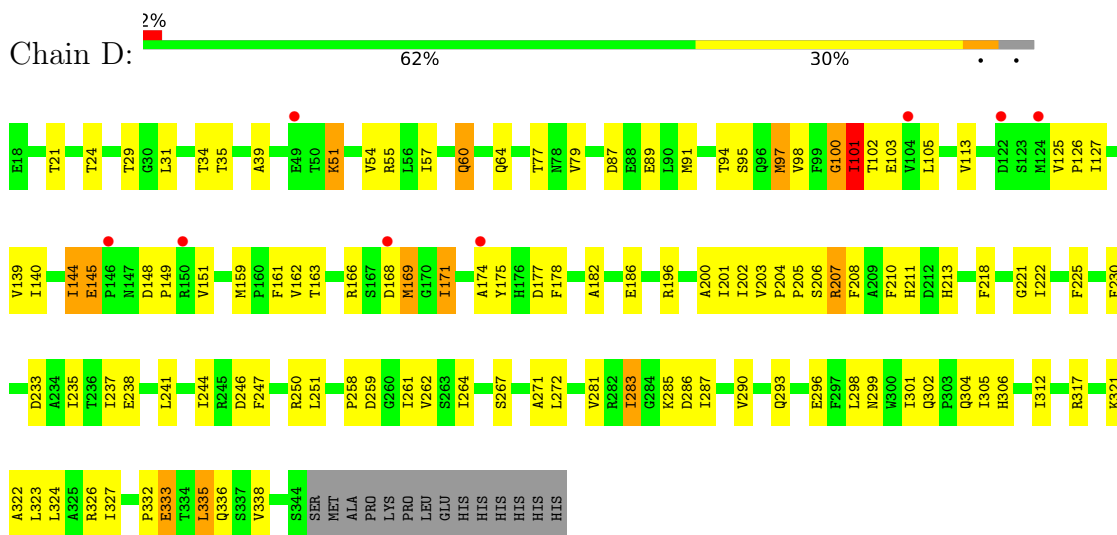


- Molecule 1: LacI-type transcription factor

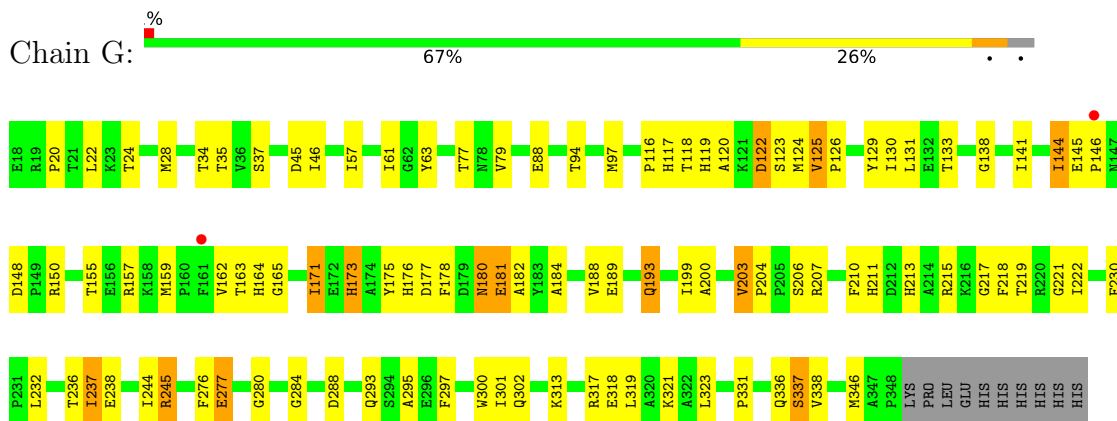




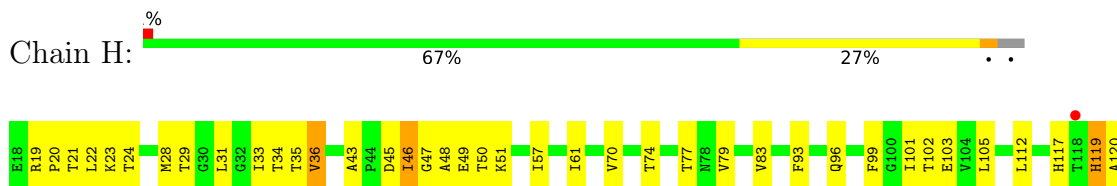
• Molecule 1: LacI-type transcription factor

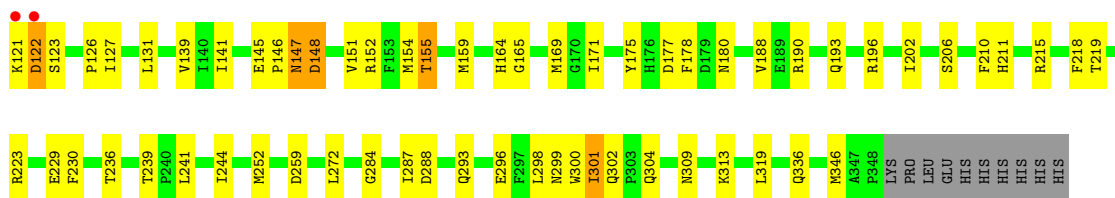


• Molecule 1: LacI-type transcription factor

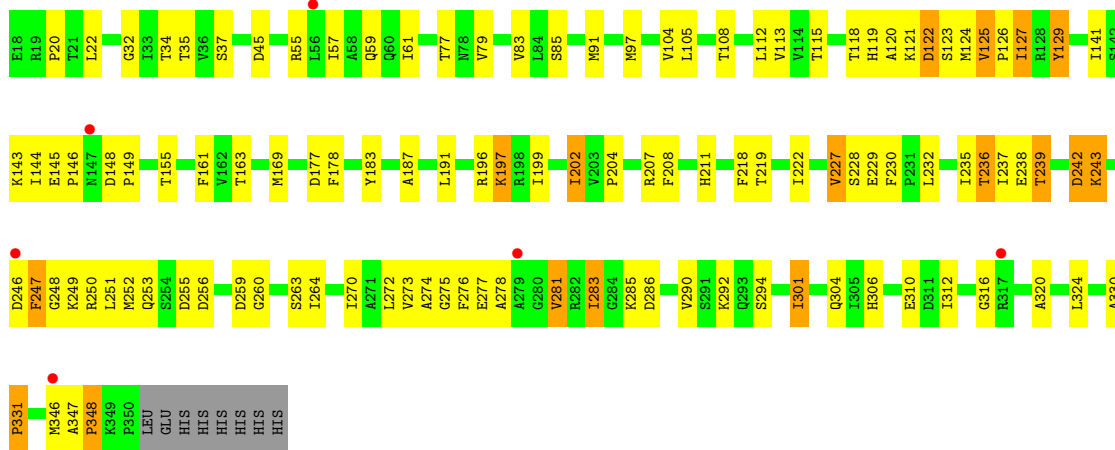


• Molecule 1: LacI-type transcription factor

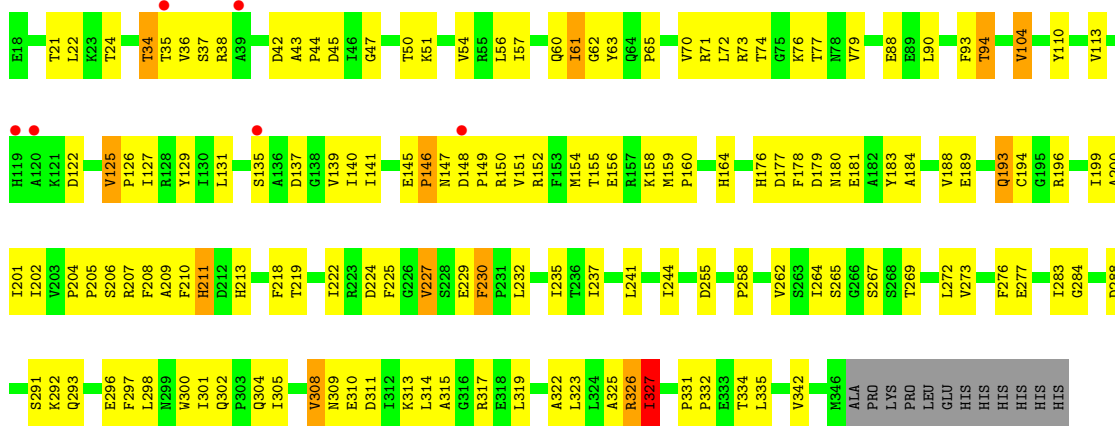




• Molecule 1: LacI-type transcription factor

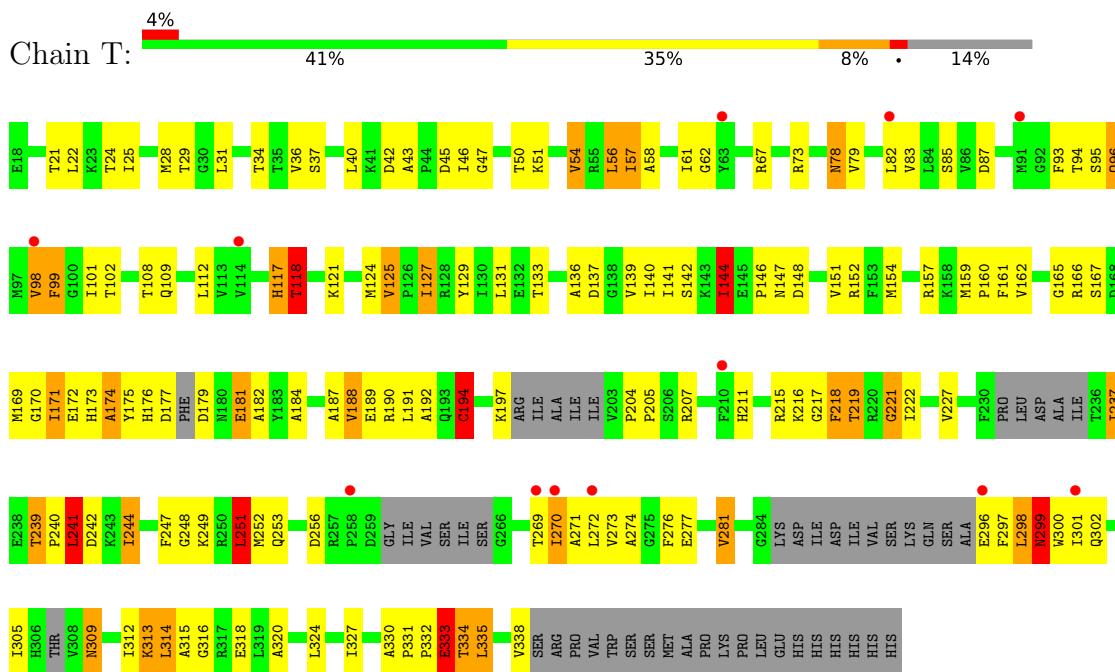


• Molecule 1: LacI-type transcription factor



• Molecule 1: LacI-type transcription factor

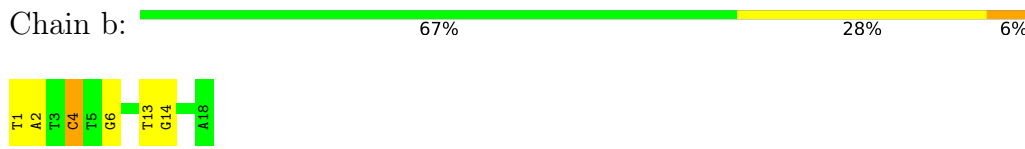




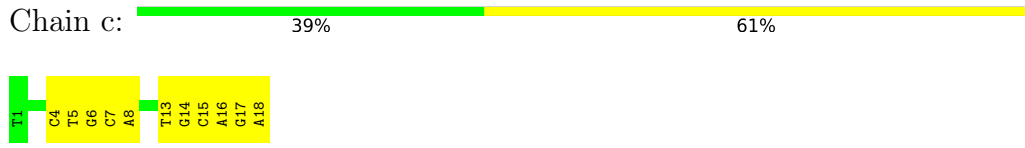
• Molecule 2: promoter DNA



• Molecule 2: promoter DNA



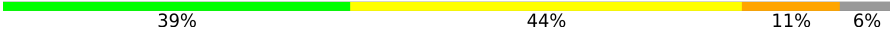
• Molecule 2: promoter DNA



• Molecule 2: promoter DNA



• Molecule 2: promoter DNA

Chain g:  39% 44% 11% 6%



• Molecule 2: promoter DNA

Chain h:  44% 50% 6%




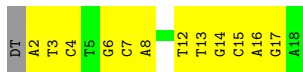
• Molecule 2: promoter DNA

Chain k:  61% 22% 11% 6%

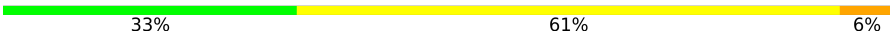


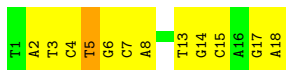
• Molecule 2: promoter DNA

Chain l:  28% 67% 6%



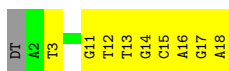
• Molecule 2: promoter DNA

Chain o:  33% 61% 6%

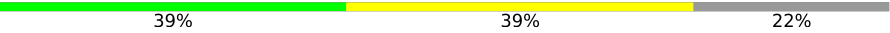


• Molecule 2: promoter DNA

Chain p:  44% 50% 6%

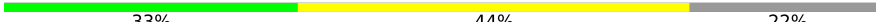


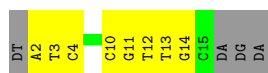
• Molecule 2: promoter DNA

Chain s:  39% 39% 22%



• Molecule 2: promoter DNA

Chain t:  33% 44% 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) 99.9 (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)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.233 , 0.281 0.246 , 0.288	Depositor DCC
R_{free} test set	5593 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	98.6	Xtrriage
Anisotropy	0.356	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 89.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 i

5.1 Standard geometry i

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.60	1/2552 (0.0%)	1.14	19/3471 (0.5%)
1	B	0.57	0/2476	1.12	9/3374 (0.3%)
1	C	0.46	0/2584	1.04	7/3509 (0.2%)
1	D	0.60	0/2471	1.17	16/3371 (0.5%)
1	G	0.52	1/2504 (0.0%)	1.14	17/3412 (0.5%)
1	H	0.45	0/2574	1.04	10/3496 (0.3%)
1	K	0.58	1/2510 (0.0%)	1.17	22/3425 (0.6%)
1	L	0.55	2/2482 (0.1%)	1.12	12/3385 (0.4%)
1	O	0.57	0/2285	1.21	22/3126 (0.7%)
1	P	0.61	0/2414	1.22	23/3293 (0.7%)
1	S	0.68	1/1796 (0.1%)	1.36	17/2458 (0.7%)
1	T	0.71	2/2024 (0.1%)	1.48	35/2770 (1.3%)
2	a	0.71	1/413 (0.2%)	0.91	1/635 (0.2%)
2	b	0.63	0/413	0.82	1/635 (0.2%)
2	c	0.37	0/413	0.66	0/635
2	d	0.31	0/413	0.62	0/635
2	g	0.45	0/391	0.88	3/601 (0.5%)
2	h	0.35	0/391	0.63	0/601
2	k	0.39	0/391	0.86	2/601 (0.3%)
2	l	0.35	0/391	0.67	0/601
2	o	0.47	0/413	0.75	1/635 (0.2%)
2	p	0.42	0/391	0.66	0/601
2	s	0.33	0/317	0.62	0/486
2	t	0.36	0/318	0.64	0/488
All	All	0.56	9/33327 (0.0%)	1.12	217/46244 (0.5%)

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	243	LYS	C-O	-5.97	1.16	1.24
1	S	271	ALA	CA-CB	-5.82	1.44	1.53
1	L	327	ILE	CA-CB	5.58	1.62	1.54
1	A	125	VAL	CA-CB	5.41	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	144	ILE	CA-CB	-5.30	1.47	1.54

The worst 5 of 217 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	98	VAL	N-CA-C	13.65	123.52	110.42
1	H	300	TRP	N-CA-C	-10.53	99.89	111.36
1	S	203	VAL	CA-C-N	-9.28	110.83	120.38
1	S	203	VAL	C-N-CA	-9.28	110.83	120.38
1	S	266	GLY	N-CA-C	8.95	125.44	113.99

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2505	0	2466	86	0
1	B	2431	0	2372	86	0
1	C	2534	0	2518	71	0
1	D	2424	0	2345	118	0
1	G	2456	0	2391	73	0
1	H	2525	0	2512	64	0
1	K	2460	0	2386	90	0
1	L	2435	0	2346	128	0
1	O	2250	0	2082	126	0
1	P	2369	0	2283	125	0
1	S	1770	0	1641	97	0
1	T	1997	0	1822	189	0
2	a	369	0	204	16	0
2	b	369	0	204	5	0
2	c	369	0	204	13	0
2	d	369	0	204	12	0
2	g	349	0	192	11	0
2	h	349	0	192	6	0
2	k	349	0	192	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	l	349	0	192	20	0
2	o	369	0	204	14	0
2	p	349	0	192	10	0
2	s	284	0	159	11	0
2	t	285	0	159	9	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	1284	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 21.

The worst 5 of 1284 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%)	21	56
1	B	326/341 (96%)	314 (96%)	11 (3%)	1 (0%)	36	68
1	C	330/341 (97%)	315 (96%)	11 (3%)	4 (1%)	10	42
1	D	325/341 (95%)	314 (97%)	10 (3%)	1 (0%)	36	68
1	G	329/341 (96%)	315 (96%)	14 (4%)	0	100	100
1	H	329/341 (96%)	319 (97%)	7 (2%)	3 (1%)	14	47
1	K	331/341 (97%)	315 (95%)	15 (4%)	1 (0%)	36	68
1	L	327/341 (96%)	318 (97%)	8 (2%)	1 (0%)	36	68
1	O	310/341 (91%)	295 (95%)	14 (4%)	1 (0%)	36	68
1	P	318/341 (93%)	302 (95%)	12 (4%)	4 (1%)	9	40
1	S	249/341 (73%)	241 (97%)	6 (2%)	2 (1%)	16	50
1	T	278/341 (82%)	258 (93%)	12 (4%)	8 (3%)	3	24
All	All	3781/4092 (92%)	3621 (96%)	132 (4%)	28 (1%)	18	52

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%)	249 (95%)	13 (5%)	22	55
1	B	249/287 (87%)	239 (96%)	10 (4%)	28	61
1	C	267/287 (93%)	259 (97%)	8 (3%)	36	66
1	D	245/287 (85%)	236 (96%)	9 (4%)	30	63
1	G	253/287 (88%)	242 (96%)	11 (4%)	26	59
1	H	266/287 (93%)	257 (97%)	9 (3%)	32	64
1	K	251/287 (88%)	241 (96%)	10 (4%)	28	61
1	L	246/287 (86%)	238 (97%)	8 (3%)	33	65
1	O	215/287 (75%)	199 (93%)	16 (7%)	13	43
1	P	238/287 (83%)	220 (92%)	18 (8%)	12	42
1	S	160/287 (56%)	150 (94%)	10 (6%)	16	48
1	T	183/287 (64%)	158 (86%)	25 (14%)	3	18
All	All	2835/3444 (82%)	2688 (95%)	147 (5%)	21	54

5 of 147 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	150	ARG
1	T	324	LEU
1	S	227	VAL
1	T	144	ILE
1	G	318	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	299	ASN
1	O	293	GLN
1	T	173	HIS
1	O	111	HIS
1	P	173	HIS

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	331/341 (97%)	0.05	3 (0%) 81 64	55, 99, 149, 231	0
1	B	328/341 (96%)	0.19	8 (2%) 59 40	49, 112, 181, 255	0
1	C	332/341 (97%)	-0.23	2 (0%) 85 73	45, 81, 125, 178	0
1	D	327/341 (95%)	0.14	8 (2%) 59 40	59, 109, 168, 236	0
1	G	331/341 (97%)	0.15	2 (0%) 85 73	46, 113, 175, 244	0
1	H	331/341 (97%)	-0.11	3 (0%) 81 64	41, 84, 139, 227	0
1	K	333/341 (97%)	0.13	6 (1%) 67 48	61, 110, 169, 238	0
1	L	329/341 (96%)	0.32	6 (1%) 67 48	66, 118, 178, 233	0
1	O	320/341 (93%)	0.52	18 (5%) 30 19	85, 143, 198, 244	0
1	P	324/341 (95%)	0.47	12 (3%) 45 28	79, 141, 191, 224	0
1	S	259/341 (75%)	0.44	13 (5%) 34 22	74, 145, 210, 255	0
1	T	292/341 (85%)	0.49	12 (4%) 41 25	84, 156, 216, 272	0
2	a	18/18 (100%)	-0.29	0 100 100	61, 77, 104, 107	0
2	b	18/18 (100%)	-0.45	0 100 100	58, 77, 102, 128	0
2	c	18/18 (100%)	-0.34	0 100 100	76, 104, 141, 159	0
2	d	18/18 (100%)	-0.40	0 100 100	71, 105, 177, 220	0
2	g	17/18 (94%)	-0.45	0 100 100	54, 85, 118, 141	0
2	h	17/18 (94%)	-0.60	0 100 100	64, 78, 111, 119	0
2	k	17/18 (94%)	-0.00	0 100 100	96, 132, 196, 200	0
2	l	17/18 (94%)	0.03	0 100 100	90, 121, 214, 226	0
2	o	18/18 (100%)	-0.09	0 100 100	111, 124, 168, 172	0
2	p	17/18 (94%)	-0.14	0 100 100	102, 123, 178, 190	0
2	s	14/18 (77%)	0.25	0 100 100	110, 144, 153, 191	0
2	t	14/18 (77%)	-0.04	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%)	0.18	93 (2%) 61 41	41, 116, 188, 272	0

The worst 5 of 93 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	124	MET	5.5
1	T	270	ILE	5.4
1	T	114	VAL	5.2
1	D	146	PRO	4.3
1	O	199	ILE	4.1

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.