Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 08:45 AM EDT

PDB ID	:	6XHR
Title	:	Crystal structure of S. aureus TarI (space group P1211)
Authors	:	Li, F.K.K.; Strynadka, N.C.J.
Deposited on	:	2020-06-19
Resolution	:	2.10 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:

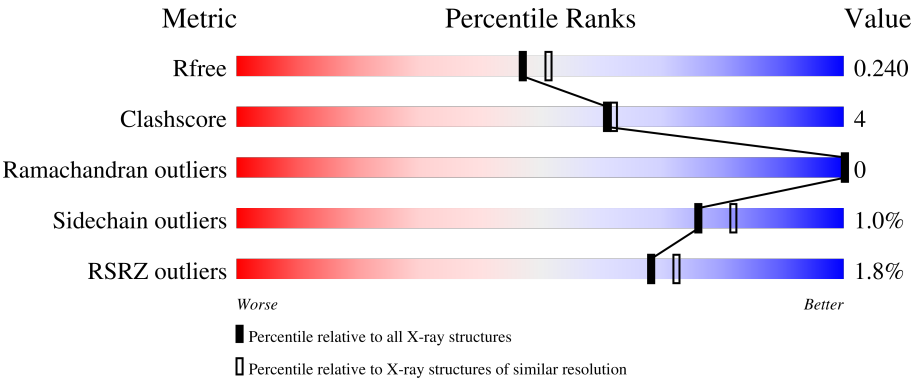
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 <=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	261	83% 7% 10%
1	B	261	75% 10% 15%
1	C	261	% 77% 14% 10%
1	D	261	2% 79% 11% 10%
1	E	261	% 78% 8% 13%

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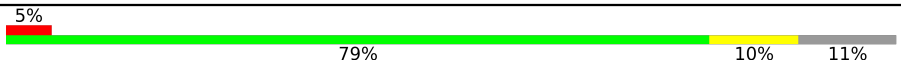
Mol	Chain	Length	Quality of chain
1	F	261	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11004 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 Ribitol-5-phosphate cytidylyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	236	Total	C	N	O	S	0	0	0
			1837	1165	311	355	6			
1	B	222	Total	C	N	O	S	0	0	0
			1700	1082	284	329	5			
1	C	236	Total	C	N	O	S	0	0	0
			1782	1129	297	350	6			
1	D	236	Total	C	N	O	S	0	0	0
			1807	1146	306	349	6			
1	E	226	Total	C	N	O	S	0	0	0
			1738	1107	289	337	5			
1	F	233	Total	C	N	O	S	0	0	0
			1732	1101	292	333	6			

There are 138 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	239	GLY	-	expression tag	UNP Q2G1C0
A	240	GLY	-	expression tag	UNP Q2G1C0
A	241	SER	-	expression tag	UNP Q2G1C0
A	242	LEU	-	expression tag	UNP Q2G1C0
A	243	VAL	-	expression tag	UNP Q2G1C0
A	244	PRO	-	expression tag	UNP Q2G1C0
A	245	ARG	-	expression tag	UNP Q2G1C0
A	246	GLY	-	expression tag	UNP Q2G1C0
A	247	SER	-	expression tag	UNP Q2G1C0
A	248	ALA	-	expression tag	UNP Q2G1C0
A	249	ALA	-	expression tag	UNP Q2G1C0
A	250	ALA	-	expression tag	UNP Q2G1C0
A	251	ALA	-	expression tag	UNP Q2G1C0
A	252	LEU	-	expression tag	UNP Q2G1C0
A	253	GLU	-	expression tag	UNP Q2G1C0
A	254	HIS	-	expression tag	UNP Q2G1C0
A	255	HIS	-	expression tag	UNP Q2G1C0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	256	HIS	-	expression tag	UNP Q2G1C0
A	257	HIS	-	expression tag	UNP Q2G1C0
A	258	HIS	-	expression tag	UNP Q2G1C0
A	259	HIS	-	expression tag	UNP Q2G1C0
A	260	HIS	-	expression tag	UNP Q2G1C0
A	261	HIS	-	expression tag	UNP Q2G1C0
B	239	GLY	-	expression tag	UNP Q2G1C0
B	240	GLY	-	expression tag	UNP Q2G1C0
B	241	SER	-	expression tag	UNP Q2G1C0
B	242	LEU	-	expression tag	UNP Q2G1C0
B	243	VAL	-	expression tag	UNP Q2G1C0
B	244	PRO	-	expression tag	UNP Q2G1C0
B	245	ARG	-	expression tag	UNP Q2G1C0
B	246	GLY	-	expression tag	UNP Q2G1C0
B	247	SER	-	expression tag	UNP Q2G1C0
B	248	ALA	-	expression tag	UNP Q2G1C0
B	249	ALA	-	expression tag	UNP Q2G1C0
B	250	ALA	-	expression tag	UNP Q2G1C0
B	251	ALA	-	expression tag	UNP Q2G1C0
B	252	LEU	-	expression tag	UNP Q2G1C0
B	253	GLU	-	expression tag	UNP Q2G1C0
B	254	HIS	-	expression tag	UNP Q2G1C0
B	255	HIS	-	expression tag	UNP Q2G1C0
B	256	HIS	-	expression tag	UNP Q2G1C0
B	257	HIS	-	expression tag	UNP Q2G1C0
B	258	HIS	-	expression tag	UNP Q2G1C0
B	259	HIS	-	expression tag	UNP Q2G1C0
B	260	HIS	-	expression tag	UNP Q2G1C0
B	261	HIS	-	expression tag	UNP Q2G1C0
C	239	GLY	-	expression tag	UNP Q2G1C0
C	240	GLY	-	expression tag	UNP Q2G1C0
C	241	SER	-	expression tag	UNP Q2G1C0
C	242	LEU	-	expression tag	UNP Q2G1C0
C	243	VAL	-	expression tag	UNP Q2G1C0
C	244	PRO	-	expression tag	UNP Q2G1C0
C	245	ARG	-	expression tag	UNP Q2G1C0
C	246	GLY	-	expression tag	UNP Q2G1C0
C	247	SER	-	expression tag	UNP Q2G1C0
C	248	ALA	-	expression tag	UNP Q2G1C0
C	249	ALA	-	expression tag	UNP Q2G1C0
C	250	ALA	-	expression tag	UNP Q2G1C0
C	251	ALA	-	expression tag	UNP Q2G1C0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	252	LEU	-	expression tag	UNP Q2G1C0
C	253	GLU	-	expression tag	UNP Q2G1C0
C	254	HIS	-	expression tag	UNP Q2G1C0
C	255	HIS	-	expression tag	UNP Q2G1C0
C	256	HIS	-	expression tag	UNP Q2G1C0
C	257	HIS	-	expression tag	UNP Q2G1C0
C	258	HIS	-	expression tag	UNP Q2G1C0
C	259	HIS	-	expression tag	UNP Q2G1C0
C	260	HIS	-	expression tag	UNP Q2G1C0
C	261	HIS	-	expression tag	UNP Q2G1C0
D	239	GLY	-	expression tag	UNP Q2G1C0
D	240	GLY	-	expression tag	UNP Q2G1C0
D	241	SER	-	expression tag	UNP Q2G1C0
D	242	LEU	-	expression tag	UNP Q2G1C0
D	243	VAL	-	expression tag	UNP Q2G1C0
D	244	PRO	-	expression tag	UNP Q2G1C0
D	245	ARG	-	expression tag	UNP Q2G1C0
D	246	GLY	-	expression tag	UNP Q2G1C0
D	247	SER	-	expression tag	UNP Q2G1C0
D	248	ALA	-	expression tag	UNP Q2G1C0
D	249	ALA	-	expression tag	UNP Q2G1C0
D	250	ALA	-	expression tag	UNP Q2G1C0
D	251	ALA	-	expression tag	UNP Q2G1C0
D	252	LEU	-	expression tag	UNP Q2G1C0
D	253	GLU	-	expression tag	UNP Q2G1C0
D	254	HIS	-	expression tag	UNP Q2G1C0
D	255	HIS	-	expression tag	UNP Q2G1C0
D	256	HIS	-	expression tag	UNP Q2G1C0
D	257	HIS	-	expression tag	UNP Q2G1C0
D	258	HIS	-	expression tag	UNP Q2G1C0
D	259	HIS	-	expression tag	UNP Q2G1C0
D	260	HIS	-	expression tag	UNP Q2G1C0
D	261	HIS	-	expression tag	UNP Q2G1C0
E	239	GLY	-	expression tag	UNP Q2G1C0
E	240	GLY	-	expression tag	UNP Q2G1C0
E	241	SER	-	expression tag	UNP Q2G1C0
E	242	LEU	-	expression tag	UNP Q2G1C0
E	243	VAL	-	expression tag	UNP Q2G1C0
E	244	PRO	-	expression tag	UNP Q2G1C0
E	245	ARG	-	expression tag	UNP Q2G1C0
E	246	GLY	-	expression tag	UNP Q2G1C0
E	247	SER	-	expression tag	UNP Q2G1C0

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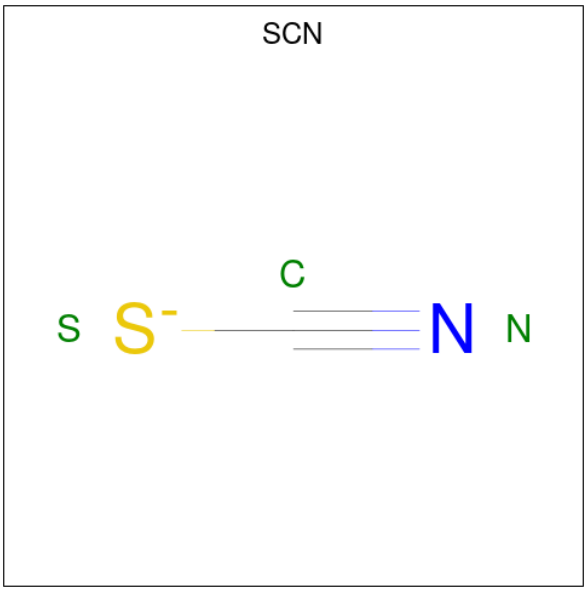
Chain	Residue	Modelled	Actual	Comment	Reference
E	248	ALA	-	expression tag	UNP Q2G1C0
E	249	ALA	-	expression tag	UNP Q2G1C0
E	250	ALA	-	expression tag	UNP Q2G1C0
E	251	ALA	-	expression tag	UNP Q2G1C0
E	252	LEU	-	expression tag	UNP Q2G1C0
E	253	GLU	-	expression tag	UNP Q2G1C0
E	254	HIS	-	expression tag	UNP Q2G1C0
E	255	HIS	-	expression tag	UNP Q2G1C0
E	256	HIS	-	expression tag	UNP Q2G1C0
E	257	HIS	-	expression tag	UNP Q2G1C0
E	258	HIS	-	expression tag	UNP Q2G1C0
E	259	HIS	-	expression tag	UNP Q2G1C0
E	260	HIS	-	expression tag	UNP Q2G1C0
E	261	HIS	-	expression tag	UNP Q2G1C0
F	239	GLY	-	expression tag	UNP Q2G1C0
F	240	GLY	-	expression tag	UNP Q2G1C0
F	241	SER	-	expression tag	UNP Q2G1C0
F	242	LEU	-	expression tag	UNP Q2G1C0
F	243	VAL	-	expression tag	UNP Q2G1C0
F	244	PRO	-	expression tag	UNP Q2G1C0
F	245	ARG	-	expression tag	UNP Q2G1C0
F	246	GLY	-	expression tag	UNP Q2G1C0
F	247	SER	-	expression tag	UNP Q2G1C0
F	248	ALA	-	expression tag	UNP Q2G1C0
F	249	ALA	-	expression tag	UNP Q2G1C0
F	250	ALA	-	expression tag	UNP Q2G1C0
F	251	ALA	-	expression tag	UNP Q2G1C0
F	252	LEU	-	expression tag	UNP Q2G1C0
F	253	GLU	-	expression tag	UNP Q2G1C0
F	254	HIS	-	expression tag	UNP Q2G1C0
F	255	HIS	-	expression tag	UNP Q2G1C0
F	256	HIS	-	expression tag	UNP Q2G1C0
F	257	HIS	-	expression tag	UNP Q2G1C0
F	258	HIS	-	expression tag	UNP Q2G1C0
F	259	HIS	-	expression tag	UNP Q2G1C0
F	260	HIS	-	expression tag	UNP Q2G1C0
F	261	HIS	-	expression tag	UNP Q2G1C0

- Molecule 2 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N S 3 1 1 1	0	0
2	A	1	Total C N S 3 1 1 1	0	0
2	C	1	Total C N S 3 1 1 1	0	0
2	C	1	Total C N S 3 1 1 1	0	0
2	D	1	Total C N S 3 1 1 1	0	0
2	D	1	Total C N S 3 1 1 1	0	0
2	F	1	Total C N S 3 1 1 1	0	0
2	F	1	Total C N S 3 1 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	122	Total O 122 122	0	0
3	B	59	Total O 59 59	0	0
3	C	54	Total O 54 54	0	0
3	D	68	Total O 68 68	0	0

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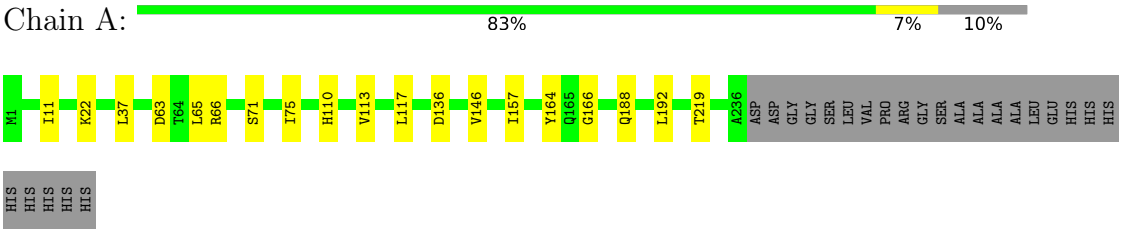
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	51	Total O 51 51	0	0
3	F	30	Total O 30 30	0	0

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.

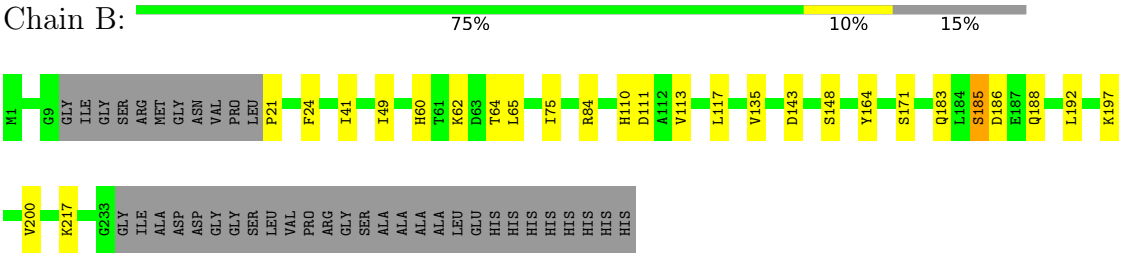
• Molecule 1: Ribitol-5-phosphate cytidylyltransferase 1

Chain A:



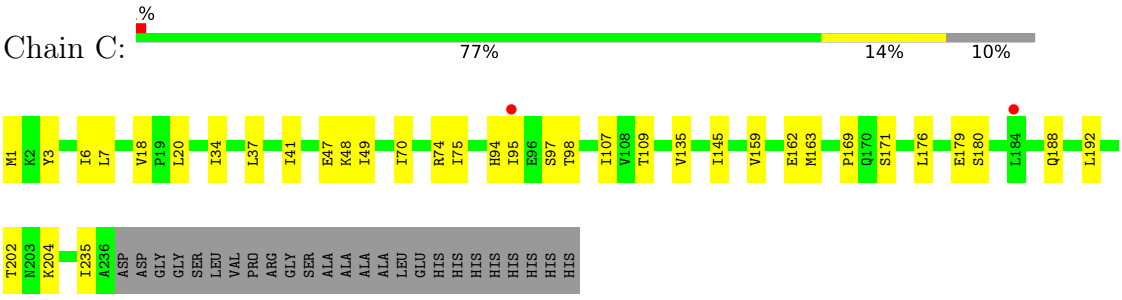
• Molecule 1: Ribitol-5-phosphate cytidylyltransferase 1

Chain B:



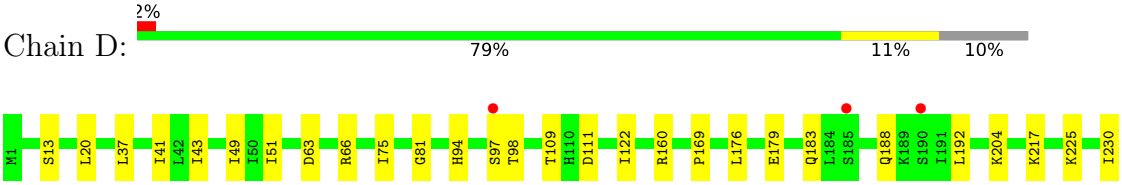
• Molecule 1: Ribitol-5-phosphate cytidylyltransferase 1

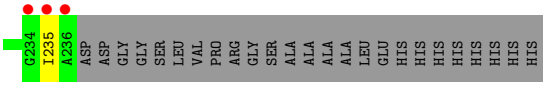
Chain C:



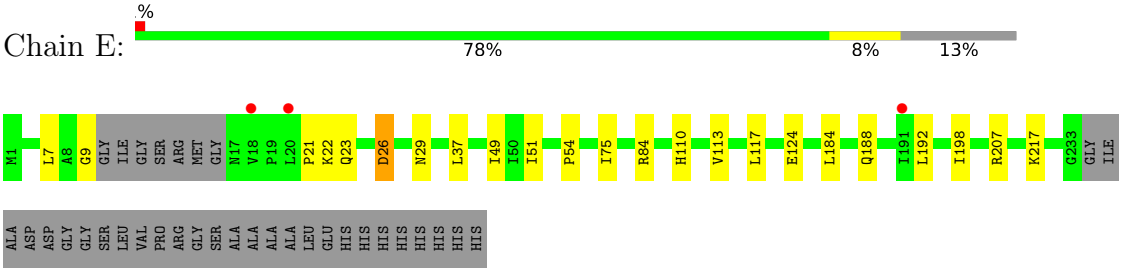
• Molecule 1: Ribitol-5-phosphate cytidylyltransferase 1

Chain D:

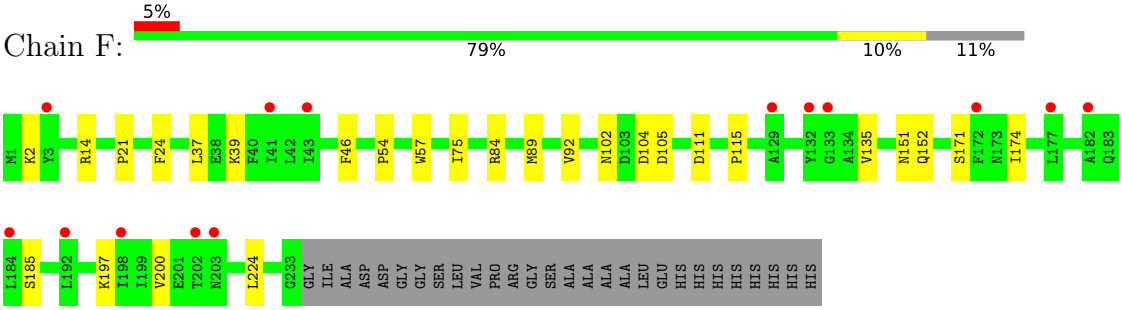




• Molecule 1: Ribitol-5-phosphate cytidylyltransferase 1



• Molecule 1: Ribitol-5-phosphate cytidylyltransferase 1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	50.52Å 138.45Å 110.11Å 90.00° 96.45° 90.00°	Depositor
Resolution (Å)	47.71 – 2.10 47.71 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.3 (47.71-2.10) 97.5 (47.71-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.36 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.198 , 0.241 0.196 , 0.240	Depositor DCC
R_{free} test set	4264 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	40.0	Xtriage
Anisotropy	0.600	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 41.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11004	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

Bond lengths and bond angles in the following residue types are not validated in this section: SCN

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	0.53	0/1864	0.72	1/2529 (0.0%)
1	B	0.46	0/1725	0.71	0/2348
1	C	0.45	0/1809	0.68	0/2468
1	D	0.49	0/1834	0.66	0/2494
1	E	0.48	0/1764	0.69	0/2402
1	F	0.46	0/1759	0.67	0/2403
All	All	0.48	0/10755	0.69	1/14644 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	136	ASP	CB-CG-OD1	5.32	123.09	118.30

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	1837	0	1871	12	0
1	B	1700	0	1691	18	0
1	C	1782	0	1749	26	0
1	D	1807	0	1811	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1738	0	1736	13	0
1	F	1732	0	1689	15	0
2	A	6	0	0	2	0
2	C	6	0	0	0	0
2	D	6	0	0	0	0
2	F	6	0	0	0	0
3	A	122	0	0	0	0
3	B	59	0	0	0	0
3	C	54	0	0	0	0
3	D	68	0	0	1	0
3	E	51	0	0	0	0
3	F	30	0	0	0	0
All	All	11004	0	10547	95	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 4.

All (95) 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:C:176:LEU:HD21	1:C:204:LYS:HD3	1.63	0.78
1:E:21:PRO:HB2	1:E:23:GLN:OE1	1.84	0.77
1:F:197:LYS:HA	1:F:200:VAL:HG12	1.66	0.75
1:D:20:LEU:HD21	1:E:124:GLU:HG2	1.68	0.72
1:C:159:VAL:HG13	1:C:162:GLU:HG3	1.74	0.68
1:C:235:ILE:HD11	1:D:225:LYS:HD3	1.77	0.67
1:B:197:LYS:HA	1:B:200:VAL:HG12	1.75	0.67
1:C:95:ILE:HA	1:C:98:THR:HG22	1.76	0.66
1:D:13:SER:HB3	1:D:20:LEU:HD11	1.79	0.64
1:E:37:LEU:HD11	1:E:51:ILE:HD11	1.80	0.63
1:D:94:HIS:O	1:D:98:THR:HG22	2.00	0.62
1:C:1:MET:CE	1:C:47:GLU:OE2	2.48	0.62
1:E:113:VAL:HG23	1:E:217:LYS:HG3	1.83	0.61
1:F:84:ARG:NH1	1:F:111:ASP:OD2	2.34	0.60
1:A:157:ILE:O	1:B:197:LYS:NZ	2.36	0.58
1:D:230:ILE:HA	1:D:235:ILE:HD12	1.85	0.58
1:C:188:GLN:O	1:C:192:LEU:HD13	2.04	0.58
1:A:37:LEU:HD21	1:A:75:ILE:HD12	1.86	0.58
1:C:18:VAL:O	1:C:20:LEU:HD22	2.05	0.57
1:D:176:LEU:HD11	1:D:204:LYS:HD3	1.87	0.57
1:F:135:VAL:CG1	1:F:171:SER:HB2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:ASP:OD1	1:D:217:LYS:HE2	2.06	0.55
1:E:26:ASP:OD1	1:E:29:ASN:HA	2.07	0.55
1:C:1:MET:HE1	1:C:47:GLU:OE2	2.05	0.55
1:B:197:LYS:HA	1:B:200:VAL:CG1	2.36	0.55
1:A:146:VAL:HG22	1:B:164:TYR:HB2	1.91	0.53
1:B:21:PRO:HB2	1:B:24:PHE:HD2	1.74	0.52
1:D:37:LEU:HD11	1:D:51:ILE:HD11	1.91	0.52
1:C:7:LEU:HD21	1:C:109:THR:HB	1.92	0.51
1:E:9:GLY:HA2	1:E:54:PRO:HD3	1.93	0.50
1:B:135:VAL:CG1	1:B:171:SER:HB2	2.41	0.50
1:E:184:LEU:HD11	1:E:198:ILE:HG23	1.93	0.49
1:F:89:MET:HA	1:F:92:VAL:HG22	1.92	0.49
1:A:63:ASP:OD1	1:A:66:ARG:NH1	2.38	0.49
1:B:60:HIS:O	1:B:64:THR:HG23	2.13	0.49
1:C:34:ILE:HD12	1:C:70:ILE:CD1	2.43	0.49
1:C:49:ILE:O	1:C:75:ILE:HA	2.12	0.49
1:F:105:ASP:HB3	1:F:174:ILE:HD12	1.95	0.49
1:F:39:LYS:HD2	1:F:115:PRO:O	2.12	0.48
1:F:102:ASN:HB2	1:F:104:ASP:OD1	2.13	0.48
1:E:7:LEU:HD12	1:E:84:ARG:NH2	2.28	0.48
1:C:94:HIS:O	1:C:98:THR:HG22	2.14	0.47
1:C:109:THR:O	1:C:169:PRO:HA	2.14	0.47
1:D:81:GLY:O	3:D:401:HOH:O	2.20	0.47
1:D:179:GLU:OE1	1:D:183:GLN:NE2	2.48	0.47
1:E:188:GLN:O	1:E:192:LEU:HG	2.14	0.47
1:F:37:LEU:HD21	1:F:75:ILE:HD12	1.97	0.47
1:C:202:THR:HG22	1:C:202:THR:O	2.16	0.46
1:F:89:MET:O	1:F:92:VAL:HG22	2.14	0.46
1:B:84:ARG:NH1	1:B:111:ASP:OD1	2.49	0.45
1:C:135:VAL:CG1	1:C:171:SER:HB2	2.46	0.45
1:C:41:ILE:HD11	1:C:75:ILE:HD11	1.97	0.45
1:C:34:ILE:HD12	1:C:70:ILE:HD13	1.98	0.45
1:F:2:LYS:O	1:F:46:PHE:HA	2.16	0.45
1:E:110:HIS:CE1	1:E:117:LEU:HD13	2.52	0.45
1:D:37:LEU:HD23	1:D:37:LEU:HA	1.83	0.44
1:C:48:LYS:HA	1:C:74:ARG:HB3	1.98	0.44
1:C:6:ILE:HD12	1:C:37:LEU:HD23	2.00	0.44
1:D:188:GLN:O	1:D:192:LEU:HG	2.18	0.44
1:A:22:LYS:HD3	2:A:302:SCN:S	2.58	0.43
1:C:3:TYR:O	1:C:107:ILE:HD12	2.18	0.43
1:E:22:LYS:HD3	1:E:22:LYS:HA	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:LYS:HA	1:B:65:LEU:HD12	2.01	0.43
1:C:6:ILE:CD1	1:C:37:LEU:HD23	2.49	0.43
1:D:49:ILE:O	1:D:75:ILE:HA	2.18	0.43
1:E:49:ILE:O	1:E:75:ILE:HA	2.18	0.43
1:D:41:ILE:HD11	1:D:75:ILE:HD11	1.99	0.43
1:E:37:LEU:HD11	1:E:51:ILE:CD1	2.46	0.43
1:B:49:ILE:O	1:B:75:ILE:HA	2.18	0.43
1:C:6:ILE:HD12	1:C:37:LEU:CD2	2.49	0.43
1:F:54:PRO:HD2	1:F:57:TRP:CE3	2.54	0.43
1:B:41:ILE:HD11	1:B:75:ILE:HD11	2.01	0.42
1:C:1:MET:HE3	1:C:47:GLU:OE2	2.17	0.42
1:F:151:ASN:C	1:F:152:GLN:HG2	2.40	0.42
1:C:95:ILE:HA	1:C:98:THR:CG2	2.48	0.42
1:A:110:HIS:CE1	1:A:117:LEU:HD13	2.54	0.42
1:A:164:TYR:CE2	1:B:148:SER:HB3	2.55	0.42
1:B:21:PRO:HB2	1:B:24:PHE:CD2	2.53	0.42
1:C:145:ILE:HB	1:C:163:MET:HE2	2.01	0.42
1:D:109:THR:O	1:D:169:PRO:HA	2.20	0.42
1:D:43:ILE:HG13	1:D:122:ILE:HG21	2.02	0.42
1:F:21:PRO:HB2	1:F:24:PHE:HD2	1.85	0.42
1:F:37:LEU:HD12	1:F:37:LEU:HA	1.88	0.41
1:A:166:GLY:O	1:B:143:ASP:HB3	2.20	0.41
1:A:188:GLN:O	1:A:192:LEU:HD23	2.20	0.41
1:B:110:HIS:CE1	1:B:117:LEU:HD13	2.55	0.41
1:A:65:LEU:HD23	1:A:65:LEU:HA	1.93	0.41
1:B:188:GLN:O	1:B:192:LEU:HG	2.20	0.41
1:A:113:VAL:HG22	2:A:301:SCN:N	2.35	0.41
1:B:185:SER:OG	1:B:186:ASP:N	2.53	0.41
1:D:63:ASP:OD2	1:D:66:ARG:NH2	2.51	0.41
1:F:224:LEU:HD23	1:F:224:LEU:HA	1.90	0.40
1:A:11:ILE:HG21	1:A:219:THR:OG1	2.21	0.40
1:B:113:VAL:HG23	1:B:217:LYS:HG3	2.04	0.40
1:C:159:VAL:CG1	1:C:162:GLU:HG3	2.45	0.40

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	234/261 (90%)	228 (97%)	6 (3%)	0	100	100
1	B	218/261 (84%)	214 (98%)	4 (2%)	0	100	100
1	C	234/261 (90%)	229 (98%)	5 (2%)	0	100	100
1	D	234/261 (90%)	230 (98%)	4 (2%)	0	100	100
1	E	222/261 (85%)	216 (97%)	6 (3%)	0	100	100
1	F	231/261 (88%)	225 (97%)	6 (3%)	0	100	100
All	All	1373/1566 (88%)	1342 (98%)	31 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	205/227 (90%)	204 (100%)	1 (0%)	88	92
1	B	185/227 (82%)	183 (99%)	2 (1%)	73	79
1	C	192/227 (85%)	189 (98%)	3 (2%)	62	69
1	D	197/227 (87%)	195 (99%)	2 (1%)	76	82
1	E	191/227 (84%)	189 (99%)	2 (1%)	76	82
1	F	182/227 (80%)	180 (99%)	2 (1%)	73	79
All	All	1152/1362 (85%)	1140 (99%)	12 (1%)	76	82

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	SER
1	B	183	GLN
1	B	185	SER
1	C	97	SER
1	C	179	GLU
1	C	180	SER
1	D	97	SER
1	D	160	ARG
1	E	26	ASP
1	E	207	ARG
1	F	14	ARG
1	F	185	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SCN	D	301	-	1,2,2	0.50	0	0,1,1	-	-
2	SCN	A	302	-	1,2,2	0.70	0	0,1,1	-	-
2	SCN	C	301	-	1,2,2	0.50	0	0,1,1	-	-
2	SCN	F	302	-	1,2,2	0.57	0	0,1,1	-	-
2	SCN	C	302	-	1,2,2	0.63	0	0,1,1	-	-
2	SCN	A	301	-	1,2,2	0.45	0	0,1,1	-	-
2	SCN	F	301	-	1,2,2	0.54	0	0,1,1	-	-
2	SCN	D	302	-	1,2,2	0.60	0	0,1,1	-	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	302	SCN	1	0
2	A	301	SCN	1	0

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, 95^{th} 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	236/261 (90%)	-0.16	0 100 100	29, 44, 64, 78	0
1	B	222/261 (85%)	-0.17	0 100 100	37, 59, 89, 140	0
1	C	236/261 (90%)	-0.10	2 (0%) 86 88	38, 63, 94, 113	0
1	D	236/261 (90%)	-0.15	6 (2%) 57 62	33, 58, 101, 121	0
1	E	226/261 (86%)	-0.13	3 (1%) 77 80	39, 59, 94, 110	0
1	F	233/261 (89%)	0.21	14 (6%) 21 27	38, 73, 117, 130	0
All	All	1389/1566 (88%)	-0.08	25 (1%) 68 72	29, 58, 101, 140	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	203	ASN	3.4
1	F	202	THR	3.4
1	E	191	ILE	3.3
1	F	129	ALA	3.3
1	C	184	LEU	3.2
1	E	20	LEU	3.1
1	F	41	ILE	3.0
1	F	182	ALA	2.9
1	F	184	LEU	2.9
1	D	234	GLY	2.8
1	F	43	ILE	2.8
1	D	190	SER	2.8
1	F	198	ILE	2.7
1	F	192	LEU	2.6
1	F	3	TYR	2.6
1	D	235	ILE	2.6
1	F	133	GLY	2.5
1	F	177	LEU	2.4
1	D	185	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	97	SER	2.2
1	E	18	VAL	2.2
1	F	172	PHE	2.1
1	F	132	TYR	2.1
1	C	95	ILE	2.0
1	D	236	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SCN	F	302	3/3	0.86	0.20	91,91,93,94	0
2	SCN	D	301	3/3	0.95	0.12	45,45,46,46	0
2	SCN	C	302	3/3	0.95	0.21	71,71,74,77	0
2	SCN	C	301	3/3	0.96	0.11	43,43,44,46	0
2	SCN	A	302	3/3	0.97	0.11	54,54,55,60	0
2	SCN	F	301	3/3	0.98	0.10	42,42,45,45	0
2	SCN	D	302	3/3	0.98	0.15	73,73,77,79	0
2	SCN	A	301	3/3	0.99	0.11	33,33,39,41	0

6.5 Other polymers (i)

There are no such residues in this entry.