



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:33 AM UTC

PDB ID : 4JYX / pdb_00004jyx
Title : Crystal structure of polyprenyl synthase PATL_3739 (TARGET EFI-509195) FROM PSEUDOALTEROMONAS ATLANTICA, COMPLEX WITH INORGANIC PHOSPHATE AND AN UNKNOWN LIGAND
Authors : Patskovsky, Y.; Toro, R.; Bhosle, R.; Hillerich, B.; Seidel, R.D.; Washington, E.; Scott Glenn, A.; Chowdhury, S.; Evans, B.; Hammonds, J.; Zencheck, W.D.; Imker, H.J.; Al Obaidi, N.; Stead, M.; Love, J.; Poulter, C.D.; Gerlt, J.A.; Almo, S.C.; Enzyme Function Initiative (EFI)
Deposited on : 2013-04-01
Resolution : 2.30 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)

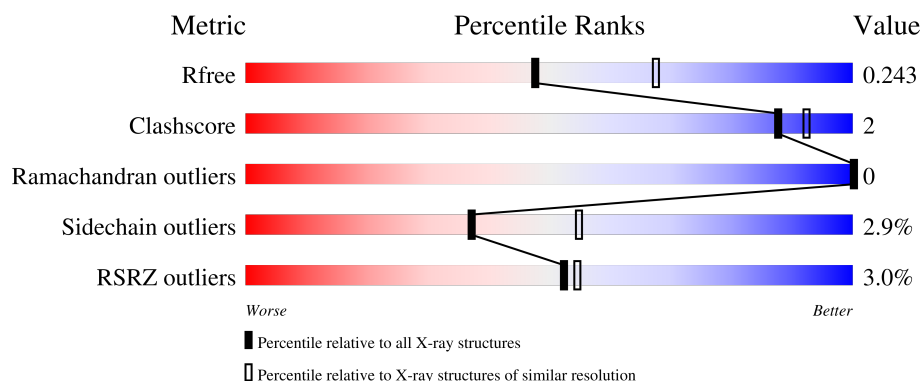
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	345	
1	B	345	
1	C	345	

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
1	D	345	4% 84% 7% 10%
1	E	345	4% 83% 7% 10%
1	F	345	4% 83% 8% 10%
1	G	345	2% 83% 8% 8%
1	H	345	3% 86% 6% 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20169 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 Trans-hexaprenyltranstransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	2	0
			2460	1539	409	496	16			
1	B	316	Total	C	N	O	S	0	0	0
			2445	1530	408	491	16			
1	C	311	Total	C	N	O	S	0	2	0
			2415	1522	396	483	14			
1	D	312	Total	C	N	O	S	0	0	0
			2411	1516	396	484	15			
1	E	310	Total	C	N	O	S	0	3	0
			2426	1526	397	489	14			
1	F	312	Total	C	N	O	S	0	1	0
			2415	1521	395	485	14			
1	G	317	Total	C	N	O	S	0	0	0
			2451	1533	409	493	16			
1	H	316	Total	C	N	O	S	0	3	0
			2463	1541	412	494	16			

There are 176 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP Q15PE7
A	-20	HIS	-	expression tag	UNP Q15PE7
A	-19	HIS	-	expression tag	UNP Q15PE7
A	-18	HIS	-	expression tag	UNP Q15PE7
A	-17	HIS	-	expression tag	UNP Q15PE7
A	-16	HIS	-	expression tag	UNP Q15PE7
A	-15	HIS	-	expression tag	UNP Q15PE7
A	-14	SER	-	expression tag	UNP Q15PE7
A	-13	SER	-	expression tag	UNP Q15PE7
A	-12	GLY	-	expression tag	UNP Q15PE7
A	-11	VAL	-	expression tag	UNP Q15PE7
A	-10	ASP	-	expression tag	UNP Q15PE7
A	-9	LEU	-	expression tag	UNP Q15PE7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	GLY	-	expression tag	UNP Q15PE7
A	-7	THR	-	expression tag	UNP Q15PE7
A	-6	GLU	-	expression tag	UNP Q15PE7
A	-5	ASN	-	expression tag	UNP Q15PE7
A	-4	LEU	-	expression tag	UNP Q15PE7
A	-3	TYR	-	expression tag	UNP Q15PE7
A	-2	PHE	-	expression tag	UNP Q15PE7
A	-1	GLN	-	expression tag	UNP Q15PE7
A	0	SER	-	expression tag	UNP Q15PE7
B	-21	MET	-	expression tag	UNP Q15PE7
B	-20	HIS	-	expression tag	UNP Q15PE7
B	-19	HIS	-	expression tag	UNP Q15PE7
B	-18	HIS	-	expression tag	UNP Q15PE7
B	-17	HIS	-	expression tag	UNP Q15PE7
B	-16	HIS	-	expression tag	UNP Q15PE7
B	-15	HIS	-	expression tag	UNP Q15PE7
B	-14	SER	-	expression tag	UNP Q15PE7
B	-13	SER	-	expression tag	UNP Q15PE7
B	-12	GLY	-	expression tag	UNP Q15PE7
B	-11	VAL	-	expression tag	UNP Q15PE7
B	-10	ASP	-	expression tag	UNP Q15PE7
B	-9	LEU	-	expression tag	UNP Q15PE7
B	-8	GLY	-	expression tag	UNP Q15PE7
B	-7	THR	-	expression tag	UNP Q15PE7
B	-6	GLU	-	expression tag	UNP Q15PE7
B	-5	ASN	-	expression tag	UNP Q15PE7
B	-4	LEU	-	expression tag	UNP Q15PE7
B	-3	TYR	-	expression tag	UNP Q15PE7
B	-2	PHE	-	expression tag	UNP Q15PE7
B	-1	GLN	-	expression tag	UNP Q15PE7
B	0	SER	-	expression tag	UNP Q15PE7
C	-21	MET	-	expression tag	UNP Q15PE7
C	-20	HIS	-	expression tag	UNP Q15PE7
C	-19	HIS	-	expression tag	UNP Q15PE7
C	-18	HIS	-	expression tag	UNP Q15PE7
C	-17	HIS	-	expression tag	UNP Q15PE7
C	-16	HIS	-	expression tag	UNP Q15PE7
C	-15	HIS	-	expression tag	UNP Q15PE7
C	-14	SER	-	expression tag	UNP Q15PE7
C	-13	SER	-	expression tag	UNP Q15PE7
C	-12	GLY	-	expression tag	UNP Q15PE7
C	-11	VAL	-	expression tag	UNP Q15PE7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	ASP	-	expression tag	UNP Q15PE7
C	-9	LEU	-	expression tag	UNP Q15PE7
C	-8	GLY	-	expression tag	UNP Q15PE7
C	-7	THR	-	expression tag	UNP Q15PE7
C	-6	GLU	-	expression tag	UNP Q15PE7
C	-5	ASN	-	expression tag	UNP Q15PE7
C	-4	LEU	-	expression tag	UNP Q15PE7
C	-3	TYR	-	expression tag	UNP Q15PE7
C	-2	PHE	-	expression tag	UNP Q15PE7
C	-1	GLN	-	expression tag	UNP Q15PE7
C	0	SER	-	expression tag	UNP Q15PE7
D	-21	MET	-	expression tag	UNP Q15PE7
D	-20	HIS	-	expression tag	UNP Q15PE7
D	-19	HIS	-	expression tag	UNP Q15PE7
D	-18	HIS	-	expression tag	UNP Q15PE7
D	-17	HIS	-	expression tag	UNP Q15PE7
D	-16	HIS	-	expression tag	UNP Q15PE7
D	-15	HIS	-	expression tag	UNP Q15PE7
D	-14	SER	-	expression tag	UNP Q15PE7
D	-13	SER	-	expression tag	UNP Q15PE7
D	-12	GLY	-	expression tag	UNP Q15PE7
D	-11	VAL	-	expression tag	UNP Q15PE7
D	-10	ASP	-	expression tag	UNP Q15PE7
D	-9	LEU	-	expression tag	UNP Q15PE7
D	-8	GLY	-	expression tag	UNP Q15PE7
D	-7	THR	-	expression tag	UNP Q15PE7
D	-6	GLU	-	expression tag	UNP Q15PE7
D	-5	ASN	-	expression tag	UNP Q15PE7
D	-4	LEU	-	expression tag	UNP Q15PE7
D	-3	TYR	-	expression tag	UNP Q15PE7
D	-2	PHE	-	expression tag	UNP Q15PE7
D	-1	GLN	-	expression tag	UNP Q15PE7
D	0	SER	-	expression tag	UNP Q15PE7
E	-21	MET	-	expression tag	UNP Q15PE7
E	-20	HIS	-	expression tag	UNP Q15PE7
E	-19	HIS	-	expression tag	UNP Q15PE7
E	-18	HIS	-	expression tag	UNP Q15PE7
E	-17	HIS	-	expression tag	UNP Q15PE7
E	-16	HIS	-	expression tag	UNP Q15PE7
E	-15	HIS	-	expression tag	UNP Q15PE7
E	-14	SER	-	expression tag	UNP Q15PE7
E	-13	SER	-	expression tag	UNP Q15PE7

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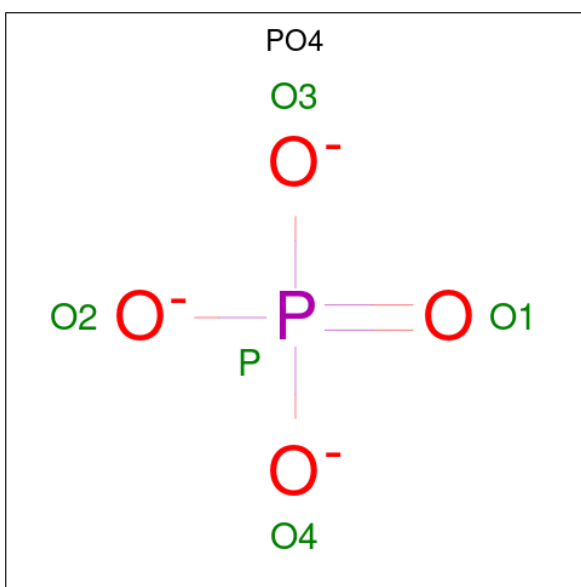
Chain	Residue	Modelled	Actual	Comment	Reference
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E	-11	VAL	-	expression tag	UNP Q15PE7
E	-10	ASP	-	expression tag	UNP Q15PE7
E	-9	LEU	-	expression tag	UNP Q15PE7
E	-8	GLY	-	expression tag	UNP Q15PE7
E	-7	THR	-	expression tag	UNP Q15PE7
E	-6	GLU	-	expression tag	UNP Q15PE7
E	-5	ASN	-	expression tag	UNP Q15PE7
E	-4	LEU	-	expression tag	UNP Q15PE7
E	-3	TYR	-	expression tag	UNP Q15PE7
E	-2	PHE	-	expression tag	UNP Q15PE7
E	-1	GLN	-	expression tag	UNP Q15PE7
E	0	SER	-	expression tag	UNP Q15PE7
F	-21	MET	-	expression tag	UNP Q15PE7
F	-20	HIS	-	expression tag	UNP Q15PE7
F	-19	HIS	-	expression tag	UNP Q15PE7
F	-18	HIS	-	expression tag	UNP Q15PE7
F	-17	HIS	-	expression tag	UNP Q15PE7
F	-16	HIS	-	expression tag	UNP Q15PE7
F	-15	HIS	-	expression tag	UNP Q15PE7
F	-14	SER	-	expression tag	UNP Q15PE7
F	-13	SER	-	expression tag	UNP Q15PE7
F	-12	GLY	-	expression tag	UNP Q15PE7
F	-11	VAL	-	expression tag	UNP Q15PE7
F	-10	ASP	-	expression tag	UNP Q15PE7
F	-9	LEU	-	expression tag	UNP Q15PE7
F	-8	GLY	-	expression tag	UNP Q15PE7
F	-7	THR	-	expression tag	UNP Q15PE7
F	-6	GLU	-	expression tag	UNP Q15PE7
F	-5	ASN	-	expression tag	UNP Q15PE7
F	-4	LEU	-	expression tag	UNP Q15PE7
F	-3	TYR	-	expression tag	UNP Q15PE7
F	-2	PHE	-	expression tag	UNP Q15PE7
F	-1	GLN	-	expression tag	UNP Q15PE7
F	0	SER	-	expression tag	UNP Q15PE7
G	-21	MET	-	expression tag	UNP Q15PE7
G	-20	HIS	-	expression tag	UNP Q15PE7
G	-19	HIS	-	expression tag	UNP Q15PE7
G	-18	HIS	-	expression tag	UNP Q15PE7
G	-17	HIS	-	expression tag	UNP Q15PE7
G	-16	HIS	-	expression tag	UNP Q15PE7
G	-15	HIS	-	expression tag	UNP Q15PE7

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-14	SER	-	expression tag	UNP Q15PE7
G	-13	SER	-	expression tag	UNP Q15PE7
G	-12	GLY	-	expression tag	UNP Q15PE7
G	-11	VAL	-	expression tag	UNP Q15PE7
G	-10	ASP	-	expression tag	UNP Q15PE7
G	-9	LEU	-	expression tag	UNP Q15PE7
G	-8	GLY	-	expression tag	UNP Q15PE7
G	-7	THR	-	expression tag	UNP Q15PE7
G	-6	GLU	-	expression tag	UNP Q15PE7
G	-5	ASN	-	expression tag	UNP Q15PE7
G	-4	LEU	-	expression tag	UNP Q15PE7
G	-3	TYR	-	expression tag	UNP Q15PE7
G	-2	PHE	-	expression tag	UNP Q15PE7
G	-1	GLN	-	expression tag	UNP Q15PE7
G	0	SER	-	expression tag	UNP Q15PE7
H	-21	MET	-	expression tag	UNP Q15PE7
H	-20	HIS	-	expression tag	UNP Q15PE7
H	-19	HIS	-	expression tag	UNP Q15PE7
H	-18	HIS	-	expression tag	UNP Q15PE7
H	-17	HIS	-	expression tag	UNP Q15PE7
H	-16	HIS	-	expression tag	UNP Q15PE7
H	-15	HIS	-	expression tag	UNP Q15PE7
H	-14	SER	-	expression tag	UNP Q15PE7
H	-13	SER	-	expression tag	UNP Q15PE7
H	-12	GLY	-	expression tag	UNP Q15PE7
H	-11	VAL	-	expression tag	UNP Q15PE7
H	-10	ASP	-	expression tag	UNP Q15PE7
H	-9	LEU	-	expression tag	UNP Q15PE7
H	-8	GLY	-	expression tag	UNP Q15PE7
H	-7	THR	-	expression tag	UNP Q15PE7
H	-6	GLU	-	expression tag	UNP Q15PE7
H	-5	ASN	-	expression tag	UNP Q15PE7
H	-4	LEU	-	expression tag	UNP Q15PE7
H	-3	TYR	-	expression tag	UNP Q15PE7
H	-2	PHE	-	expression tag	UNP Q15PE7
H	-1	GLN	-	expression tag	UNP Q15PE7
H	0	SER	-	expression tag	UNP Q15PE7

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	G	1	Total	O	P	0	0
			5	4	1		
2	G	1	Total	O	P	0	0
			5	4	1		
2	H	1	Total	O	P	0	0
			5	4	1		
2	H	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 8 7 1	0	0
3	B	1	Total C N 8 7 1	0	0
3	G	1	Total C N 8 7 1	0	0
3	H	1	Total C N 8 7 1	0	0

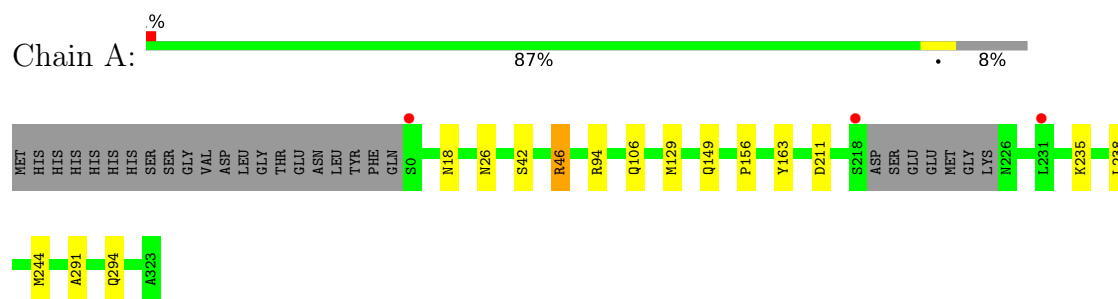
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	100	Total O 100 100	0	0
4	B	97	Total O 97 97	0	0
4	C	63	Total O 63 63	0	0
4	D	84	Total O 84 84	0	0
4	E	44	Total O 44 44	0	0
4	F	59	Total O 59 59	0	0
4	G	76	Total O 76 76	0	0
4	H	63	Total O 63 63	0	0

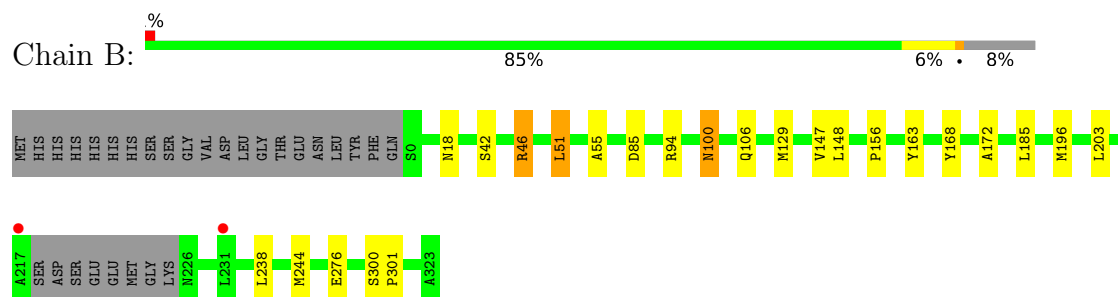
3 Residue-property plots [i](#)

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.

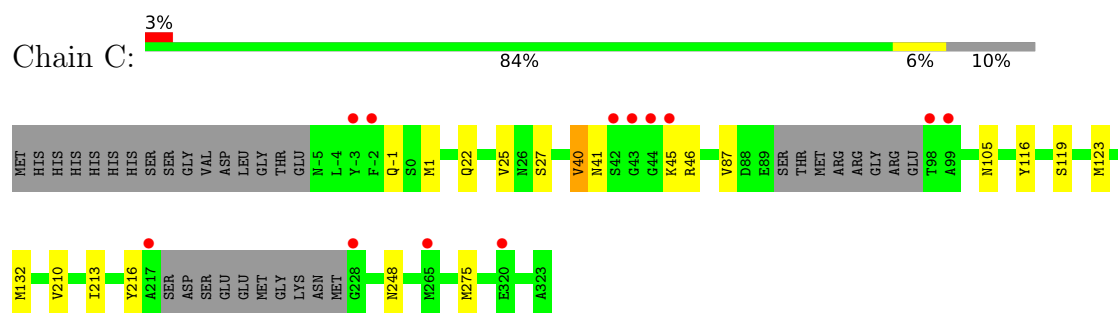
- Molecule 1: Trans-hexaprenyltranstransferase



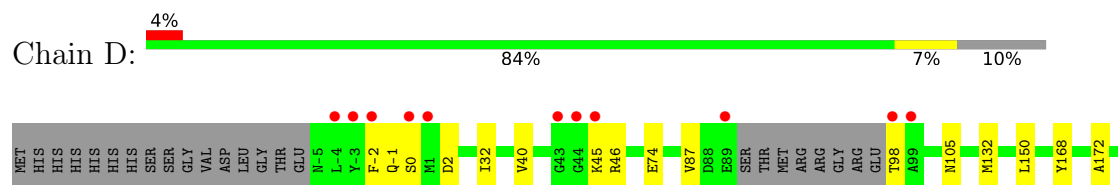
- Molecule 1: Trans-hexaprenyltranstransferase

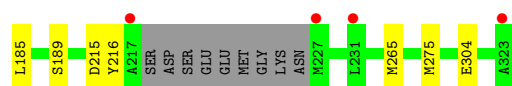


- Molecule 1: Trans-hexaprenyltranstransferase

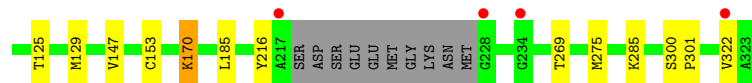
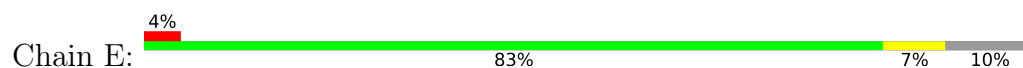


- Molecule 1: Trans-hexaprenyltranstransferase

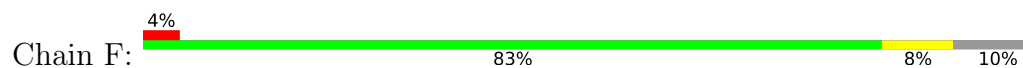




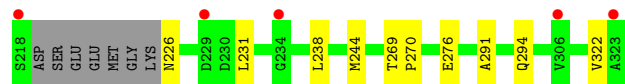
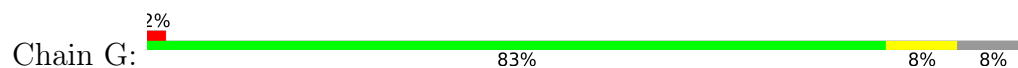
- Molecule 1: Trans-hexaprenyltranstransferase



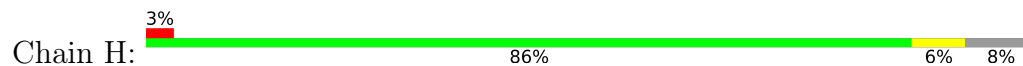
- Molecule 1: Trans-hexaprenyltranstransferase



- Molecule 1: Trans-hexaprenyltranstransferase



- Molecule 1: Trans-hexaprenyltranstransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.10Å 152.91Å 284.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.40 – 2.30 48.40 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.40-2.30) 99.6 (48.40-2.30)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.177 , 0.239 0.185 , 0.243	Depositor DCC
R_{free} test set	4257 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å ²)	35.6	Xtriage
Anisotropy	0.664	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	20169	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.66 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.4507e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: UNL, PO4

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	0.47	0/2497	0.74	0/3384
1	B	0.47	0/2476	0.74	0/3356
1	C	0.45	0/2453	0.74	0/3327
1	D	0.44	0/2442	0.78	2/3312 (0.1%)
1	E	0.42	0/2457	0.71	0/3332
1	F	0.44	0/2450	0.72	0/3324
1	G	0.46	0/2482	0.73	0/3364
1	H	0.43	0/2503	0.75	0/3392
All	All	0.45	0/19760	0.74	2/26791 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	-2	PHE	N-CA-C	7.91	119.98	111.36
1	D	-1	GLN	N-CA-C	7.58	119.19	111.07

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	2460	0	2445	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2445	0	2429	16	0
1	C	2415	0	2401	8	0
1	D	2411	0	2389	9	0
1	E	2426	0	2398	11	0
1	F	2415	0	2390	9	0
1	G	2451	0	2434	14	0
1	H	2463	0	2452	10	0
2	A	15	0	0	0	0
2	B	10	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	10	0	0	0	0
2	H	10	0	0	0	0
3	A	8	0	0	0	0
3	B	8	0	0	0	0
3	G	8	0	0	0	0
3	H	8	0	0	0	0
4	A	100	0	0	2	0
4	B	97	0	0	0	0
4	C	63	0	0	1	0
4	D	84	0	0	0	0
4	E	44	0	0	0	0
4	F	59	0	0	1	0
4	G	76	0	0	0	0
4	H	63	0	0	1	0
All	All	20169	0	19338	79	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 2.

All (79) 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:A:149:GLN:HE21	1:A:235:LYS:NZ	1.86	0.73
1:A:149:GLN:HE21	1:A:235:LYS:HZ3	1.41	0.69
1:A:42:SER:OG	1:A:94:ARG:NH1	2.25	0.69
1:D:87:VAL:H	1:D:105:ASN:HD21	1.44	0.66
1:A:18:ASN:OD1	1:A:46:ARG:NH2	2.32	0.63
1:F:129:MET:N	1:G:129:MET:HE1	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:LEU:HD11	1:B:203:LEU:CD2	2.31	0.60
1:G:24:GLN:HG2	1:G:122:MET:SD	2.41	0.60
1:C:87:VAL:H	1:C:105:ASN:HD21	1.50	0.60
1:A:235:LYS:HE3	4:A:555:HOH:O	2.02	0.60
1:B:55:ALA:HB1	1:B:196:MET:CE	2.32	0.59
1:B:156:PRO:O	1:B:244:MET:HE1	2.04	0.58
1:A:235:LYS:NZ	4:A:593:HOH:O	2.37	0.58
1:B:42:SER:OG	1:B:94:ARG:NH1	2.31	0.57
1:A:149:GLN:NE2	1:A:235:LYS:CE	2.68	0.55
1:B:18:ASN:OD1	1:B:46:ARG:NH2	2.39	0.55
1:E:129:MET:N	1:H:129:MET:HE1	2.22	0.54
1:F:216:TYR:CE1	1:F:275:MET:HE1	2.43	0.53
1:G:231:LEU:C	1:G:231:LEU:HD23	2.34	0.52
1:B:100:ASN:HD22	1:B:100:ASN:H	1.58	0.52
1:A:149:GLN:HE22	1:A:235:LYS:HE2	1.74	0.52
1:H:163:TYR:OH	1:H:212:ASP:OD2	2.21	0.52
1:A:149:GLN:NE2	1:A:235:LYS:HE2	2.24	0.51
1:D:189:SER:HB2	1:G:125:THR:HG22	1.93	0.51
1:E:24:GLN:HG2	1:E:122:MET:HE3	1.92	0.50
1:A:149:GLN:NE2	1:A:235:LYS:NZ	2.56	0.50
1:G:42:SER:OG	1:G:94:ARG:NH1	2.44	0.50
1:F:269:THR:HB	1:F:270:PRO:HD3	1.93	0.49
1:B:51:LEU:HD11	1:B:203:LEU:HD21	1.94	0.48
1:C:119:SER:O	1:C:123:MET:HG3	2.13	0.48
1:A:156:PRO:O	1:A:244:MET:HE1	2.12	0.48
1:B:129:MET:HE1	1:D:132:MET:CG	2.43	0.48
1:F:254:ILE:HG23	1:F:267:ASN:HD22	1.76	0.48
1:B:85:ASP:HB3	1:B:100:ASN:HD21	1.78	0.48
1:D:168:TYR:HA	1:D:172:ALA:HB3	1.96	0.48
1:H:156:PRO:O	1:H:244:MET:HE1	2.14	0.47
1:B:163:TYR:CE2	1:B:238:LEU:HB2	2.50	0.47
1:F:289:LEU:HD23	1:F:319:VAL:HG21	1.97	0.46
1:G:81:LEU:HD22	1:G:93:ARG:CZ	2.46	0.46
1:F:163:TYR:OH	1:F:212:ASP:OD2	2.32	0.45
1:B:106:GLN:HG2	1:D:150:LEU:HD13	1.98	0.45
1:H:39:ILE:HD11	1:H:81:LEU:HD22	1.97	0.45
1:H:265:MET:HB2	4:H:549:HOH:O	2.15	0.44
1:B:300:SER:HB2	1:B:301:PRO:HD3	1.99	0.44
1:B:129:MET:HE1	1:D:132:MET:HG2	1.99	0.44
1:G:163:TYR:CE2	1:G:238:LEU:HB2	2.53	0.44
1:C:45[A]:LYS:NZ	4:C:562:HOH:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:71:ALA:HB1	1:E:122:MET:HE1	2.00	0.43
1:E:216:TYR:CE1	1:E:275:MET:HE1	2.53	0.43
1:B:168:TYR:HA	1:B:172:ALA:HB3	2.01	0.43
1:B:147:VAL:HG11	1:D:32:ILE:HG13	2.00	0.43
1:C:25:VAL:HG21	1:C:40:VAL:HG21	2.00	0.43
1:E:106:GLN:HG2	1:H:87:VAL:HG13	2.01	0.43
1:A:129:MET:HE1	1:C:132:MET:CG	2.48	0.43
1:E:32:ILE:HG13	1:H:147:VAL:HG11	2.01	0.43
1:H:291:ALA:HA	1:H:294:GLN:HE21	1.84	0.43
1:C:248:ASN:C	1:C:248:ASN:OD1	2.61	0.42
1:D:45:LYS:HG2	1:D:74:GLU:HG2	2.01	0.42
1:G:156:PRO:O	1:G:244:MET:HE1	2.19	0.42
1:D:216:TYR:CE1	1:D:275:MET:HE1	2.54	0.42
1:E:84:ASP:OD2	1:E:170:LYS:NZ	2.52	0.42
1:G:291:ALA:HA	1:G:294:GLN:HE21	1.85	0.42
1:A:163:TYR:CE2	1:A:238:LEU:HB2	2.55	0.42
1:B:100:ASN:H	1:B:100:ASN:ND2	2.17	0.41
1:C:216:TYR:CE1	1:C:275:MET:HE1	2.56	0.41
1:F:285:LYS:HG2	1:F:322:VAL:HG13	2.02	0.41
1:G:269:THR:HB	1:G:270:PRO:HD3	2.02	0.41
1:F:147:VAL:HG11	1:G:32:ILE:HG13	2.03	0.41
1:G:168:TYR:HA	1:G:172:ALA:HB3	2.03	0.41
1:E:122:MET:O	1:E:125:THR:OG1	2.35	0.41
4:F:537:HOH:O	1:G:146:GLU:HG3	2.21	0.40
1:G:35:LEU:HD22	1:G:111:VAL:HG11	2.03	0.40
1:A:291:ALA:HA	1:A:294:GLN:HE21	1.86	0.40
1:E:300:SER:N	1:E:301:PRO:HD2	2.36	0.40
1:H:81:LEU:HD21	1:H:93:ARG:CD	2.52	0.40
1:C:210:VAL:HA	1:C:213:ILE:HD12	2.03	0.40
1:E:147:VAL:HG11	1:H:32:ILE:HG13	2.03	0.40
1:E:285:LYS:HG2	1:E:322:VAL:HG13	2.03	0.40
1:F:71:ALA:CB	1:F:122:MET:HE1	2.51	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	315/345 (91%)	312 (99%)	3 (1%)	0	100	100
1	B	312/345 (90%)	306 (98%)	6 (2%)	0	100	100
1	C	307/345 (89%)	303 (99%)	4 (1%)	0	100	100
1	D	306/345 (89%)	301 (98%)	5 (2%)	0	100	100
1	E	305/345 (88%)	298 (98%)	7 (2%)	0	100	100
1	F	307/345 (89%)	303 (99%)	4 (1%)	0	100	100
1	G	313/345 (91%)	311 (99%)	2 (1%)	0	100	100
1	H	315/345 (91%)	311 (99%)	4 (1%)	0	100	100
All	All	2480/2760 (90%)	2445 (99%)	35 (1%)	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	270/293 (92%)	266 (98%)	4 (2%)	57	75
1	B	267/293 (91%)	261 (98%)	6 (2%)	45	65
1	C	264/293 (90%)	256 (97%)	8 (3%)	36	53
1	D	263/293 (90%)	254 (97%)	9 (3%)	32	49
1	E	265/293 (90%)	255 (96%)	10 (4%)	29	44
1	F	263/293 (90%)	252 (96%)	11 (4%)	26	40
1	G	268/293 (92%)	262 (98%)	6 (2%)	45	65
1	H	270/293 (92%)	262 (97%)	8 (3%)	36	53
All	All	2130/2344 (91%)	2068 (97%)	62 (3%)	37	55

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	46	ARG
1	A	106	GLN
1	A	211	ASP
1	B	46	ARG
1	B	51	LEU
1	B	100	ASN
1	B	148	LEU
1	B	185	LEU
1	B	276	GLU
1	C	-1	GLN
1	C	1	MET
1	C	22	GLN
1	C	27	SER
1	C	40	VAL
1	C	41	ASN
1	C	46	ARG
1	C	116	TYR
1	D	0	SER
1	D	2	ASP
1	D	40	VAL
1	D	46	ARG
1	D	98	THR
1	D	185	LEU
1	D	215	ASP
1	D	265	MET
1	D	304	GLU
1	E	-4	LEU
1	E	2	ASP
1	E	15	LEU
1	E	27	SER
1	E	100	ASN
1	E	116	TYR
1	E	153	CYS
1	E	170	LYS
1	E	185	LEU
1	E	269	THR
1	F	-1	GLN
1	F	22	GLN
1	F	40	VAL
1	F	45	LYS
1	F	46	ARG
1	F	116	TYR

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Mol	Chain	Res	Type
1	F	133	GLN
1	F	211	ASP
1	F	276	GLU
1	F	304[A]	GLU
1	F	304[B]	GLU
1	G	20	LEU
1	G	27	SER
1	G	211	ASP
1	G	226	ASN
1	G	276	GLU
1	G	322	VAL
1	H	46	ARG
1	H	148	LEU
1	H	185	LEU
1	H	211	ASP
1	H	229	ASP
1	H	265	MET
1	H	276	GLU
1	H	322	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	22	GLN
1	A	34	GLN
1	A	106	GLN
1	A	149	GLN
1	A	194	ASN
1	A	294	GLN
1	B	100	ASN
1	B	105	ASN
1	B	106	GLN
1	B	194	ASN
1	C	19	GLN
1	C	24	GLN
1	C	105	ASN
1	C	194	ASN
1	C	250	GLN
1	C	267	ASN
1	D	19	GLN
1	D	24	GLN

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Mol	Chain	Res	Type
1	D	65	GLN
1	D	105	ASN
1	D	149	GLN
1	D	152	ASN
1	D	194	ASN
1	D	267	ASN
1	D	294	GLN
1	E	-1	GLN
1	E	5	HIS
1	E	24	GLN
1	E	152	ASN
1	E	194	ASN
1	F	-5	ASN
1	F	-1	GLN
1	F	19	GLN
1	F	22	GLN
1	F	65	GLN
1	F	133	GLN
1	F	152	ASN
1	F	263	ASN
1	F	267	ASN
1	G	34	GLN
1	G	194	ASN
1	G	226	ASN
1	G	294	GLN
1	H	19	GLN
1	H	65	GLN
1	H	194	ASN
1	H	263	ASN
1	H	294	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

Of 17 ligands modelled in this entry, 4 are unknown - leaving 13 for Mogul analysis.

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	PO4	C	401	-	4,4,4	0.89	0	6,6,6	0.54	0
2	PO4	G	402	-	4,4,4	0.94	0	6,6,6	0.48	0
2	PO4	H	402	-	4,4,4	0.91	0	6,6,6	0.56	0
2	PO4	E	401	-	4,4,4	0.89	0	6,6,6	0.51	0
2	PO4	G	401	-	4,4,4	0.90	0	6,6,6	0.65	0
2	PO4	H	401	-	4,4,4	0.99	0	6,6,6	0.59	0
2	PO4	B	401	-	4,4,4	0.92	0	6,6,6	0.57	0
2	PO4	F	401	-	4,4,4	0.86	0	6,6,6	0.56	0
2	PO4	A	402	-	4,4,4	0.91	0	6,6,6	0.58	0
2	PO4	B	402	-	4,4,4	0.95	0	6,6,6	0.46	0
2	PO4	D	401	-	4,4,4	0.92	0	6,6,6	0.52	0
2	PO4	A	401	-	4,4,4	0.91	0	6,6,6	0.80	0
2	PO4	A	403	-	4,4,4	0.95	0	6,6,6	0.47	0

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 ⓘ

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	317/345 (91%)	-0.26	3 (0%) 81 82	22, 40, 71, 107	2 (0%)
1	B	316/345 (91%)	-0.22	2 (0%) 85 86	26, 42, 70, 98	0
1	C	311/345 (90%)	0.00	12 (3%) 43 45	20, 46, 86, 120	2 (0%)
1	D	312/345 (90%)	0.03	15 (4%) 35 37	25, 46, 96, 143	0
1	E	310/345 (89%)	0.11	14 (4%) 38 40	22, 50, 91, 131	3 (0%)
1	F	312/345 (90%)	0.10	13 (4%) 40 42	26, 49, 89, 125	1 (0%)
1	G	317/345 (91%)	0.01	6 (1%) 66 68	29, 45, 76, 106	0
1	H	316/345 (91%)	0.17	10 (3%) 50 52	30, 51, 80, 104	3 (0%)
All	All	2511/2760 (90%)	-0.01	75 (2%) 52 54	20, 46, 83, 143	11 (0%)

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	-3	TYR	5.8
1	G	0	SER	4.7
1	D	-4	LEU	4.6
1	C	45[A]	LYS	4.5
1	D	-3	TYR	4.3
1	D	45	LYS	4.2
1	D	98	THR	4.1
1	F	218	SER	3.9
1	A	218	SER	3.9
1	F	45	LYS	3.6
1	F	322	VAL	3.6
1	F	44	GLY	3.6
1	E	43	GLY	3.4
1	E	228	GLY	3.4
1	G	218	SER	3.4
1	E	98	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	1	MET	3.3
1	F	98	THR	3.3
1	F	103	PHE	3.2
1	B	217	ALA	3.2
1	F	89	GLU	3.2
1	E	-4	LEU	3.2
1	H	321[A]	ARG	3.2
1	H	218	SER	3.0
1	F	228	GLY	3.0
1	E	-2	PHE	2.9
1	A	0	SER	2.8
1	D	-2	PHE	2.8
1	D	43	GLY	2.8
1	C	217	ALA	2.8
1	E	45	LYS	2.7
1	D	217	ALA	2.7
1	D	1	MET	2.7
1	H	228	GLY	2.6
1	G	306	VAL	2.6
1	D	231	LEU	2.5
1	C	44	GLY	2.5
1	H	148	LEU	2.5
1	H	265	MET	2.5
1	F	100	ASN	2.5
1	E	322	VAL	2.5
1	H	5	HIS	2.5
1	C	-3	TYR	2.5
1	D	0	SER	2.4
1	G	234	GLY	2.4
1	D	89	GLU	2.4
1	E	234	GLY	2.4
1	D	227	MET	2.4
1	C	98	THR	2.4
1	E	42	SER	2.4
1	C	320	GLU	2.4
1	C	228	GLY	2.3
1	E	217	ALA	2.3
1	H	323	ALA	2.3
1	C	265	MET	2.3
1	E	-1	GLN	2.3
1	F	43	GLY	2.3
1	C	43	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	229	ASP	2.2
1	H	229	ASP	2.2
1	C	-2	PHE	2.2
1	D	44	GLY	2.2
1	C	42	SER	2.2
1	F	231	LEU	2.2
1	E	100	ASN	2.2
1	G	323	ALA	2.2
1	B	231	LEU	2.2
1	F	-5	ASN	2.1
1	C	99	ALA	2.1
1	D	99	ALA	2.1
1	D	323	ALA	2.1
1	F	99	ALA	2.0
1	H	306	VAL	2.0
1	H	227	MET	2.0
1	A	231	LEU	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 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($\text{\AA}^2$)	Q<0.9
2	PO4	A	402	5/5	0.74	0.12	68,76,97,152	0
2	PO4	H	402	5/5	0.81	0.09	53,61,99,122	0
2	PO4	D	401	5/5	0.85	0.10	48,51,78,140	0
2	PO4	A	403	5/5	0.85	0.10	43,126,139,170	0
2	PO4	E	401	5/5	0.86	0.08	51,67,99,113	0
2	PO4	B	402	5/5	0.86	0.09	72,79,93,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PO4	F	401	5/5	0.88	0.08	48,62,102,111	0
2	PO4	G	402	5/5	0.89	0.08	59,79,103,137	0
2	PO4	C	401	5/5	0.89	0.10	63,63,79,82	0
3	UNL	B	403	8/-	0.89	0.16	33,40,49,52	0
3	UNL	A	404	8/-	0.92	0.17	45,45,62,64	0
3	UNL	G	403	8/-	0.92	0.16	43,53,66,74	0
3	UNL	H	403	8/-	0.94	0.16	40,53,59,66	0
2	PO4	G	401	5/5	0.96	0.08	47,47,56,60	0
2	PO4	H	401	5/5	0.97	0.07	44,55,66,72	0
2	PO4	A	401	5/5	0.97	0.07	40,44,53,55	0
2	PO4	B	401	5/5	0.98	0.07	35,42,54,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.