Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 06:06 PM EDT

PDB ID	:	6SXN
Title	:	Crystal structure of P212121 apo form of CrtE
Authors	:	Feng, Y.; Morgan, R.M.L.; Nixon, P.J.
Deposited on	:	2019-09-26
Resolution	:	2.66 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:

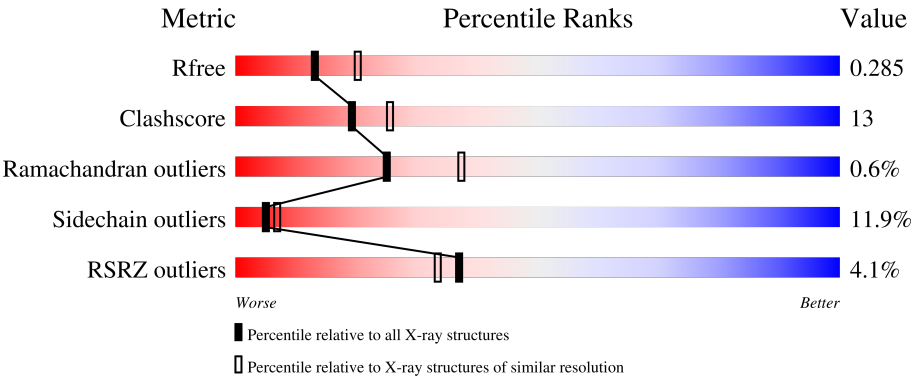
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.66 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	267	3% 76% 20% .
2	B	259	% 76% 20% .
3	C	258	2% 76% 21% .
4	D	267	7% 77% 20% .
5	E	259	7% 73% 23% .

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Mol	Chain	Length	Quality of chain
6	F	253	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 11367 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 Geranylgeranyl pyrophosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	267	1931	1221	328	371	11	0	0	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	THR	deletion	UNP B1XJV9
A	?	-	ALA	deletion	UNP B1XJV9
A	?	-	THR	deletion	UNP B1XJV9
A	?	-	ALA	deletion	UNP B1XJV9
A	?	-	GLU	deletion	UNP B1XJV9
A	?	-	GLU	deletion	UNP B1XJV9
A	?	-	LEU	deletion	UNP B1XJV9
A	?	-	GLY	deletion	UNP B1XJV9
A	?	-	LYS	deletion	UNP B1XJV9
A	?	-	THR	deletion	UNP B1XJV9
A	?	-	ALA	deletion	UNP B1XJV9
A	?	-	GLY	deletion	UNP B1XJV9
A	?	-	LYS	deletion	UNP B1XJV9
A	?	-	ASP	deletion	UNP B1XJV9
A	?	-	LEU	deletion	UNP B1XJV9
A	?	-	GLU	deletion	UNP B1XJV9
A	?	-	ALA	deletion	UNP B1XJV9
A	?	-	GLN	deletion	UNP B1XJV9
A	?	-	LYS	deletion	UNP B1XJV9
A	?	-	SER	deletion	UNP B1XJV9
A	?	-	LEU	deletion	UNP B1XJV9
A	?	-	TRP	deletion	UNP B1XJV9
A	?	-	GLY	deletion	UNP B1XJV9
A	?	-	ILE	deletion	UNP B1XJV9
A	?	-	GLU	deletion	UNP B1XJV9
A	300	ALA	-	expression tag	UNP B1XJV9

- Molecule 2 is a protein called Geranylgeranyl pyrophosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	259	Total	C	N	O	S	0	0	0
			1884	1192	319	362	11			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLY	deletion	UNP B1XJV9
B	?	-	LYS	deletion	UNP B1XJV9
B	258	SER	ASP	conflict	UNP B1XJV9
B	?	-	ILE	deletion	UNP B1XJV9
B	?	-	THR	deletion	UNP B1XJV9
B	?	-	ALA	deletion	UNP B1XJV9
B	?	-	THR	deletion	UNP B1XJV9
B	?	-	ALA	deletion	UNP B1XJV9
B	?	-	GLU	deletion	UNP B1XJV9
B	?	-	GLU	deletion	UNP B1XJV9
B	?	-	LEU	deletion	UNP B1XJV9
B	?	-	GLY	deletion	UNP B1XJV9
B	?	-	LYS	deletion	UNP B1XJV9
B	?	-	THR	deletion	UNP B1XJV9
B	?	-	ALA	deletion	UNP B1XJV9
B	?	-	GLY	deletion	UNP B1XJV9
B	?	-	LYS	deletion	UNP B1XJV9
B	?	-	ASP	deletion	UNP B1XJV9
B	?	-	LEU	deletion	UNP B1XJV9
B	?	-	GLU	deletion	UNP B1XJV9
B	?	-	ALA	deletion	UNP B1XJV9
B	?	-	GLN	deletion	UNP B1XJV9
B	?	-	LYS	deletion	UNP B1XJV9
B	?	-	VAL	deletion	UNP B1XJV9
B	?	-	THR	deletion	UNP B1XJV9
B	?	-	TYR	deletion	UNP B1XJV9
B	?	-	PRO	deletion	UNP B1XJV9
B	?	-	SER	deletion	UNP B1XJV9
B	?	-	LEU	deletion	UNP B1XJV9
B	?	-	TRP	deletion	UNP B1XJV9
B	?	-	GLY	deletion	UNP B1XJV9
B	259	LEU	ILE	conflict	UNP B1XJV9

- Molecule 3 is a protein called Geranylgeranyl pyrophosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	258	Total	C	N	O	S	0	0	0
			1877	1187	318	361	11			

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	LYS	deletion	UNP B1XJV9
C	?	-	THR	deletion	UNP B1XJV9
C	?	-	ASP	deletion	UNP B1XJV9
C	?	-	VAL	deletion	UNP B1XJV9
C	?	-	ALA	deletion	UNP B1XJV9
C	?	-	ASP	deletion	UNP B1XJV9
C	?	-	ILE	deletion	UNP B1XJV9
C	?	-	THR	deletion	UNP B1XJV9
C	?	-	ALA	deletion	UNP B1XJV9
C	?	-	THR	deletion	UNP B1XJV9
C	?	-	ALA	deletion	UNP B1XJV9
C	?	-	GLU	deletion	UNP B1XJV9
C	?	-	GLU	deletion	UNP B1XJV9
C	?	-	LEU	deletion	UNP B1XJV9
C	?	-	GLY	deletion	UNP B1XJV9
C	?	-	LYS	deletion	UNP B1XJV9
C	?	-	THR	deletion	UNP B1XJV9
C	?	-	ALA	deletion	UNP B1XJV9
C	?	-	GLY	deletion	UNP B1XJV9
C	?	-	LYS	deletion	UNP B1XJV9
C	?	-	ASP	deletion	UNP B1XJV9
C	?	-	LEU	deletion	UNP B1XJV9
C	?	-	GLU	deletion	UNP B1XJV9
C	?	-	ALA	deletion	UNP B1XJV9
C	?	-	GLN	deletion	UNP B1XJV9
C	?	-	LYS	deletion	UNP B1XJV9
C	?	-	VAL	deletion	UNP B1XJV9
C	?	-	THR	deletion	UNP B1XJV9
C	?	-	TYR	deletion	UNP B1XJV9
C	?	-	PRO	deletion	UNP B1XJV9
C	?	-	SER	deletion	UNP B1XJV9

- Molecule 4 is a protein called Geranylgeranyl pyrophosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	267	Total	C	N	O	S	0	0	0
			1918	1212	327	368	11			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	ASP	deletion	UNP B1XJV9
D	?	-	ILE	deletion	UNP B1XJV9
D	?	-	THR	deletion	UNP B1XJV9
D	?	-	ALA	deletion	UNP B1XJV9
D	?	-	THR	deletion	UNP B1XJV9
D	?	-	ALA	deletion	UNP B1XJV9
D	?	-	GLU	deletion	UNP B1XJV9
D	?	-	GLU	deletion	UNP B1XJV9
D	?	-	LEU	deletion	UNP B1XJV9
D	?	-	GLY	deletion	UNP B1XJV9
D	?	-	LYS	deletion	UNP B1XJV9
D	?	-	THR	deletion	UNP B1XJV9
D	?	-	ALA	deletion	UNP B1XJV9
D	?	-	GLY	deletion	UNP B1XJV9
D	?	-	LYS	deletion	UNP B1XJV9
D	?	-	ASP	deletion	UNP B1XJV9
D	?	-	LEU	deletion	UNP B1XJV9
D	?	-	GLU	deletion	UNP B1XJV9
D	?	-	ALA	deletion	UNP B1XJV9
D	?	-	GLN	deletion	UNP B1XJV9
D	?	-	LYS	deletion	UNP B1XJV9
D	?	-	VAL	deletion	UNP B1XJV9

- Molecule 5 is a protein called Geranylgeranyl pyrophosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	259	Total	C	N	O	S	0	0	0
			1859	1175	320	353	11			

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	GLY	deletion	UNP B1XJV9
E	?	-	LYS	deletion	UNP B1XJV9
E	?	-	THR	deletion	UNP B1XJV9
E	?	-	ASP	deletion	UNP B1XJV9
E	?	-	ASP	deletion	UNP B1XJV9
E	?	-	ASP	deletion	UNP B1XJV9
E	?	-	ILE	deletion	UNP B1XJV9
E	?	-	LEU	deletion	UNP B1XJV9
E	?	-	ASP	deletion	UNP B1XJV9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	ILE	deletion	UNP B1XJV9
E	?	-	THR	deletion	UNP B1XJV9
E	?	-	ALA	deletion	UNP B1XJV9
E	?	-	THR	deletion	UNP B1XJV9
E	?	-	ALA	deletion	UNP B1XJV9
E	?	-	GLU	deletion	UNP B1XJV9
E	?	-	GLU	deletion	UNP B1XJV9
E	?	-	LEU	deletion	UNP B1XJV9
E	?	-	GLY	deletion	UNP B1XJV9
E	?	-	LYS	deletion	UNP B1XJV9
E	?	-	THR	deletion	UNP B1XJV9
E	?	-	ALA	deletion	UNP B1XJV9
E	?	-	GLY	deletion	UNP B1XJV9
E	?	-	LYS	deletion	UNP B1XJV9
E	?	-	ASP	deletion	UNP B1XJV9
E	?	-	LEU	deletion	UNP B1XJV9
E	?	-	GLU	deletion	UNP B1XJV9
E	?	-	ALA	deletion	UNP B1XJV9
E	?	-	GLN	deletion	UNP B1XJV9
E	?	-	LYS	deletion	UNP B1XJV9
E	?	-	VAL	deletion	UNP B1XJV9
E	?	-	THR	deletion	UNP B1XJV9
E	?	-	TYR	deletion	UNP B1XJV9
E	?	-	PRO	deletion	UNP B1XJV9
E	?	-	SER	deletion	UNP B1XJV9
E	?	-	LEU	deletion	UNP B1XJV9
E	?	-	TRP	deletion	UNP B1XJV9
E	?	-	GLY	deletion	UNP B1XJV9
E	?	-	ILE	deletion	UNP B1XJV9
E	?	-	GLU	deletion	UNP B1XJV9

- Molecule 6 is a protein called Geranylgeranyl pyrophosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	253	Total	C	N	O	S	0	0	0
			1852	1172	314	355	11			

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	THR	deletion	UNP B1XJV9
F	?	-	ASP	deletion	UNP B1XJV9

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Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	VAL	deletion	UNP B1XJV9
F	?	-	ALA	deletion	UNP B1XJV9
F	?	-	VAL	deletion	UNP B1XJV9
F	?	-	ILE	deletion	UNP B1XJV9
F	?	-	LEU	deletion	UNP B1XJV9
F	?	-	ASP	deletion	UNP B1XJV9
F	?	-	ILE	deletion	UNP B1XJV9
F	?	-	THR	deletion	UNP B1XJV9
F	?	-	ALA	deletion	UNP B1XJV9
F	?	-	THR	deletion	UNP B1XJV9
F	?	-	ALA	deletion	UNP B1XJV9
F	?	-	GLU	deletion	UNP B1XJV9
F	?	-	GLU	deletion	UNP B1XJV9
F	?	-	LEU	deletion	UNP B1XJV9
F	?	-	GLY	deletion	UNP B1XJV9
F	?	-	LYS	deletion	UNP B1XJV9
F	?	-	THR	deletion	UNP B1XJV9
F	?	-	ALA	deletion	UNP B1XJV9
F	?	-	GLY	deletion	UNP B1XJV9
F	?	-	LYS	deletion	UNP B1XJV9
F	?	-	ASP	deletion	UNP B1XJV9
F	?	-	LEU	deletion	UNP B1XJV9
F	?	-	GLU	deletion	UNP B1XJV9
F	?	-	ALA	deletion	UNP B1XJV9
F	?	-	GLN	deletion	UNP B1XJV9
F	?	-	LYS	deletion	UNP B1XJV9
F	?	-	VAL	deletion	UNP B1XJV9
F	?	-	THR	deletion	UNP B1XJV9
F	?	-	TYR	deletion	UNP B1XJV9
F	?	-	PRO	deletion	UNP B1XJV9
F	?	-	SER	deletion	UNP B1XJV9
F	?	-	LEU	deletion	UNP B1XJV9
F	?	-	TRP	deletion	UNP B1XJV9
F	?	-	GLY	deletion	UNP B1XJV9
F	?	-	ILE	deletion	UNP B1XJV9
F	?	-	GLU	deletion	UNP B1XJV9
F	?	-	LYS	deletion	UNP B1XJV9

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	11	Total O 11 11	0	0

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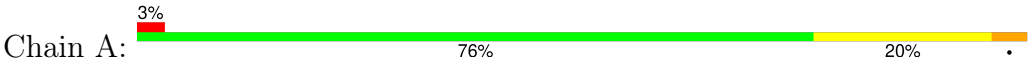
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	12	Total O 12 12	0	0
7	C	5	Total O 5 5	0	0
7	D	2	Total O 2 2	0	0
7	E	9	Total O 9 9	0	0
7	F	7	Total O 7 7	0	0

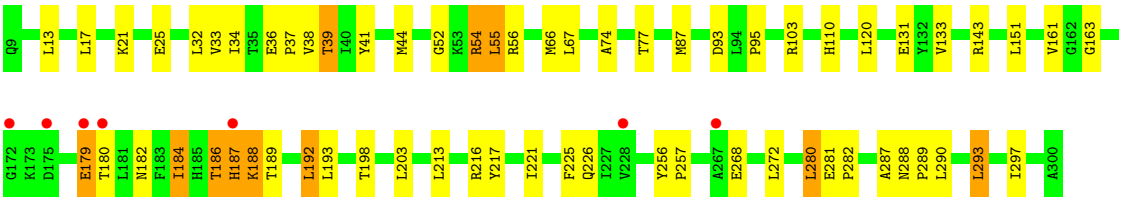
3 Residue-property plots (i)

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: Geranylgeranyl pyrophosphate synthase

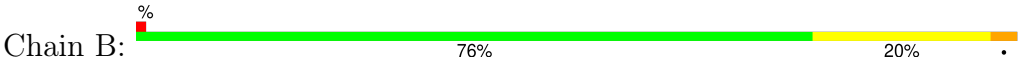
Chain A:

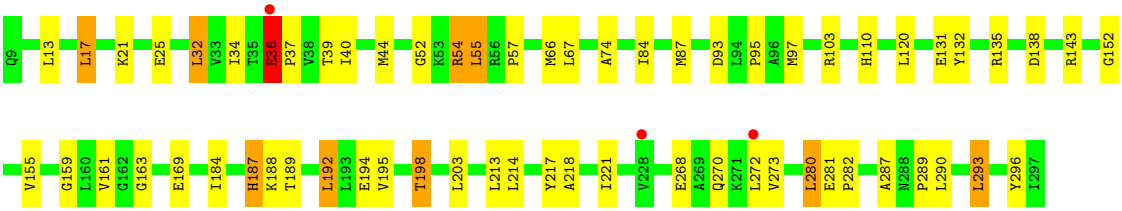




• Molecule 2: Geranylgeranyl pyrophosphate synthase

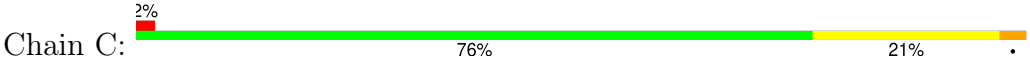
Chain B:

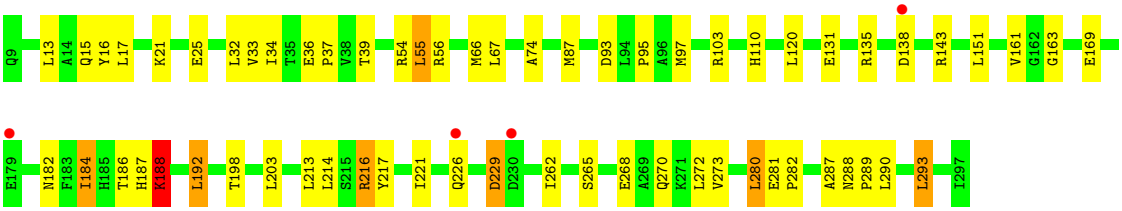




• Molecule 3: Geranylgeranyl pyrophosphate synthase

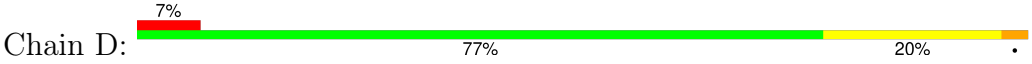
Chain C:

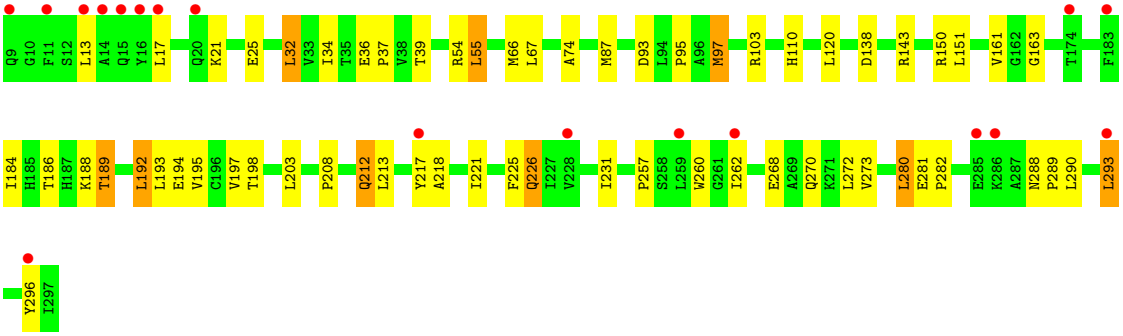




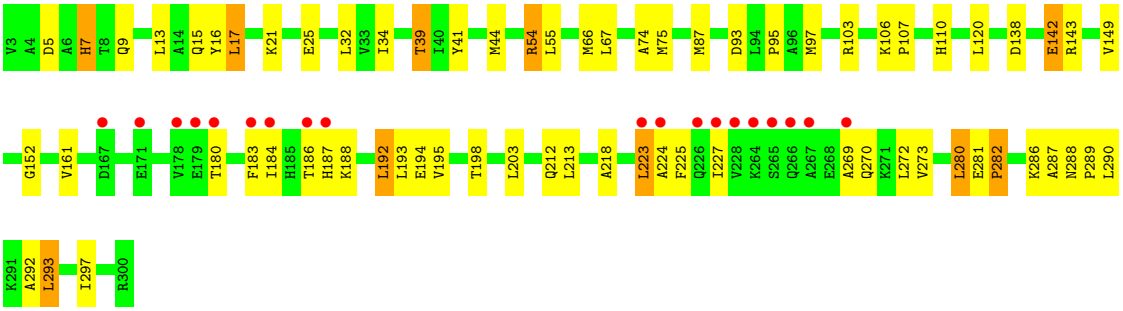
• Molecule 4: Geranylgeranyl pyrophosphate synthase

Chain D:

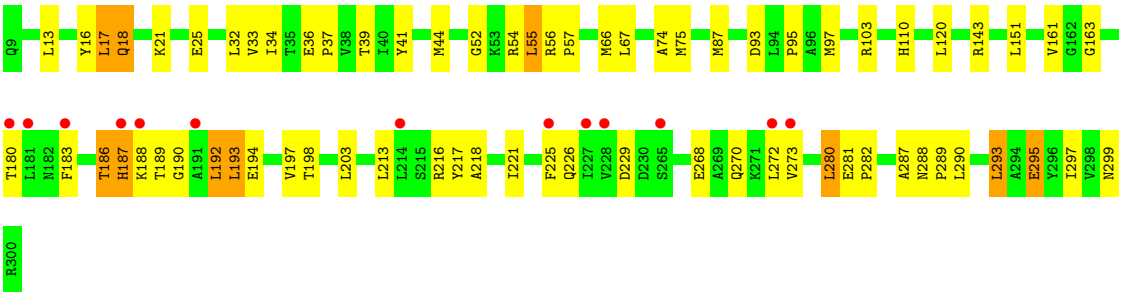




• Molecule 5: Geranylgeranyl pyrophosphate synthase



• Molecule 6: Geranylgeranyl pyrophosphate synthase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	102.56Å 122.97Å 134.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.02 – 2.66 67.92 – 2.66	Depositor EDS
% Data completeness (in resolution range)	99.2 (68.02-2.66) 99.3 (67.92-2.66)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.228 , 0.285 0.230 , 0.285	Depositor DCC
R_{free} test set	2407 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	57.0	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 66.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11367	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.56% 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

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	0.49	0/1954	0.78	0/2656
2	B	0.48	0/1906	0.78	0/2589
3	C	0.52	1/1900 (0.1%)	0.83	2/2581 (0.1%)
4	D	0.45	0/1943	0.79	1/2644 (0.0%)
5	E	0.50	0/1882	0.83	2/2559 (0.1%)
6	F	0.48	0/1875	0.79	0/2547
All	All	0.49	1/11460 (0.0%)	0.80	5/15576 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	188	LYS	C-O	5.75	1.34	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	216	ARG	CG-CD-NE	10.49	133.82	111.80
5	E	186	THR	CB-CA-C	7.30	131.31	111.60
4	D	212	GLN	CB-CA-C	5.62	121.65	110.40
3	C	229	ASP	CB-CA-C	5.32	121.04	110.40
5	E	212	GLN	CB-CA-C	5.16	120.73	110.40

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	1931	0	1891	53	0
2	B	1884	0	1853	49	0
3	C	1877	0	1849	47	0
4	D	1918	0	1867	53	0
5	E	1859	0	1816	52	3
6	F	1852	0	1839	56	3
7	A	11	0	0	4	0
7	B	12	0	0	1	0
7	C	5	0	0	1	0
7	D	2	0	0	1	0
7	E	9	0	0	2	0
7	F	7	0	0	1	0
All	All	11367	0	11115	289	3

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 13.

All (289) 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)
2:B:36:GLU:HB3	2:B:37:PRO:CD	1.52	1.30
2:B:36:GLU:HB3	2:B:37:PRO:HD2	1.28	1.14
4:D:66:MET:HE3	4:D:290:LEU:HD12	1.21	1.14
6:F:186:THR:CG2	6:F:226:GLN:NE2	2.11	1.13
6:F:186:THR:HG23	6:F:226:GLN:NE2	1.64	1.10
6:F:18:GLN:HE21	6:F:18:GLN:HA	1.15	1.07
1:A:39:THR:HG21	2:B:169:GLU:OE2	1.55	1.07
2:B:36:GLU:HB3	2:B:37:PRO:HD3	1.37	1.04
2:B:36:GLU:CB	2:B:37:PRO:CD	2.42	0.98
2:B:198:THR:HG21	7:B:302:HOH:O	1.66	0.92
1:A:182:ASN:O	1:A:186:THR:HG23	1.71	0.90
3:C:56:ARG:HD3	3:C:192:LEU:HD13	1.53	0.90
4:D:280:LEU:HA	7:D:301:HOH:O	1.70	0.89
3:C:169:GLU:OE1	5:E:39:THR:HG21	1.73	0.89
2:B:36:GLU:CB	2:B:37:PRO:HD2	2.03	0.88
1:A:188:LYS:HD3	1:A:188:LYS:N	1.87	0.88
6:F:18:GLN:HA	6:F:18:GLN:NE2	1.86	0.88
6:F:66:MET:HE2	6:F:287:ALA:HA	1.56	0.86
3:C:56:ARG:HD3	3:C:192:LEU:CD1	2.06	0.84
7:A:406:HOH:O	3:C:273:VAL:HG11	1.77	0.83
1:A:38:VAL:CG1	4:D:212:GLN:HB3	2.09	0.83
3:C:188:LYS:HD3	3:C:188:LYS:N	1.91	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:66:MET:HE2	5:E:287:ALA:HA	1.61	0.83
1:A:39:THR:CG2	2:B:169:GLU:OE2	2.27	0.82
2:B:66:MET:HE3	2:B:290:LEU:HD12	1.61	0.82
4:D:188:LYS:HD3	4:D:188:LYS:N	1.94	0.82
6:F:56:ARG:HD3	6:F:192:LEU:HD13	1.62	0.81
3:C:184:ILE:HG13	3:C:188:LYS:HE3	1.63	0.80
5:E:55:LEU:HD21	5:E:297:ILE:HG12	1.64	0.80
6:F:225:PHE:HD2	6:F:297:ILE:HG23	1.47	0.79
1:A:184:ILE:HG13	1:A:188:LYS:HE3	1.65	0.79
1:A:66:MET:HE2	1:A:287:ALA:HA	1.64	0.78
6:F:194:GLU:HA	6:F:218:ALA:HB1	1.65	0.77
3:C:66:MET:HE2	3:C:287:ALA:HA	1.66	0.77
6:F:186:THR:HG23	6:F:226:GLN:HE22	1.46	0.75
3:C:66:MET:HE1	3:C:290:LEU:HD12	1.69	0.75
5:E:223:LEU:HD23	5:E:273:VAL:HG21	1.69	0.74
1:A:38:VAL:CG1	4:D:212:GLN:CB	2.65	0.73
3:C:66:MET:CE	3:C:290:LEU:HD12	2.18	0.73
1:A:38:VAL:HG11	4:D:212:GLN:CB	2.19	0.73
3:C:192:LEU:HD22	3:C:192:LEU:O	1.90	0.72
6:F:186:THR:HG23	6:F:226:GLN:HE21	1.51	0.71
1:A:66:MET:CE	1:A:290:LEU:HD12	2.20	0.71
5:E:66:MET:CE	5:E:290:LEU:HD12	2.21	0.71
5:E:224:ALA:HB2	5:E:273:VAL:HG12	1.73	0.71
1:A:66:MET:HE3	1:A:290:LEU:HD12	1.71	0.71
2:B:281:GLU:N	2:B:282:PRO:HD2	2.06	0.71
2:B:34:ILE:HD12	2:B:34:ILE:H	1.56	0.70
3:C:34:ILE:HD12	3:C:34:ILE:H	1.57	0.70
4:D:163:GLY:HA3	4:D:188:LYS:CB	2.22	0.70
5:E:66:MET:HE1	5:E:290:LEU:HD12	1.74	0.69
1:A:217:TYR:CZ	1:A:221:ILE:HD12	2.27	0.69
1:A:110:HIS:HD2	7:A:407:HOH:O	1.74	0.69
4:D:34:ILE:H	4:D:34:ILE:HD12	1.57	0.69
4:D:163:GLY:N	4:D:188:LYS:HG3	2.08	0.69
2:B:66:MET:HE2	2:B:287:ALA:HA	1.74	0.69
5:E:34:ILE:HD12	5:E:34:ILE:H	1.55	0.69
4:D:217:TYR:CZ	4:D:221:ILE:HD12	2.28	0.68
1:A:34:ILE:HD12	1:A:34:ILE:H	1.57	0.68
5:E:192:LEU:O	5:E:195:VAL:HG12	1.94	0.68
4:D:66:MET:HE3	4:D:290:LEU:CD1	2.12	0.67
6:F:34:ILE:HD12	6:F:34:ILE:H	1.58	0.67
2:B:66:MET:CE	2:B:290:LEU:HD12	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:163:GLY:HA3	4:D:188:LYS:HB2	1.75	0.67
6:F:66:MET:CE	6:F:290:LEU:HD12	2.24	0.66
4:D:194:GLU:HA	4:D:218:ALA:HB1	1.76	0.66
1:A:163:GLY:HA3	1:A:188:LYS:CB	2.25	0.66
3:C:36:GLU:HG3	3:C:37:PRO:HA	1.79	0.65
5:E:281:GLU:N	5:E:282:PRO:HD2	2.12	0.64
1:A:38:VAL:HG11	4:D:212:GLN:HB2	1.79	0.64
6:F:183:PHE:O	6:F:187:HIS:HB2	1.98	0.64
4:D:192:LEU:O	4:D:195:VAL:HG12	1.98	0.64
1:A:34:ILE:HD13	4:D:208:PRO:HB3	1.80	0.64
4:D:36:GLU:HG3	4:D:37:PRO:HA	1.79	0.63
4:D:194:GLU:HA	4:D:218:ALA:CB	2.28	0.63
5:E:93:ASP:OD1	5:E:103:ARG:NH1	2.31	0.63
2:B:192:LEU:O	2:B:195:VAL:HG12	1.99	0.62
3:C:93:ASP:OD1	3:C:103:ARG:NH1	2.33	0.62
5:E:224:ALA:HB2	5:E:270:GLN:HA	1.82	0.62
2:B:93:ASP:OD1	2:B:103:ARG:NH1	2.32	0.62
2:B:217:TYR:CZ	2:B:221:ILE:HD12	2.35	0.61
1:A:163:GLY:HA3	1:A:188:LYS:HB2	1.82	0.61
6:F:93:ASP:OD1	6:F:103:ARG:NH1	2.34	0.61
1:A:36:GLU:HG3	1:A:37:PRO:HA	1.83	0.60
1:A:217:TYR:CZ	1:A:221:ILE:CD1	2.84	0.60
2:B:131:GLU:O	2:B:135:ARG:HG3	2.00	0.60
6:F:36:GLU:HG3	6:F:37:PRO:HA	1.84	0.60
5:E:192:LEU:O	5:E:192:LEU:HD23	2.02	0.59
1:A:120:LEU:HB3	2:B:161:VAL:HG13	1.84	0.59
6:F:281:GLU:N	6:F:282:PRO:HD2	2.17	0.59
4:D:163:GLY:CA	4:D:188:LYS:CG	2.81	0.59
5:E:269:ALA:HA	5:E:272:LEU:HD12	1.83	0.59
1:A:38:VAL:HG11	4:D:212:GLN:HB3	1.79	0.59
2:B:188:LYS:HD3	2:B:188:LYS:N	2.18	0.58
5:E:55:LEU:HD21	5:E:297:ILE:CG1	2.33	0.58
2:B:184:ILE:HG13	2:B:188:LYS:HE3	1.84	0.58
3:C:56:ARG:CD	3:C:192:LEU:HD13	2.29	0.58
2:B:268:GLU:O	2:B:272:LEU:HG	2.04	0.58
1:A:93:ASP:OD1	1:A:103:ARG:NH1	2.35	0.58
6:F:268:GLU:O	6:F:272:LEU:HG	2.03	0.58
6:F:186:THR:CG2	6:F:226:GLN:HE21	2.07	0.57
5:E:224:ALA:HB1	5:E:270:GLN:CB	2.35	0.57
1:A:268:GLU:O	1:A:272:LEU:HG	2.04	0.57
1:A:55:LEU:HD23	1:A:55:LEU:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:268:GLU:O	4:D:272:LEU:HG	2.03	0.57
5:E:289:PRO:O	5:E:293:LEU:HB2	2.04	0.57
3:C:163:GLY:HA3	3:C:188:LYS:HB2	1.86	0.57
2:B:217:TYR:CZ	2:B:221:ILE:CD1	2.88	0.57
4:D:257:PRO:HD2	4:D:260:TRP:CB	2.35	0.57
4:D:217:TYR:CZ	4:D:221:ILE:CD1	2.88	0.57
3:C:110:HIS:HD2	7:C:305:HOH:O	1.88	0.56
3:C:281:GLU:N	3:C:282:PRO:HD2	2.20	0.56
1:A:187:HIS:HB3	1:A:188:LYS:HD3	1.87	0.56
1:A:281:GLU:N	1:A:282:PRO:CD	2.69	0.56
5:E:224:ALA:HB2	5:E:273:VAL:CG1	2.34	0.56
6:F:225:PHE:CD2	6:F:297:ILE:HG23	2.34	0.56
1:A:217:TYR:CE1	1:A:221:ILE:HD12	2.40	0.56
6:F:56:ARG:HD3	6:F:192:LEU:CD1	2.32	0.56
4:D:281:GLU:N	4:D:282:PRO:CD	2.68	0.56
4:D:55:LEU:HD23	4:D:55:LEU:H	1.71	0.56
1:A:281:GLU:N	1:A:282:PRO:HD2	2.21	0.56
6:F:281:GLU:N	6:F:282:PRO:CD	2.69	0.56
4:D:225:PHE:CE2	4:D:296:TYR:CE2	2.95	0.56
6:F:18:GLN:HE21	6:F:18:GLN:CA	2.04	0.56
2:B:289:PRO:O	2:B:293:LEU:HB2	2.07	0.55
3:C:281:GLU:N	3:C:282:PRO:CD	2.70	0.55
3:C:289:PRO:O	3:C:293:LEU:HB2	2.06	0.55
4:D:163:GLY:H	4:D:188:LYS:HG3	1.69	0.55
4:D:93:ASP:OD1	4:D:103:ARG:NH1	2.37	0.55
1:A:289:PRO:O	1:A:293:LEU:HB2	2.07	0.55
3:C:268:GLU:O	3:C:272:LEU:HG	2.06	0.55
4:D:161:VAL:HG13	6:F:120:LEU:HB3	1.89	0.55
6:F:217:TYR:CZ	6:F:221:ILE:CD1	2.90	0.55
5:E:281:GLU:N	5:E:282:PRO:CD	2.70	0.55
6:F:289:PRO:O	6:F:293:LEU:HB2	2.07	0.54
3:C:56:ARG:CD	3:C:192:LEU:CD1	2.83	0.54
6:F:55:LEU:HD23	6:F:55:LEU:H	1.71	0.54
6:F:66:MET:HE1	6:F:290:LEU:HD12	1.89	0.54
3:C:55:LEU:HD23	3:C:55:LEU:H	1.73	0.54
4:D:289:PRO:O	4:D:293:LEU:HB2	2.08	0.54
6:F:217:TYR:CZ	6:F:221:ILE:HD12	2.42	0.54
2:B:55:LEU:H	2:B:55:LEU:HD23	1.72	0.54
2:B:184:ILE:O	2:B:188:LYS:HG2	2.08	0.54
5:E:110:HIS:HD2	7:E:404:HOH:O	1.91	0.53
3:C:217:TYR:CZ	3:C:221:ILE:CD1	2.92	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:189:THR:HG21	4:D:226:GLN:OE1	2.08	0.53
1:A:41:TYR:HA	1:A:44:MET:HE3	1.91	0.53
3:C:217:TYR:CZ	3:C:221:ILE:HD12	2.44	0.53
6:F:66:MET:HE3	6:F:290:LEU:HD12	1.91	0.53
6:F:186:THR:CA	6:F:226:GLN:HE22	2.19	0.53
5:E:75:MET:HG3	7:E:405:HOH:O	2.10	0.52
5:E:224:ALA:CB	5:E:270:GLN:HA	2.39	0.51
5:E:9:GLN:O	5:E:9:GLN:HG3	2.10	0.51
6:F:295:GLU:OE1	6:F:299:ASN:ND2	2.43	0.51
4:D:281:GLU:N	4:D:282:PRO:HD2	2.26	0.51
5:E:225:PHE:CD2	5:E:225:PHE:C	2.85	0.51
4:D:225:PHE:CE2	4:D:296:TYR:HE2	2.29	0.51
6:F:163:GLY:N	6:F:188:LYS:HG3	2.25	0.51
1:A:38:VAL:CG1	4:D:212:GLN:HB2	2.39	0.50
5:E:7:HIS:N	5:E:7:HIS:CD2	2.78	0.50
2:B:281:GLU:N	2:B:282:PRO:CD	2.72	0.50
4:D:186:THR:HA	4:D:189:THR:HG23	1.94	0.49
2:B:194:GLU:HA	2:B:218:ALA:HB1	1.93	0.49
5:E:269:ALA:HA	5:E:272:LEU:CD1	2.42	0.49
3:C:217:TYR:CE1	3:C:221:ILE:HD12	2.48	0.48
6:F:186:THR:CG2	6:F:226:GLN:HE22	2.02	0.48
6:F:217:TYR:CE1	6:F:221:ILE:HD12	2.48	0.48
1:A:38:VAL:HG12	4:D:212:GLN:CB	2.41	0.48
4:D:163:GLY:HA3	4:D:188:LYS:CG	2.43	0.48
4:D:197:VAL:CG2	4:D:218:ALA:HB2	2.44	0.48
2:B:194:GLU:HA	2:B:218:ALA:CB	2.44	0.47
5:E:41:TYR:HA	5:E:44:MET:HE3	1.97	0.47
6:F:41:TYR:HA	6:F:44:MET:HE3	1.95	0.47
4:D:74:ALA:HA	4:D:203:LEU:HD13	1.95	0.47
5:E:142:GLU:H	5:E:142:GLU:HG2	1.45	0.47
2:B:159:GLY:O	2:B:188:LYS:HB3	2.14	0.46
3:C:34:ILE:HD12	3:C:34:ILE:N	2.29	0.46
5:E:106:LYS:HG3	5:E:107:PRO:HD2	1.97	0.46
3:C:135:ARG:NH2	5:E:149:VAL:CG1	2.79	0.46
7:A:406:HOH:O	3:C:273:VAL:HG21	2.13	0.46
5:E:280:LEU:C	5:E:282:PRO:HD2	2.36	0.46
1:A:34:ILE:HD12	1:A:34:ILE:N	2.28	0.46
1:A:163:GLY:CA	1:A:188:LYS:CB	2.94	0.46
4:D:21:LYS:O	4:D:25:GLU:HG3	2.16	0.46
6:F:21:LYS:HE2	6:F:52:GLY:O	2.16	0.46
3:C:21:LYS:O	3:C:25:GLU:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:188:LYS:N	5:E:188:LYS:HD3	2.31	0.46
2:B:280:LEU:C	2:B:282:PRO:HD2	2.36	0.46
5:E:34:ILE:HD12	5:E:34:ILE:N	2.29	0.46
1:A:256:TYR:N	1:A:257:PRO:HD3	2.31	0.45
4:D:217:TYR:CE2	4:D:221:ILE:HD12	2.51	0.45
3:C:169:GLU:OE1	5:E:39:THR:CG2	2.56	0.45
6:F:280:LEU:C	6:F:282:PRO:HD2	2.37	0.45
5:E:224:ALA:HA	5:E:227:ILE:HD12	1.98	0.45
5:E:95:PRO:HD3	5:E:110:HIS:CE1	2.52	0.45
6:F:186:THR:HG21	6:F:226:GLN:HB2	1.98	0.45
1:A:95:PRO:HD3	1:A:110:HIS:CE1	2.51	0.45
3:C:16:TYR:CZ	3:C:289:PRO:HB3	2.52	0.45
6:F:197:VAL:CG2	6:F:218:ALA:HB2	2.47	0.45
2:B:34:ILE:HD12	2:B:34:ILE:N	2.29	0.45
4:D:151:LEU:HD12	4:D:151:LEU:HA	1.84	0.45
5:E:74:ALA:HA	5:E:203:LEU:HD13	1.99	0.45
1:A:225:PHE:CD2	1:A:297:ILE:HG23	2.51	0.45
3:C:288:ASN:N	3:C:289:PRO:CD	2.80	0.45
4:D:36:GLU:CG	4:D:37:PRO:HA	2.46	0.45
3:C:163:GLY:HA3	3:C:188:LYS:CB	2.46	0.44
4:D:95:PRO:HD3	4:D:110:HIS:CE1	2.52	0.44
3:C:131:GLU:HB2	5:E:152:GLY:HA3	1.99	0.44
6:F:16:TYR:CZ	6:F:289:PRO:HB3	2.53	0.44
6:F:95:PRO:HD3	6:F:110:HIS:CE1	2.53	0.44
4:D:13:LEU:HD11	4:D:293:LEU:HD13	2.00	0.44
2:B:74:ALA:HA	2:B:203:LEU:HD13	1.99	0.44
3:C:120:LEU:HB3	5:E:161:VAL:HG13	1.99	0.44
2:B:13:LEU:HG	2:B:17:LEU:HD22	2.00	0.44
5:E:21:LYS:O	5:E:25:GLU:HG3	2.18	0.44
5:E:288:ASN:N	5:E:289:PRO:CD	2.81	0.44
5:E:194:GLU:HA	5:E:218:ALA:HB1	1.99	0.44
5:E:223:LEU:CD2	5:E:273:VAL:HG21	2.45	0.44
5:E:225:PHE:O	5:E:225:PHE:CG	2.70	0.44
2:B:163:GLY:HA3	2:B:188:LYS:HB2	2.00	0.43
3:C:95:PRO:HD3	3:C:110:HIS:CE1	2.53	0.43
4:D:97:MET:HE3	4:D:97:MET:HB3	1.92	0.43
2:B:13:LEU:HD11	2:B:293:LEU:HD13	2.00	0.43
2:B:21:LYS:O	2:B:25:GLU:HG3	2.17	0.43
4:D:150:ARG:HH11	4:D:150:ARG:HD2	1.67	0.43
6:F:74:ALA:HA	6:F:203:LEU:HD13	1.99	0.43
2:B:187:HIS:HB3	2:B:188:LYS:HE2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:66:MET:HE3	5:E:290:LEU:HD12	2.00	0.43
6:F:163:GLY:CA	6:F:188:LYS:HG3	2.49	0.43
2:B:21:LYS:HE2	2:B:52:GLY:O	2.18	0.43
2:B:95:PRO:HD3	2:B:110:HIS:CE1	2.53	0.43
3:C:36:GLU:CG	3:C:37:PRO:HA	2.47	0.43
3:C:182:ASN:O	3:C:186:THR:HG23	2.19	0.43
4:D:270:GLN:O	4:D:273:VAL:HG12	2.18	0.43
6:F:186:THR:HA	6:F:226:GLN:OE1	2.18	0.43
1:A:21:LYS:O	1:A:25:GLU:HG3	2.18	0.43
6:F:75:MET:HG3	7:F:403:HOH:O	2.19	0.42
1:A:151:LEU:HD12	1:A:151:LEU:HA	1.82	0.42
1:A:179:GLU:OE1	1:A:180:THR:N	2.51	0.42
5:E:17:LEU:HD12	5:E:17:LEU:HA	1.89	0.42
1:A:13:LEU:HD11	1:A:293:LEU:HD13	2.01	0.42
6:F:13:LEU:HD11	6:F:293:LEU:HD13	2.02	0.42
1:A:56:ARG:HD3	1:A:192:LEU:HD13	2.01	0.42
5:E:13:LEU:HD13	5:E:292:ALA:HB1	2.02	0.42
6:F:194:GLU:HA	6:F:218:ALA:CB	2.43	0.42
7:A:406:HOH:O	3:C:273:VAL:CG1	2.52	0.42
3:C:13:LEU:HD11	3:C:293:LEU:HD13	2.01	0.42
4:D:192:LEU:O	4:D:192:LEU:HD23	2.19	0.42
4:D:288:ASN:HD22	4:D:288:ASN:HA	1.68	0.42
6:F:270:GLN:O	6:F:273:VAL:HG12	2.20	0.42
1:A:161:VAL:HG13	2:B:120:LEU:HB3	2.02	0.42
2:B:66:MET:HE3	2:B:290:LEU:CD1	2.39	0.42
4:D:32:LEU:HD12	4:D:32:LEU:HA	1.91	0.42
2:B:217:TYR:CE2	2:B:221:ILE:HD12	2.55	0.42
5:E:286:LYS:HE3	5:E:286:LYS:HB2	1.89	0.42
1:A:77:THR:HA	1:A:133:VAL:HG22	2.01	0.41
1:A:280:LEU:C	1:A:282:PRO:HD2	2.41	0.41
2:B:270:GLN:O	2:B:273:VAL:HG12	2.20	0.41
3:C:270:GLN:O	3:C:273:VAL:HG12	2.19	0.41
3:C:280:LEU:C	3:C:282:PRO:HD2	2.40	0.41
5:E:21:LYS:HG3	5:E:54:ARG:HG3	2.02	0.41
1:A:74:ALA:HA	1:A:203:LEU:HD13	2.02	0.41
3:C:161:VAL:HG13	5:E:120:LEU:HB3	2.01	0.41
5:E:16:TYR:CZ	5:E:289:PRO:HB3	2.55	0.41
6:F:21:LYS:O	6:F:25:GLU:HG3	2.21	0.41
6:F:190:GLY:HA2	6:F:193:LEU:HB2	2.02	0.41
3:C:74:ALA:HA	3:C:203:LEU:HD13	2.02	0.41
4:D:120:LEU:HB3	6:F:161:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:LYS:HG3	2:B:54:ARG:HG3	2.02	0.41
3:C:151:LEU:HD12	3:C:151:LEU:HA	1.83	0.41
6:F:151:LEU:HD12	6:F:151:LEU:HA	1.80	0.41
1:A:131:GLU:HB2	2:B:152:GLY:HA3	2.03	0.41
5:E:293:LEU:HD12	5:E:293:LEU:HA	1.78	0.41
1:A:66:MET:HE1	1:A:290:LEU:HD12	1.99	0.41
1:A:225:PHE:HD2	1:A:297:ILE:HG12	1.86	0.41
6:F:34:ILE:HD12	6:F:34:ILE:N	2.30	0.41
6:F:36:GLU:CG	6:F:37:PRO:HA	2.50	0.41
3:C:66:MET:HE3	3:C:290:LEU:HD12	1.98	0.41
3:C:214:LEU:HD13	3:C:214:LEU:HA	1.96	0.41
1:A:21:LYS:HG3	1:A:54:ARG:HG3	2.03	0.40
1:A:288:ASN:N	1:A:289:PRO:CD	2.84	0.40
2:B:40:ILE:O	2:B:44:MET:HG3	2.21	0.40
2:B:214:LEU:HD13	2:B:214:LEU:HA	1.94	0.40
6:F:17:LEU:HD12	6:F:17:LEU:HA	1.86	0.40
1:A:21:LYS:HE2	1:A:52:GLY:O	2.21	0.40
2:B:32:LEU:HD12	2:B:32:LEU:HA	1.94	0.40
2:B:84:ILE:HG21	2:B:155:VAL:HG22	2.03	0.40
4:D:34:ILE:HD12	4:D:34:ILE:N	2.30	0.40
6:F:288:ASN:N	6:F:289:PRO:CD	2.84	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:180:THR:CB	6:F:187:HIS:NE2[1_655]	1.70	0.50
5:E:180:THR:N	6:F:187:HIS:NE2[1_655]	2.12	0.08
5:E:180:THR:CA	6:F:187:HIS:NE2[1_655]	2.18	0.02

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	259/267 (97%)	249 (96%)	10 (4%)	0	100 100
2	B	251/259 (97%)	237 (94%)	12 (5%)	2 (1%)	19 29
3	C	252/258 (98%)	240 (95%)	11 (4%)	1 (0%)	34 48
4	D	263/267 (98%)	247 (94%)	14 (5%)	2 (1%)	19 29
5	E	253/259 (98%)	237 (94%)	12 (5%)	4 (2%)	9 14
6	F	247/253 (98%)	239 (97%)	8 (3%)	0	100 100
All	All	1525/1563 (98%)	1449 (95%)	67 (4%)	9 (1%)	25 37

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	36	GLU
3	C	262	ILE
4	D	262	ILE
2	B	296	TYR
4	D	231	ILE
5	E	5	ASP
5	E	183	PHE
5	E	282	PRO
5	E	184	ILE

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	187/211 (89%)	164 (88%)	23 (12%)	4 6
2	B	184/205 (90%)	164 (89%)	20 (11%)	6 9
3	C	184/203 (91%)	160 (87%)	24 (13%)	4 5
4	D	183/211 (87%)	164 (90%)	19 (10%)	7 10
5	E	176/203 (87%)	156 (89%)	20 (11%)	5 8
6	F	184/199 (92%)	159 (86%)	25 (14%)	3 5
All	All	1098/1232 (89%)	967 (88%)	131 (12%)	5 7

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	32	LEU
1	A	33	VAL
1	A	39	THR
1	A	54	ARG
1	A	55	LEU
1	A	67	LEU
1	A	87	MET
1	A	143	ARG
1	A	179	GLU
1	A	184	ILE
1	A	186	THR
1	A	187	HIS
1	A	188	LYS
1	A	189	THR
1	A	192	LEU
1	A	193	LEU
1	A	198	THR
1	A	213	LEU
1	A	216	ARG
1	A	226	GLN
1	A	280	LEU
1	A	293	LEU
2	B	17	LEU
2	B	32	LEU
2	B	36	GLU
2	B	39	THR
2	B	54	ARG
2	B	55	LEU
2	B	57	PRO
2	B	67	LEU
2	B	87	MET
2	B	97	MET
2	B	132	TYR
2	B	138	ASP
2	B	143	ARG
2	B	187	HIS
2	B	189	THR
2	B	192	LEU
2	B	198	THR
2	B	213	LEU
2	B	280	LEU

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Mol	Chain	Res	Type
2	B	293	LEU
3	C	15	GLN
3	C	17	LEU
3	C	32	LEU
3	C	33	VAL
3	C	39	THR
3	C	54	ARG
3	C	55	LEU
3	C	67	LEU
3	C	87	MET
3	C	97	MET
3	C	138	ASP
3	C	143	ARG
3	C	184	ILE
3	C	187	HIS
3	C	188	LYS
3	C	192	LEU
3	C	198	THR
3	C	213	LEU
3	C	216	ARG
3	C	226	GLN
3	C	229	ASP
3	C	265	SER
3	C	280	LEU
3	C	293	LEU
4	D	17	LEU
4	D	32	LEU
4	D	39	THR
4	D	54	ARG
4	D	55	LEU
4	D	67	LEU
4	D	87	MET
4	D	97	MET
4	D	138	ASP
4	D	143	ARG
4	D	184	ILE
4	D	189	THR
4	D	192	LEU
4	D	193	LEU
4	D	198	THR
4	D	213	LEU
4	D	226	GLN

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Mol	Chain	Res	Type
4	D	280	LEU
4	D	293	LEU
5	E	7	HIS
5	E	15	GLN
5	E	17	LEU
5	E	32	LEU
5	E	39	THR
5	E	54	ARG
5	E	67	LEU
5	E	87	MET
5	E	97	MET
5	E	138	ASP
5	E	142	GLU
5	E	143	ARG
5	E	187	HIS
5	E	192	LEU
5	E	193	LEU
5	E	198	THR
5	E	213	LEU
5	E	223	LEU
5	E	280	LEU
5	E	293	LEU
6	F	17	LEU
6	F	18	GLN
6	F	32	LEU
6	F	33	VAL
6	F	39	THR
6	F	54	ARG
6	F	55	LEU
6	F	57	PRO
6	F	67	LEU
6	F	87	MET
6	F	97	MET
6	F	143	ARG
6	F	180	THR
6	F	186	THR
6	F	187	HIS
6	F	189	THR
6	F	192	LEU
6	F	193	LEU
6	F	198	THR
6	F	213	LEU

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Mol	Chain	Res	Type
6	F	216	ARG
6	F	229	ASP
6	F	280	LEU
6	F	293	LEU
6	F	295	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	288	ASN
2	B	153	GLN
2	B	164	GLN
2	B	226	GLN
2	B	288	ASN
3	C	153	GLN
3	C	164	GLN
3	C	288	ASN
4	D	153	GLN
4	D	164	GLN
4	D	288	ASN
5	E	7	HIS
5	E	110	HIS
5	E	164	GLN
5	E	226	GLN
5	E	288	ASN
6	F	18	GLN
6	F	153	GLN
6	F	164	GLN
6	F	226	GLN
6	F	288	ASN

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)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3
2	B	3
3	C	2
5	E	2
6	F	2
4	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	235:THR	C	254:VAL	N	15.68
1	D	232:LEU	C	255:THR	N	14.53
1	C	232:LEU	C	259:LEU	N	12.09
1	A	257:PRO	C	264:LYS	N	12.08
1	E	228:VAL	C	264:LYS	N	11.77
1	F	173:LYS	C	179:GLU	N	11.41
1	F	230:ASP	C	265:SER	N	10.32
1	E	171:GLU	C	176:VAL	N	10.08
1	B	232:LEU	C	258:SER	N	9.74
1	C	172:GLY	C	178:VAL	N	8.76
1	A	173:LYS	C	175:ASP	N	5.13
1	B	259:LEU	C	263:GLU	N	4.80
1	B	171:GLU	C	174:THR	N	4.01

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	267/267 (100%)	0.09	7 (2%)	56	52	32, 61, 127, 191	0
2	B	259/259 (100%)	0.04	3 (1%)	79	77	29, 55, 109, 156	0
3	C	258/258 (100%)	0.04	4 (1%)	72	69	30, 52, 119, 165	0
4	D	267/267 (100%)	0.38	18 (6%)	17	14	41, 79, 137, 178	0
5	E	259/259 (100%)	0.24	19 (7%)	15	12	31, 59, 158, 239	0
6	F	253/253 (100%)	0.25	13 (5%)	28	25	34, 64, 144, 192	0
All	All	1563/1563 (100%)	0.17	64 (4%)	37	33	29, 63, 132, 239	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	183	PHE	6.4
4	D	9	GLN	6.1
6	F	228	VAL	5.6
5	E	184	ILE	5.2
5	E	226	GLN	5.1
4	D	262	ILE	5.1
5	E	267	ALA	5.0
4	D	11	PHE	4.9
6	F	181	LEU	4.7
6	F	272	LEU	4.4
4	D	285	GLU	4.1
5	E	224	ALA	3.9
2	B	36	GLU	3.8
5	E	187	HIS	3.8
6	F	183	PHE	3.8
5	E	228	VAL	3.7
1	A	179	GLU	3.6
5	E	223	LEU	3.6
2	B	272	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
5	E	264	LYS	3.4
4	D	13	LEU	3.4
3	C	226	GLN	3.4
4	D	15	GLN	3.3
4	D	296	TYR	3.3
5	E	266	GLN	3.3
5	E	179	GLU	3.3
6	F	187	HIS	3.2
4	D	228	VAL	3.2
6	F	180	THR	3.1
6	F	273	VAL	3.0
5	E	227	ILE	2.9
6	F	214	LEU	2.8
5	E	186	THR	2.8
4	D	286	LYS	2.8
5	E	180	THR	2.7
4	D	183	PHE	2.7
4	D	16	TYR	2.7
5	E	269	ALA	2.6
6	F	265	SER	2.6
4	D	20	GLN	2.5
6	F	188	LYS	2.4
6	F	191	ALA	2.4
5	E	178	VAL	2.4
1	A	187	HIS	2.3
5	E	265	SER	2.3
6	F	225	PHE	2.3
1	A	175	ASP	2.2
1	A	172	GLY	2.2
4	D	17	LEU	2.2
4	D	293	LEU	2.2
4	D	217	TYR	2.2
6	F	227	ILE	2.2
1	A	267	ALA	2.1
1	A	180	THR	2.1
1	A	228	VAL	2.1
3	C	138	ASP	2.1
5	E	167	ASP	2.1
5	E	171	GLU	2.1
3	C	179	GLU	2.1
4	D	259	LEU	2.0
2	B	228	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
4	D	14	ALA	2.0
3	C	230	ASP	2.0
4	D	174	THR	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.