



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:45 AM UTC

PDB ID : 4UOO / pdb_00004uoo
Title : Structure of lipoteichoic acid synthase LtaS from *Listeria monocytogenes*
Authors : Campeotto, I.; Freemont, P.; Grundling, A.
Deposited on : 2014-06-06
Resolution : 3.00 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

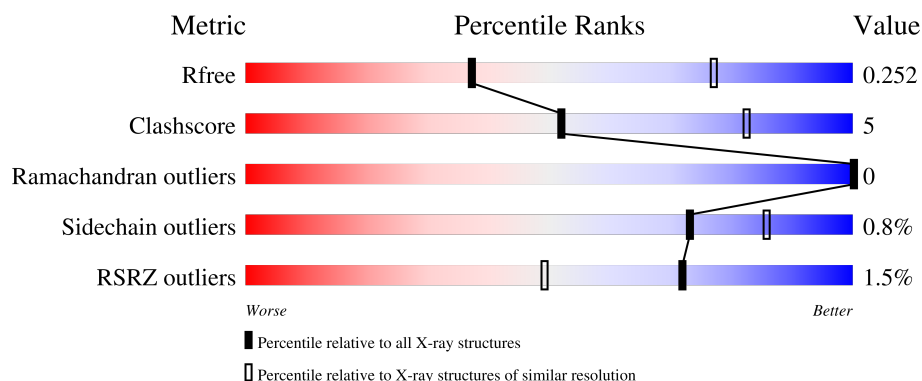
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	459	80% 10% 10%
1	B	459	2% 78% 12% 10%
1	C	459	80% 11% 10%
1	D	459	2% 77% 13% 10%
1	E	459	80% 11% 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16745 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 LIPOTEICHOIC ACID SYNTHASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	415	Total	C	N	O	P	S	0	0	0
			3348	2142	532	665	1	8			
1	B	415	Total	C	N	O	P	S	0	0	0
			3348	2142	532	665	1	8			
1	C	415	Total	C	N	O	P	S	0	0	0
			3348	2142	532	665	1	8			
1	D	415	Total	C	N	O	P	S	0	0	0
			3348	2142	532	665	1	8			
1	E	415	Total	C	N	O	P	S	0	0	0
			3348	2142	532	665	1	8			

There are 155 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	195	MET	-	expression tag	UNP Q8Y8H6
A	196	SER	-	expression tag	UNP Q8Y8H6
A	197	TYR	-	expression tag	UNP Q8Y8H6
A	198	TYR	-	expression tag	UNP Q8Y8H6
A	199	HIS	-	expression tag	UNP Q8Y8H6
A	200	HIS	-	expression tag	UNP Q8Y8H6
A	201	HIS	-	expression tag	UNP Q8Y8H6
A	202	HIS	-	expression tag	UNP Q8Y8H6
A	203	HIS	-	expression tag	UNP Q8Y8H6
A	204	HIS	-	expression tag	UNP Q8Y8H6
A	205	ASP	-	expression tag	UNP Q8Y8H6
A	206	TYR	-	expression tag	UNP Q8Y8H6
A	207	ASP	-	expression tag	UNP Q8Y8H6
A	208	ILE	-	expression tag	UNP Q8Y8H6
A	209	PRO	-	expression tag	UNP Q8Y8H6
A	210	THR	-	expression tag	UNP Q8Y8H6
A	211	THR	-	expression tag	UNP Q8Y8H6
A	212	GLU	-	expression tag	UNP Q8Y8H6
A	213	ASN	-	expression tag	UNP Q8Y8H6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	214	LEU	-	expression tag	UNP Q8Y8H6
A	215	TYR	-	expression tag	UNP Q8Y8H6
A	216	PHE	-	expression tag	UNP Q8Y8H6
A	217	GLN	-	expression tag	UNP Q8Y8H6
A	218	GLY	-	expression tag	UNP Q8Y8H6
A	219	ALA	-	expression tag	UNP Q8Y8H6
A	220	MET	-	expression tag	UNP Q8Y8H6
A	221	GLY	-	expression tag	UNP Q8Y8H6
A	222	SER	-	expression tag	UNP Q8Y8H6
A	223	GLY	-	expression tag	UNP Q8Y8H6
A	224	ILE	-	expression tag	UNP Q8Y8H6
A	225	GLN	-	expression tag	UNP Q8Y8H6
B	195	MET	-	expression tag	UNP Q8Y8H6
B	196	SER	-	expression tag	UNP Q8Y8H6
B	197	TYR	-	expression tag	UNP Q8Y8H6
B	198	TYR	-	expression tag	UNP Q8Y8H6
B	199	HIS	-	expression tag	UNP Q8Y8H6
B	200	HIS	-	expression tag	UNP Q8Y8H6
B	201	HIS	-	expression tag	UNP Q8Y8H6
B	202	HIS	-	expression tag	UNP Q8Y8H6
B	203	HIS	-	expression tag	UNP Q8Y8H6
B	204	HIS	-	expression tag	UNP Q8Y8H6
B	205	ASP	-	expression tag	UNP Q8Y8H6
B	206	TYR	-	expression tag	UNP Q8Y8H6
B	207	ASP	-	expression tag	UNP Q8Y8H6
B	208	ILE	-	expression tag	UNP Q8Y8H6
B	209	PRO	-	expression tag	UNP Q8Y8H6
B	210	THR	-	expression tag	UNP Q8Y8H6
B	211	THR	-	expression tag	UNP Q8Y8H6
B	212	GLU	-	expression tag	UNP Q8Y8H6
B	213	ASN	-	expression tag	UNP Q8Y8H6
B	214	LEU	-	expression tag	UNP Q8Y8H6
B	215	TYR	-	expression tag	UNP Q8Y8H6
B	216	PHE	-	expression tag	UNP Q8Y8H6
B	217	GLN	-	expression tag	UNP Q8Y8H6
B	218	GLY	-	expression tag	UNP Q8Y8H6
B	219	ALA	-	expression tag	UNP Q8Y8H6
B	220	MET	-	expression tag	UNP Q8Y8H6
B	221	GLY	-	expression tag	UNP Q8Y8H6
B	222	SER	-	expression tag	UNP Q8Y8H6
B	223	GLY	-	expression tag	UNP Q8Y8H6
B	224	ILE	-	expression tag	UNP Q8Y8H6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	225	GLN	-	expression tag	UNP Q8Y8H6
C	195	MET	-	expression tag	UNP Q8Y8H6
C	196	SER	-	expression tag	UNP Q8Y8H6
C	197	TYR	-	expression tag	UNP Q8Y8H6
C	198	TYR	-	expression tag	UNP Q8Y8H6
C	199	HIS	-	expression tag	UNP Q8Y8H6
C	200	HIS	-	expression tag	UNP Q8Y8H6
C	201	HIS	-	expression tag	UNP Q8Y8H6
C	202	HIS	-	expression tag	UNP Q8Y8H6
C	203	HIS	-	expression tag	UNP Q8Y8H6
C	204	HIS	-	expression tag	UNP Q8Y8H6
C	205	ASP	-	expression tag	UNP Q8Y8H6
C	206	TYR	-	expression tag	UNP Q8Y8H6
C	207	ASP	-	expression tag	UNP Q8Y8H6
C	208	ILE	-	expression tag	UNP Q8Y8H6
C	209	PRO	-	expression tag	UNP Q8Y8H6
C	210	THR	-	expression tag	UNP Q8Y8H6
C	211	THR	-	expression tag	UNP Q8Y8H6
C	212	GLU	-	expression tag	UNP Q8Y8H6
C	213	ASN	-	expression tag	UNP Q8Y8H6
C	214	LEU	-	expression tag	UNP Q8Y8H6
C	215	TYR	-	expression tag	UNP Q8Y8H6
C	216	PHE	-	expression tag	UNP Q8Y8H6
C	217	GLN	-	expression tag	UNP Q8Y8H6
C	218	GLY	-	expression tag	UNP Q8Y8H6
C	219	ALA	-	expression tag	UNP Q8Y8H6
C	220	MET	-	expression tag	UNP Q8Y8H6
C	221	GLY	-	expression tag	UNP Q8Y8H6
C	222	SER	-	expression tag	UNP Q8Y8H6
C	223	GLY	-	expression tag	UNP Q8Y8H6
C	224	ILE	-	expression tag	UNP Q8Y8H6
C	225	GLN	-	expression tag	UNP Q8Y8H6
D	195	MET	-	expression tag	UNP Q8Y8H6
D	196	SER	-	expression tag	UNP Q8Y8H6
D	197	TYR	-	expression tag	UNP Q8Y8H6
D	198	TYR	-	expression tag	UNP Q8Y8H6
D	199	HIS	-	expression tag	UNP Q8Y8H6
D	200	HIS	-	expression tag	UNP Q8Y8H6
D	201	HIS	-	expression tag	UNP Q8Y8H6
D	202	HIS	-	expression tag	UNP Q8Y8H6
D	203	HIS	-	expression tag	UNP Q8Y8H6
D	204	HIS	-	expression tag	UNP Q8Y8H6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	205	ASP	-	expression tag	UNP Q8Y8H6
D	206	TYR	-	expression tag	UNP Q8Y8H6
D	207	ASP	-	expression tag	UNP Q8Y8H6
D	208	ILE	-	expression tag	UNP Q8Y8H6
D	209	PRO	-	expression tag	UNP Q8Y8H6
D	210	THR	-	expression tag	UNP Q8Y8H6
D	211	THR	-	expression tag	UNP Q8Y8H6
D	212	GLU	-	expression tag	UNP Q8Y8H6
D	213	ASN	-	expression tag	UNP Q8Y8H6
D	214	LEU	-	expression tag	UNP Q8Y8H6
D	215	TYR	-	expression tag	UNP Q8Y8H6
D	216	PHE	-	expression tag	UNP Q8Y8H6
D	217	GLN	-	expression tag	UNP Q8Y8H6
D	218	GLY	-	expression tag	UNP Q8Y8H6
D	219	ALA	-	expression tag	UNP Q8Y8H6
D	220	MET	-	expression tag	UNP Q8Y8H6
D	221	GLY	-	expression tag	UNP Q8Y8H6
D	222	SER	-	expression tag	UNP Q8Y8H6
D	223	GLY	-	expression tag	UNP Q8Y8H6
D	224	ILE	-	expression tag	UNP Q8Y8H6
D	225	GLN	-	expression tag	UNP Q8Y8H6
E	195	MET	-	expression tag	UNP Q8Y8H6
E	196	SER	-	expression tag	UNP Q8Y8H6
E	197	TYR	-	expression tag	UNP Q8Y8H6
E	198	TYR	-	expression tag	UNP Q8Y8H6
E	199	HIS	-	expression tag	UNP Q8Y8H6
E	200	HIS	-	expression tag	UNP Q8Y8H6
E	201	HIS	-	expression tag	UNP Q8Y8H6
E	202	HIS	-	expression tag	UNP Q8Y8H6
E	203	HIS	-	expression tag	UNP Q8Y8H6
E	204	HIS	-	expression tag	UNP Q8Y8H6
E	205	ASP	-	expression tag	UNP Q8Y8H6
E	206	TYR	-	expression tag	UNP Q8Y8H6
E	207	ASP	-	expression tag	UNP Q8Y8H6
E	208	ILE	-	expression tag	UNP Q8Y8H6
E	209	PRO	-	expression tag	UNP Q8Y8H6
E	210	THR	-	expression tag	UNP Q8Y8H6
E	211	THR	-	expression tag	UNP Q8Y8H6
E	212	GLU	-	expression tag	UNP Q8Y8H6
E	213	ASN	-	expression tag	UNP Q8Y8H6
E	214	LEU	-	expression tag	UNP Q8Y8H6
E	215	TYR	-	expression tag	UNP Q8Y8H6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	216	PHE	-	expression tag	UNP Q8Y8H6
E	217	GLN	-	expression tag	UNP Q8Y8H6
E	218	GLY	-	expression tag	UNP Q8Y8H6
E	219	ALA	-	expression tag	UNP Q8Y8H6
E	220	MET	-	expression tag	UNP Q8Y8H6
E	221	GLY	-	expression tag	UNP Q8Y8H6
E	222	SER	-	expression tag	UNP Q8Y8H6
E	223	GLY	-	expression tag	UNP Q8Y8H6
E	224	ILE	-	expression tag	UNP Q8Y8H6
E	225	GLN	-	expression tag	UNP Q8Y8H6

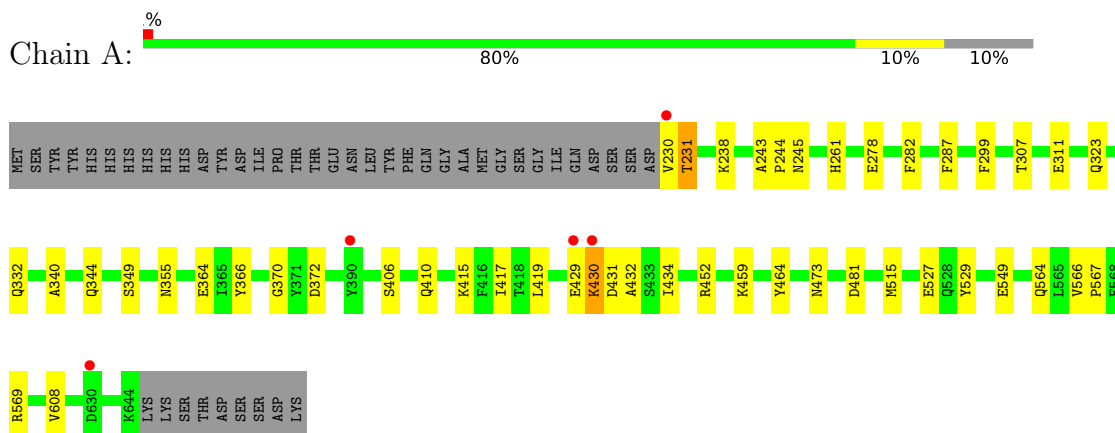
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0

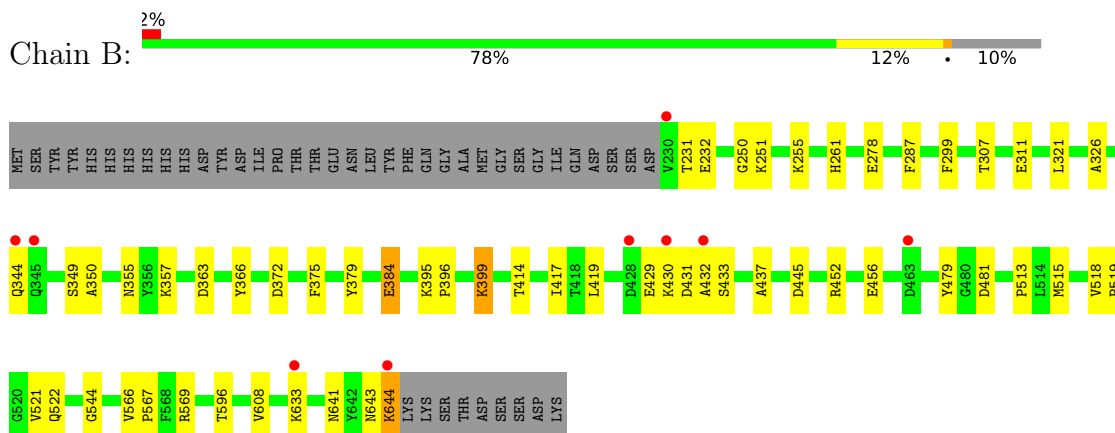
3 Residue-property plots

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.

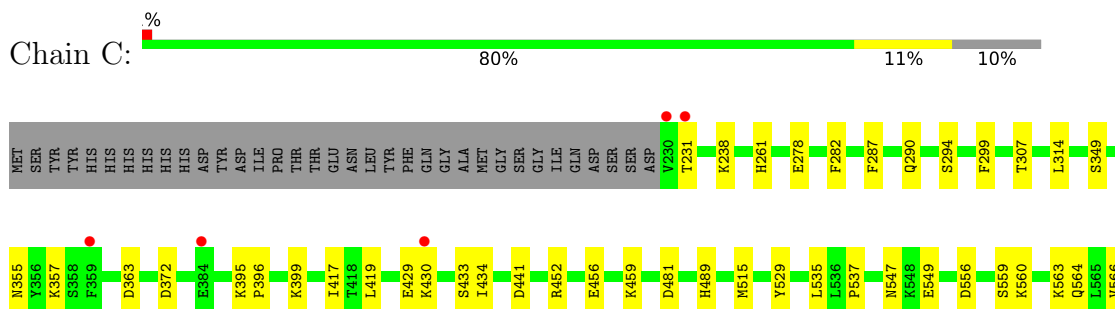
• Molecule 1: LIPOTEICHOIC ACID SYNTHASE



• Molecule 1: LIPOTEICHOIC ACID SYNTHASE

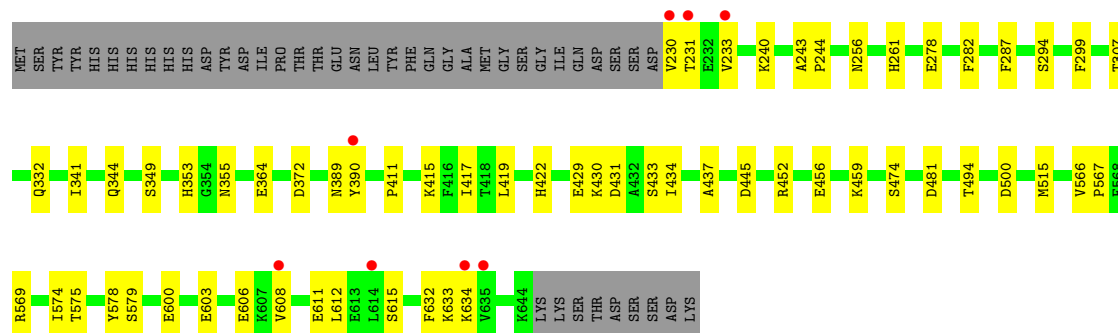
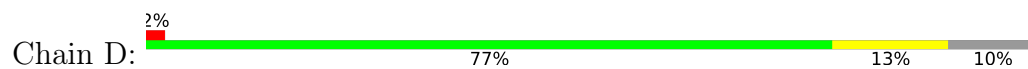


• Molecule 1: LIPOTEICHOIC ACID SYNTHASE

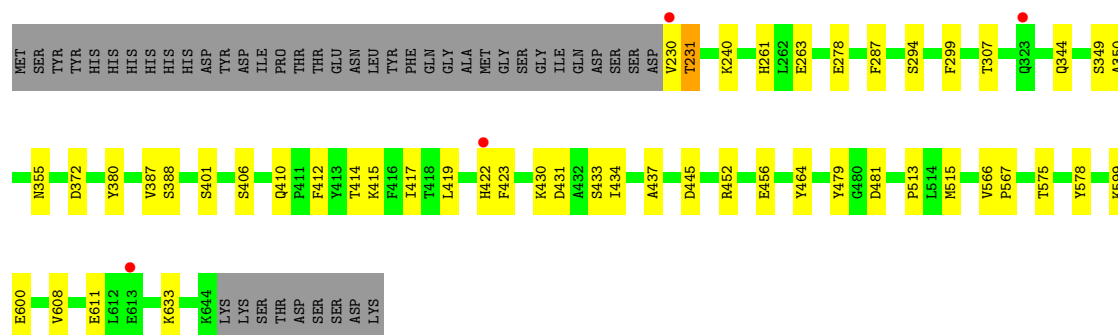
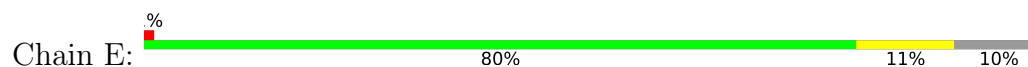




• Molecule 1: LIPOTEICHOIC ACID SYNTHASE



• Molecule 1: LIPOTEICHOIC ACID SYNTHASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	119.76Å 119.76Å 473.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	108.88 – 3.00 108.88 – 3.00	Depositor EDS
% Data completeness (in resolution range)	90.7 (108.88-3.00) 90.6 (108.88-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.222 , 0.260 0.216 , 0.252	Depositor DCC
R_{free} test set	3201 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	56.9	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	16745	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.32% 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

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

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	0.31	0/3422	0.70	5/4629 (0.1%)
1	B	0.35	0/3422	0.71	2/4629 (0.0%)
1	C	0.27	0/3422	0.68	3/4629 (0.1%)
1	D	0.35	0/3422	0.72	3/4629 (0.1%)
1	E	0.28	0/3422	0.70	3/4629 (0.1%)
All	All	0.31	0/17110	0.70	16/23145 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	431	ASP	N-CA-C	-8.27	102.22	111.82
1	E	431	ASP	N-CA-C	-7.84	103.51	113.23
1	B	231	THR	N-CA-C	-7.63	103.33	114.39
1	E	231	THR	N-CA-C	-7.42	103.81	114.12
1	A	430	LYS	CA-CB-CG	7.41	128.92	114.10
1	B	431	ASP	N-CA-C	-6.75	104.52	112.89
1	D	431	ASP	N-CA-C	-6.60	105.53	113.97
1	C	231	THR	N-CA-C	-6.30	105.25	114.39
1	A	231	THR	N-CA-C	-6.05	105.20	113.30
1	E	423	PHE	N-CA-C	5.44	115.85	109.60
1	D	615	SER	CA-C-N	5.33	127.69	120.44
1	D	615	SER	C-N-CA	5.33	127.69	120.44
1	C	592	GLU	CA-C-N	5.02	125.29	119.92
1	C	592	GLU	C-N-CA	5.02	125.29	119.92
1	A	245	ASN	CA-C-N	5.01	125.28	119.47
1	A	245	ASN	C-N-CA	5.01	125.28	119.47

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	3348	0	3178	27	0
1	B	3348	0	3178	34	0
1	C	3348	0	3178	26	0
1	D	3348	0	3178	46	0
1	E	3348	0	3178	33	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
All	All	16745	0	15890	165	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 5.

All (165) 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:D:567:PRO:HB3	1:D:608:VAL:CG2	1.58	1.32
1:A:429:GLU:HG3	1:A:430:LYS:HB3	1.31	1.09
1:D:567:PRO:HB3	1:D:608:VAL:HG21	1.27	1.07
1:D:567:PRO:HB3	1:D:608:VAL:HG23	1.44	0.95
1:D:567:PRO:CB	1:D:608:VAL:CG2	2.50	0.87
1:D:344:GLN:HE22	1:D:633:LYS:H	1.25	0.84
1:E:419:LEU:O	1:E:422:HIS:ND1	2.11	0.81
1:D:569:ARG:NH1	1:D:612:LEU:HD13	1.96	0.79
1:B:349:SER:HB2	1:B:372:ASP:H	1.49	0.78
1:A:238:LYS:NZ	1:A:549:GLU:OE2	2.18	0.77
1:D:567:PRO:CB	1:D:608:VAL:HG21	2.11	0.76
1:B:344:GLN:HE22	1:B:633:LYS:HD2	1.48	0.76
1:D:567:PRO:CB	1:D:608:VAL:HG23	2.13	0.75
1:A:230:VAL:HG23	1:A:231:THR:H	1.52	0.74
1:E:263:GLU:HG2	1:E:422:HIS:CE1	2.22	0.74
1:A:349:SER:HB2	1:A:372:ASP:H	1.53	0.74
1:D:349:SER:HB2	1:D:372:ASP:H	1.53	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:349:SER:HB2	1:E:372:ASP:H	1.55	0.71
1:E:419:LEU:HA	1:E:422:HIS:HE1	1.56	0.69
1:B:429:GLU:HB2	1:B:430:LYS:HG2	1.73	0.69
1:D:344:GLN:HE22	1:D:633:LYS:N	1.92	0.67
1:B:251:LYS:HZ1	1:B:521:VAL:HB	1.61	0.66
1:D:240:LYS:NZ	1:D:611:GLU:OE1	2.25	0.65
1:A:429:GLU:HG3	1:A:430:LYS:CB	2.18	0.64
1:E:344:GLN:HE22	1:E:633:LYS:H	1.47	0.63
1:E:263:GLU:CD	1:E:422:HIS:NE2	2.57	0.63
1:E:344:GLN:NE2	1:E:633:LYS:H	1.96	0.62
1:E:419:LEU:HA	1:E:422:HIS:CE1	2.33	0.62
1:C:278:GLU:O	1:C:452:ARG:NH2	2.33	0.61
1:D:287:PHE:HD1	1:D:515:MET:HE2	1.66	0.61
1:C:355:ASN:HB2	1:C:419:LEU:HD11	1.83	0.60
1:E:355:ASN:HB2	1:E:419:LEU:HD11	1.83	0.60
1:D:230:VAL:HG23	1:D:231:THR:H	1.67	0.60
1:A:355:ASN:HB2	1:A:419:LEU:HD11	1.84	0.59
1:C:299:PHE:HB2	1:C:566:VAL:HG11	1.85	0.58
1:C:349:SER:HB2	1:C:372:ASP:H	1.68	0.58
1:E:567:PRO:HB3	1:E:608:VAL:HG13	1.85	0.57
1:A:299:PHE:HB2	1:A:566:VAL:HG11	1.86	0.56
1:B:384:GLU:H	1:B:384:GLU:CD	2.12	0.56
1:D:344:GLN:NE2	1:D:633:LYS:H	2.02	0.55
1:A:430:LYS:HB2	1:A:432:ALA:O	2.06	0.55
1:B:287:PHE:HD1	1:B:515:MET:HE2	1.72	0.55
1:D:389:ASN:OD1	1:D:390:TYR:N	2.38	0.55
1:D:567:PRO:CG	1:D:608:VAL:HG23	2.37	0.55
1:D:433:SER:OG	1:D:456:GLU:OE2	2.23	0.55
1:B:355:ASN:HB2	1:B:419:LEU:HD11	1.90	0.54
1:D:389:ASN:CG	1:D:390:TYR:HD1	2.15	0.54
1:D:261:HIS:CE1	1:D:481:ASP:HB3	2.43	0.54
1:B:430:LYS:HB3	1:B:432:ALA:O	2.09	0.53
1:D:569:ARG:HH11	1:D:612:LEU:HD13	1.73	0.53
1:B:567:PRO:HB3	1:B:608:VAL:HG13	1.91	0.53
1:D:575:THR:OG1	1:D:578:TYR:O	2.24	0.53
1:B:261:HIS:HB3	1:B:417:ILE:HA	1.90	0.53
1:B:437:ALA:HB3	1:B:445:ASP:HA	1.91	0.53
1:D:355:ASN:HB2	1:D:419:LEU:HD11	1.91	0.53
1:E:387:VAL:HG12	1:E:388:SER:O	2.09	0.52
1:B:379:TYR:CD2	1:B:644:LYS:HE2	2.44	0.52
1:E:263:GLU:HG2	1:E:422:HIS:NE2	2.25	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:TYR:CG	1:B:644:LYS:HE2	2.45	0.52
1:A:434:ILE:HB	1:A:452:ARG:HD2	1.92	0.52
1:C:261:HIS:CE1	1:C:481:ASP:HB3	2.45	0.52
1:C:441:ASP:OD2	1:C:489:HIS:ND1	2.41	0.51
1:E:287:PHE:HD2	1:E:515:MET:HE2	1.75	0.51
1:B:311:GLU:OE1	1:B:366:TYR:OH	2.23	0.51
1:C:575:THR:OG1	1:C:578:TYR:O	2.22	0.51
1:D:261:HIS:HB3	1:D:417:ILE:HA	1.92	0.51
1:E:575:THR:OG1	1:E:578:TYR:O	2.19	0.51
1:B:278:GLU:O	1:B:452:ARG:NH2	2.44	0.51
1:E:278:GLU:O	1:E:452:ARG:NH2	2.44	0.51
1:B:299:PHE:HB2	1:B:566:VAL:HG11	1.93	0.50
1:B:375:PHE:HD1	1:B:379:TYR:CD2	2.29	0.50
1:C:287:PHE:HD1	1:C:515:MET:HE2	1.77	0.50
1:D:278:GLU:O	1:D:452:ARG:NH2	2.44	0.50
1:E:299:PHE:HB2	1:E:566:VAL:HG11	1.94	0.49
1:A:567:PRO:HB3	1:A:608:VAL:HG13	1.95	0.49
1:C:357:LYS:HB2	1:C:363:ASP:HB2	1.93	0.49
1:A:261:HIS:CE1	1:A:481:ASP:HB3	2.48	0.49
1:A:332:GLN:NE2	1:A:364:GLU:OE2	2.45	0.49
1:E:261:HIS:HB3	1:E:417:ILE:HA	1.93	0.49
1:B:641:ASN:OD1	1:B:643:ASN:ND2	2.43	0.48
1:D:389:ASN:CG	1:D:390:TYR:CD1	2.91	0.48
1:A:370:GLY:O	1:E:599:LYS:NZ	2.46	0.47
1:A:415:LYS:HE3	1:A:417:ILE:HD11	1.96	0.47
1:A:429:GLU:HA	1:A:430:LYS:HA	1.50	0.47
1:A:238:LYS:CE	1:A:549:GLU:OE2	2.63	0.47
1:A:406:SER:OG	1:A:464:TYR:OH	2.28	0.47
1:C:567:PRO:HB3	1:C:608:VAL:HG13	1.95	0.47
1:E:433:SER:OG	1:E:456:GLU:OE2	2.24	0.47
1:A:340:ALA:O	1:A:344:GLN:HG2	2.15	0.47
1:B:518:VAL:O	1:B:521:VAL:HG12	2.15	0.47
1:B:375:PHE:HA	1:B:379:TYR:CD1	2.49	0.46
1:C:282:PHE:CG	1:C:459:LYS:HB2	2.50	0.46
1:A:261:HIS:HB3	1:A:417:ILE:HA	1.96	0.46
1:D:494:THR:HG23	1:D:500:ASP:HA	1.97	0.46
1:C:592:GLU:HA	1:C:593:PRO:HD3	1.81	0.46
1:A:287:PHE:HD1	1:A:515:MET:HE2	1.79	0.46
1:C:429:GLU:HA	1:C:430:LYS:HA	1.56	0.46
1:E:350:ALA:HB3	1:E:414:THR:HG22	1.97	0.46
1:B:399:LYS:HB2	1:B:399:LYS:HE3	1.55	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:537:PRO:HB3	1:C:547:ASN:HD21	1.81	0.46
1:E:287:PHE:CE2	1:E:294:SER:HB3	2.51	0.46
1:A:278:GLU:O	1:A:452:ARG:NH2	2.49	0.46
1:D:389:ASN:OD1	1:D:390:TYR:HD1	1.99	0.46
1:C:261:HIS:HB3	1:C:417:ILE:HA	1.98	0.45
1:D:429:GLU:HA	1:D:430:LYS:HA	1.53	0.45
1:E:434:ILE:HB	1:E:452:ARG:HD2	1.99	0.45
1:E:261:HIS:CE1	1:E:481:ASP:HB3	2.52	0.45
1:A:282:PHE:CD1	1:A:459:LYS:HG3	2.52	0.45
1:A:311:GLU:OE1	1:A:366:TYR:OH	2.24	0.45
1:B:261:HIS:CE1	1:B:481:ASP:HB3	2.52	0.45
1:C:529:TYR:HB2	1:C:564:GLN:HB3	1.99	0.45
1:D:341:ILE:HA	1:D:632:PHE:HE1	1.82	0.44
1:B:429:GLU:HA	1:B:430:LYS:HA	1.42	0.44
1:C:238:LYS:NZ	1:C:549:GLU:OE2	2.32	0.44
1:D:574:ILE:HD13	1:D:579:SER:HB3	1.99	0.44
1:B:521:VAL:HG22	1:B:522:GLN:N	2.33	0.44
1:E:263:GLU:CG	1:E:422:HIS:NE2	2.80	0.43
1:B:350:ALA:HB3	1:B:414:THR:HG22	1.99	0.43
1:B:433:SER:OG	1:B:456:GLU:OE2	2.30	0.43
1:D:481:ASP:OD1	1:D:481:ASP:N	2.51	0.43
1:E:406:SER:HG	1:E:464:TYR:HH	1.58	0.43
1:D:332:GLN:NE2	1:D:364:GLU:OE2	2.51	0.43
1:B:357:LYS:HB2	1:B:363:ASP:HB2	2.00	0.43
1:C:433:SER:OG	1:C:456:GLU:OE2	2.29	0.43
1:E:380:TYR:OH	1:E:401:SER:HB3	2.19	0.43
1:C:314:LEU:HG	1:C:535:LEU:HD23	2.01	0.43
1:A:529:TYR:HB2	1:A:564:GLN:HB3	2.00	0.42
1:E:600:GLU:H	1:E:600:GLU:CD	2.27	0.42
1:B:569:ARG:HA	1:B:569:ARG:HD2	1.80	0.42
1:B:250:GLY:HA2	1:B:544:GLY:CA	2.49	0.42
1:D:299:PHE:HB2	1:D:566:VAL:HG11	2.01	0.42
1:A:410:GLN:OE1	1:A:473:ASN:ND2	2.48	0.42
1:B:395:LYS:HB2	1:B:396:PRO:HD3	2.01	0.42
1:E:415:LYS:HE3	1:E:417:ILE:HD11	2.02	0.42
1:D:282:PHE:CD1	1:D:459:LYS:HG3	2.53	0.42
1:A:243:ALA:HA	1:A:244:PRO:HD3	1.94	0.42
1:D:287:PHE:CD1	1:D:515:MET:HE2	2.52	0.42
1:D:569:ARG:HD2	1:D:569:ARG:HA	1.86	0.42
1:C:287:PHE:CE1	1:C:294:SER:HB3	2.55	0.42
1:D:353:HIS:ND1	1:D:417:ILE:HB	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:243:ALA:HA	1:D:244:PRO:HD3	1.90	0.42
1:D:434:ILE:HB	1:D:452:ARG:HD2	2.02	0.42
1:D:415:LYS:HE3	1:D:417:ILE:HD11	2.02	0.41
1:E:240:LYS:HE3	1:E:611:GLU:OE1	2.19	0.41
1:B:321:LEU:HG	1:B:326:ALA:HB2	2.01	0.41
1:D:287:PHE:CE1	1:D:294:SER:HB3	2.55	0.41
1:E:230:VAL:HG13	1:E:231:THR:N	2.35	0.41
1:C:569:ARG:HA	1:C:569:ARG:HD2	1.76	0.41
1:C:556:ASP:HB3	1:C:559:SER:HB2	2.02	0.41
1:D:569:ARG:HH12	1:D:612:LEU:HD13	1.83	0.41
1:C:434:ILE:HB	1:C:452:ARG:HD2	2.02	0.41
1:B:255:LYS:HE2	1:B:519:PRO:HG2	2.03	0.41
1:B:232:GLU:H	1:B:232:GLU:HG3	1.64	0.41
1:E:437:ALA:HB3	1:E:445:ASP:HA	2.03	0.41
1:D:256:ASN:OD1	1:D:411:PRO:HA	2.21	0.41
1:E:410:GLN:HG2	1:E:412:PHE:CE2	2.56	0.41
1:C:481:ASP:OD1	1:C:481:ASP:N	2.48	0.41
1:D:256:ASN:HB2	1:D:474:SER:OG	2.21	0.41
1:E:479:TYR:HA	1:E:513:PRO:O	2.21	0.41
1:A:569:ARG:HD2	1:A:569:ARG:HA	1.78	0.40
1:C:395:LYS:HB2	1:C:396:PRO:HD3	2.03	0.40
1:C:560:LYS:HB3	1:C:560:LYS:HE2	1.82	0.40
1:B:479:TYR:HA	1:B:513:PRO:O	2.22	0.40
1:D:437:ALA:HB3	1:D:445:ASP:HA	2.04	0.40
1:D:600:GLU:H	1:D:600:GLU:CD	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	412/459 (90%)	401 (97%)	11 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	412/459 (90%)	398 (97%)	14 (3%)	0	100	100
1	C	412/459 (90%)	398 (97%)	14 (3%)	0	100	100
1	D	412/459 (90%)	397 (96%)	15 (4%)	0	100	100
1	E	412/459 (90%)	400 (97%)	12 (3%)	0	100	100
All	All	2060/2295 (90%)	1994 (97%)	66 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	A	363/403 (90%)	361 (99%)	2 (1%)	78	88
1	B	363/403 (90%)	359 (99%)	4 (1%)	65	83
1	C	363/403 (90%)	360 (99%)	3 (1%)	73	86
1	D	363/403 (90%)	358 (99%)	5 (1%)	59	80
1	E	363/403 (90%)	362 (100%)	1 (0%)	86	91
All	All	1815/2015 (90%)	1800 (99%)	15 (1%)	73	86

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	323	GLN
1	A	527	GLU
1	B	384	GLU
1	B	399	LYS
1	B	596	THR
1	B	644	LYS
1	C	290	GLN
1	C	399	LYS
1	C	563	LYS
1	D	233	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	422	HIS
1	D	603	GLU
1	D	606	GLU
1	D	634	LYS
1	E	430	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	291	ASN
1	A	449	GLN
1	A	506	ASN
1	B	344	GLN
1	B	422	HIS
1	B	449	GLN
1	B	473	ASN
1	B	506	ASN
1	C	344	GLN
1	C	449	GLN
1	C	506	ASN
1	C	541	HIS
1	C	589	GLN
1	D	344	GLN
1	D	506	ASN
1	E	235	ASN
1	E	345	GLN
1	E	589	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	TPO	E	307	2,1	8,10,11	1.12	0	10,14,16	2.09	1 (10%)
1	TPO	A	307	2,1	8,10,11	1.12	0	10,14,16	2.10	1 (10%)
1	TPO	D	307	2,1	8,10,11	1.08	0	10,14,16	2.24	1 (10%)
1	TPO	C	307	2,1	8,10,11	1.13	0	10,14,16	2.06	1 (10%)
1	TPO	B	307	2,1	8,10,11	1.10	0	10,14,16	2.08	1 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	E	307	2,1	-	2/9/11/13	-
1	TPO	A	307	2,1	-	2/9/11/13	-
1	TPO	D	307	2,1	-	2/9/11/13	-
1	TPO	C	307	2,1	-	2/9/11/13	-
1	TPO	B	307	2,1	-	2/9/11/13	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	307	TPO	P-OG1-CB	-6.47	105.75	123.33
1	E	307	TPO	P-OG1-CB	-6.09	106.77	123.33
1	A	307	TPO	P-OG1-CB	-6.06	106.85	123.33
1	B	307	TPO	P-OG1-CB	-6.02	106.98	123.33
1	C	307	TPO	P-OG1-CB	-5.91	107.28	123.33

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	307	TPO	O-C-CA-CB
1	B	307	TPO	O-C-CA-CB
1	C	307	TPO	O-C-CA-CB
1	D	307	TPO	O-C-CA-CB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	E	307	TPO	O-C-CA-CB
1	A	307	TPO	CB-OG1-P-O2P
1	B	307	TPO	CB-OG1-P-O2P
1	C	307	TPO	CB-OG1-P-O2P
1	D	307	TPO	CB-OG1-P-O2P
1	E	307	TPO	CB-OG1-P-O2P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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	414/459 (90%)	-0.32	5 (1%) 76 55	27, 42, 63, 84	0
1	B	414/459 (90%)	0.07	9 (2%) 62 39	24, 55, 82, 96	0
1	C	414/459 (90%)	-0.12	5 (1%) 76 55	33, 49, 70, 96	0
1	D	414/459 (90%)	0.03	8 (1%) 66 43	38, 54, 80, 102	0
1	E	414/459 (90%)	-0.32	4 (0%) 79 59	30, 44, 62, 84	0
All	All	2070/2295 (90%)	-0.13	31 (1%) 72 49	24, 48, 74, 102	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	230	VAL	6.0
1	C	230	VAL	5.9
1	E	230	VAL	5.4
1	A	230	VAL	4.8
1	B	230	VAL	4.3
1	D	608	VAL	3.5
1	B	633	LYS	3.0
1	E	422	HIS	2.7
1	D	614	LEU	2.6
1	B	432	ALA	2.6
1	E	613	GLU	2.6
1	A	630	ASP	2.6
1	D	635	VAL	2.6
1	A	390	TYR	2.5
1	B	430	LYS	2.5
1	D	231	THR	2.5
1	B	428	ASP	2.5
1	B	644	LYS	2.4
1	A	429	GLU	2.4
1	C	231	THR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	463	ASP	2.3
1	B	344	GLN	2.2
1	C	384	GLU	2.2
1	B	345	GLN	2.2
1	E	323	GLN	2.2
1	A	430	LYS	2.2
1	C	430	LYS	2.2
1	C	359	PHE	2.1
1	D	233	VAL	2.1
1	D	390	TYR	2.0
1	D	634	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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, 95th 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
1	TPO	C	307	11/12	0.95	0.08	41,49,60,69	0
1	TPO	B	307	11/12	0.97	0.07	27,45,51,58	0
1	TPO	D	307	11/12	0.97	0.07	42,55,61,64	0
1	TPO	A	307	11/12	0.98	0.07	33,44,57,60	0
1	TPO	E	307	11/12	0.98	0.06	41,46,54,60	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th 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	MG	C	1645	1/1	0.98	0.04	45,45,45,45	0
2	MG	B	1645	1/1	0.99	0.03	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	A	1645	1/1	0.99	0.03	40,40,40,40	0
2	MG	D	1645	1/1	0.99	0.04	53,53,53,53	0
2	MG	E	1645	1/1	0.99	0.03	48,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.