



wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 03:00 PM GMT

PDB ID : 3AQ0
Title : Ligand-bound form of Arabidopsis medium/long-chain length prenyl pyrophosphate synthase (surface polar residue mutant)
Authors : Hsieh, F.-L.; Chang, T.-H.; Ko, T.-P.; Wang, A.H.-J.
Deposited on : 2010-10-24
Resolution : 2.65 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

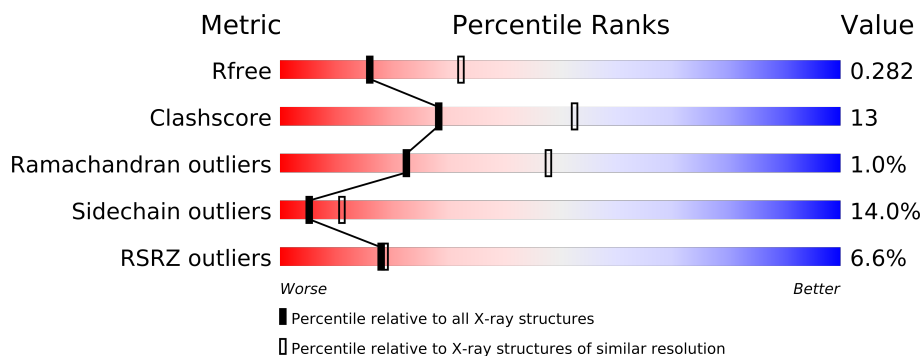
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.65 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}	66092	2232 (2.70-2.62)
Clashscore	79885	2700 (2.70-2.62)
Ramachandran outliers	78287	2657 (2.70-2.62)
Sidechain outliers	78261	2657 (2.70-2.62)
RSRZ outliers	66119	2234 (2.70-2.62)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	348	
1	B	348	
1	C	348	
1	D	348	
1	E	348	
1	F	348	
1	G	348	
1	H	348	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	MG	C	1000	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Geometry	Electron density
6	PEG	B	1002	-	X
6	PEG	D	1002	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 20426 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Geranyl diphosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2488	1563	434	479	12			
1	B	313	Total	C	N	O	S	0	0	0
			2394	1507	414	461	12			
1	C	327	Total	C	N	O	S	0	0	0
			2496	1567	434	483	12			
1	D	312	Total	C	N	O	S	0	0	0
			2388	1506	410	460	12			
1	E	325	Total	C	N	O	S	0	0	0
			2478	1556	432	478	12			
1	F	310	Total	C	N	O	S	0	0	0
			2368	1492	408	456	12			
1	G	314	Total	C	N	O	S	0	0	0
			2400	1514	415	459	12			
1	H	324	Total	C	N	O	S	0	0	0
			2471	1552	431	476	12			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	EXPRESSION TAG	UNP Q9FT89
A	178	ALA	GLU	ENGINEERED MUTATION	UNP Q9FT89
A	179	ALA	GLN	ENGINEERED MUTATION	UNP Q9FT89
A	281	ALA	GLU	ENGINEERED MUTATION	UNP Q9FT89
A	282	ALA	LYS	ENGINEERED MUTATION	UNP Q9FT89
B	1	GLY	-	EXPRESSION TAG	UNP Q9FT89
B	178	ALA	GLU	ENGINEERED MUTATION	UNP Q9FT89
B	179	ALA	GLN	ENGINEERED MUTATION	UNP Q9FT89
B	281	ALA	GLU	ENGINEERED MUTATION	UNP Q9FT89
B	282	ALA	LYS	ENGINEERED MUTATION	UNP Q9FT89
C	1	GLY	-	EXPRESSION TAG	UNP Q9FT89
C	178	ALA	GLU	ENGINEERED MUTATION	UNP Q9FT89
C	179	ALA	GLN	ENGINEERED MUTATION	UNP Q9FT89

Continued on next page...

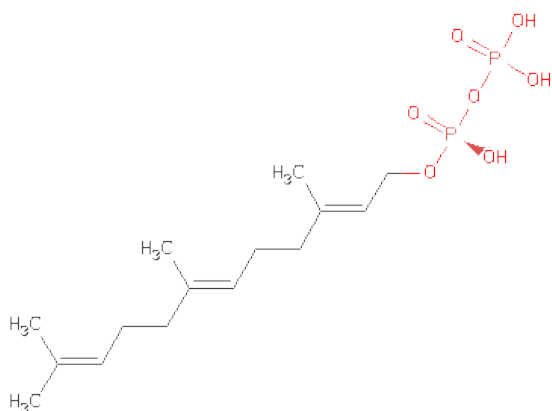
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	281	ALA	GLU	ENGINEERED MUTATION	UNP Q9FT89
C	282	ALA	LYS	ENGINEERED MUTATION	UNP Q9FT89
D	1	GLY	-	EXPRESSION TAG	UNP Q9FT89
D	178	ALA	GLU	ENGINEERED MUTATION	UNP Q9FT89
D	179	ALA	GLN	ENGINEERED MUTATION	UNP Q9FT89
D	281	ALA	GLU	ENGINEERED MUTATION	UNP Q9FT89
D	282	ALA	LYS	ENGINEERED MUTATION	UNP Q9FT89
E	1	GLY	-	EXPRESSION TAG	UNP Q9FT89
E	178	ALA	GLU	ENGINEERED MUTATION	UNP Q9FT89
E	179	ALA	GLN	ENGINEERED MUTATION	UNP Q9FT89
E	281	ALA	GLU	ENGINEERED MUTATION	UNP Q9FT89
E	282	ALA	LYS	ENGINEERED MUTATION	UNP Q9FT89
F	1	GLY	-	EXPRESSION TAG	UNP Q9FT89
F	178	ALA	GLU	ENGINEERED MUTATION	UNP Q9FT89
F	179	ALA	GLN	ENGINEERED MUTATION	UNP Q9FT89
F	281	ALA	GLU	ENGINEERED MUTATION	UNP Q9FT89
F	282	ALA	LYS	ENGINEERED MUTATION	UNP Q9FT89
G	1	GLY	-	EXPRESSION TAG	UNP Q9FT89
G	178	ALA	GLU	ENGINEERED MUTATION	UNP Q9FT89
G	179	ALA	GLN	ENGINEERED MUTATION	UNP Q9FT89
G	281	ALA	GLU	ENGINEERED MUTATION	UNP Q9FT89
G	282	ALA	LYS	ENGINEERED MUTATION	UNP Q9FT89
H	1	GLY	-	EXPRESSION TAG	UNP Q9FT89
H	178	ALA	GLU	ENGINEERED MUTATION	UNP Q9FT89
H	179	ALA	GLN	ENGINEERED MUTATION	UNP Q9FT89
H	281	ALA	GLU	ENGINEERED MUTATION	UNP Q9FT89
H	282	ALA	LYS	ENGINEERED MUTATION	UNP Q9FT89

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

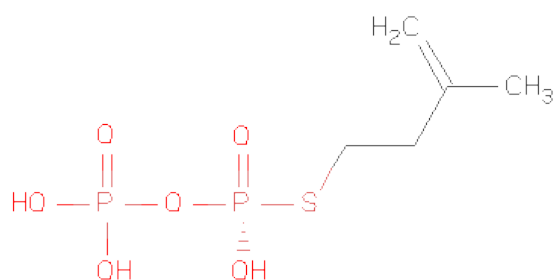
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	2	Total Mg 2 2	0	0
2	A	2	Total Mg 2 2	0	0
2	C	2	Total Mg 2 2	0	0
2	E	2	Total Mg 2 2	0	0

- Molecule 3 is FARNESYL DIPHOSPHATE (three-letter code: FPP) (formula: C₁₅H₂₈O₇P₂).



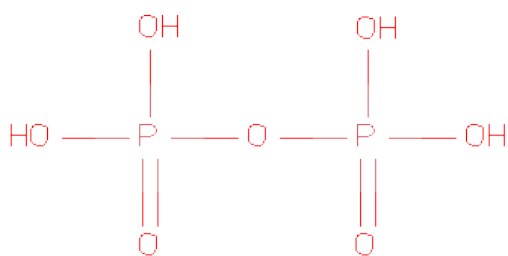
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			24	15	7	2		
3	B	1	Total	C	O	P	0	0
			24	15	7	2		
3	C	1	Total	C	O	P	0	0
			24	15	7	2		
3	E	1	Total	C	O	P	0	0
			24	15	7	2		
3	G	1	Total	C	O	P	0	0
			24	15	7	2		
3	H	1	Total	C	O	P	0	0
			24	15	7	2		

- Molecule 4 is 3-METHYLBUT-3-ENYLSULFANYL(PHOSPHONOOXY)PHOSPHINIC ACID (three-letter code: ISY) (formula: C₅H₁₂O₆P₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	O	P	S	0	0
			14	5	6	2	1		
4	H	1	Total	C	O	P	S	0	0
			14	5	6	2	1		

- Molecule 5 is PYROPHOSPHATE (three-letter code: PPV) (formula: $\text{H}_4\text{O}_7\text{P}_2$).



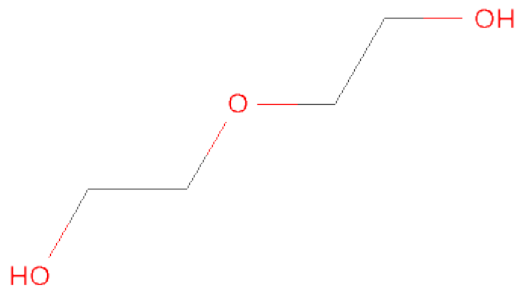
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	P	0	0
			9	7	2		
5	C	1	Total	O	P	0	0
			9	7	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	O	P	0	0
			9	7	2		
5	E	1	Total	O	P	0	0
			9	7	2		
5	F	1	Total	O	P	0	0
			9	7	2		
5	G	1	Total	O	P	0	0
			9	7	2		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			7	4	3		
6	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	83	Total	O	0	0
			83	83		
7	B	98	Total	O	0	0
			98	98		
7	C	116	Total	O	0	0
			116	116		

Continued on next page...

Continued from previous page...

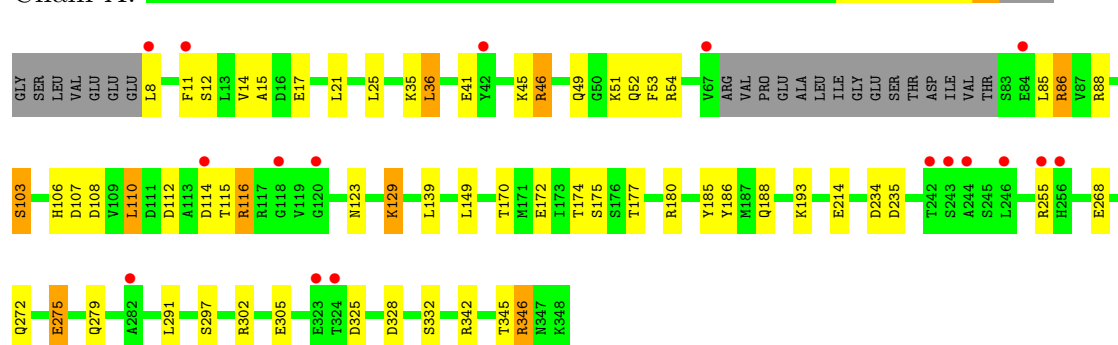
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	100	Total 100	O 100	0	0
7	E	67	Total 67	O 67	0	0
7	F	78	Total 78	O 78	0	0
7	G	77	Total 77	O 77	0	0
7	H	76	Total 76	O 76	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

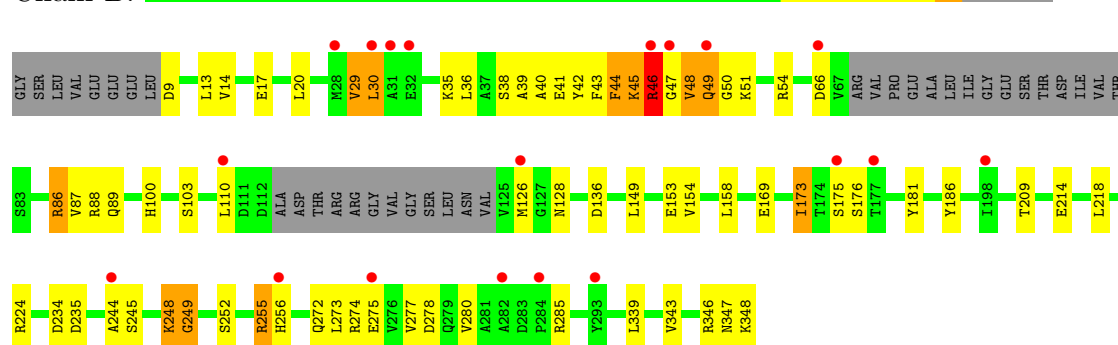
- Molecule 1: Geranyl diphosphate synthase

Chain A:



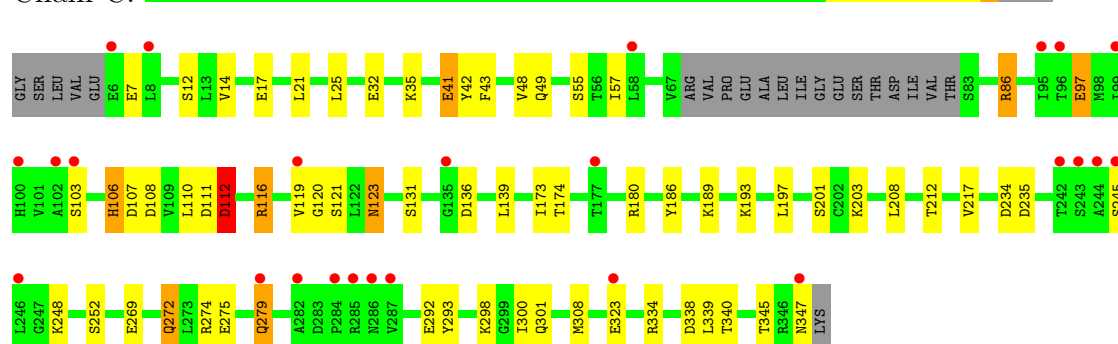
- Molecule 1: Geranyl diphosphate synthase

Chain B:



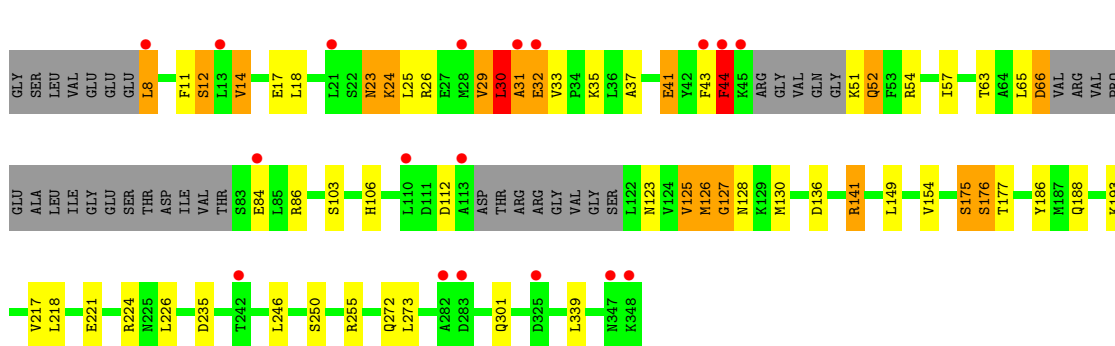
- Molecule 1: Geranyl diphosphate synthase

Chain C:



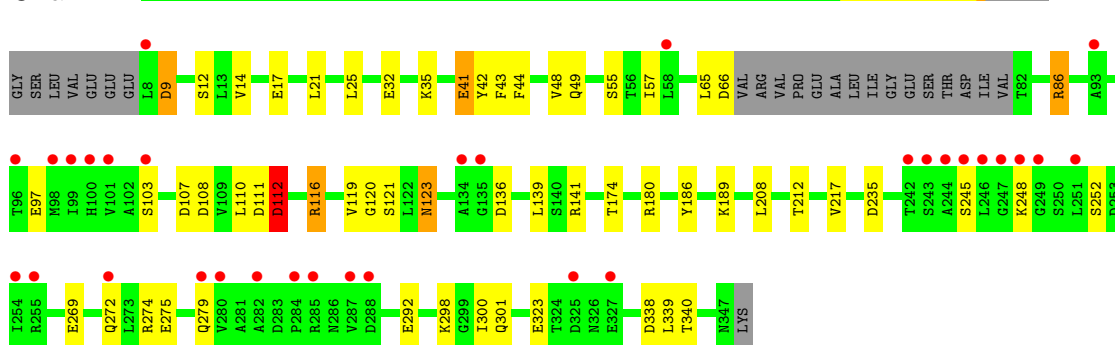
- Molecule 1: Geranyl diphosphate synthase

Chain D:



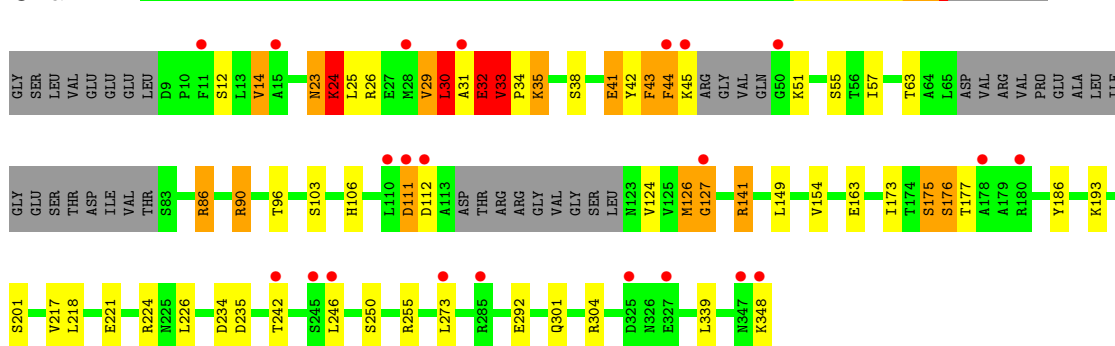
- Molecule 1: Geranyl diphosphate synthase

Chain E:



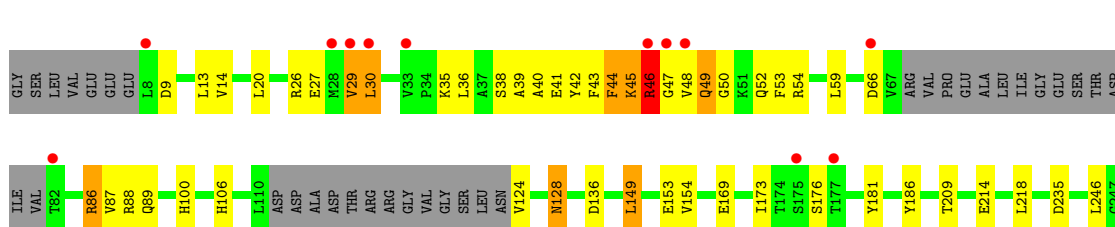
- Molecule 1: Geranyl diphosphate synthase

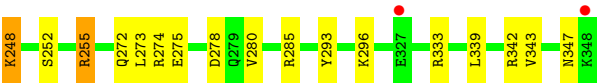
Chain F:



- Molecule 1: Geranyl diphosphate synthase

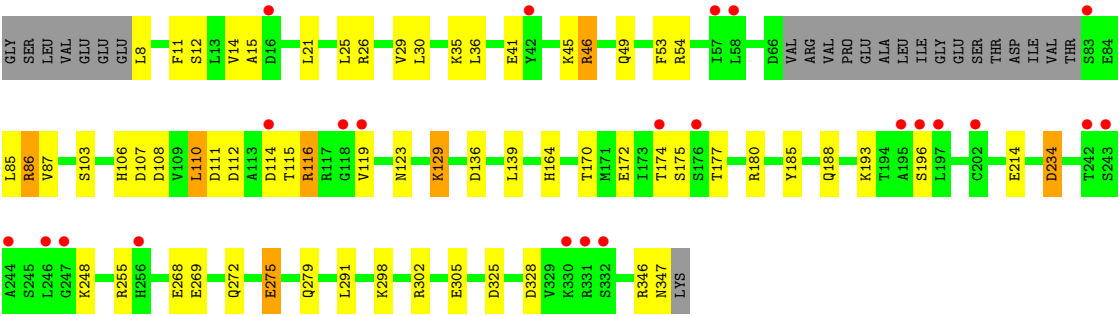
Chain G:





● Molecule 1: Geranyl diphosphate synthase

Chain H: A horizontal bar chart for Chain H showing the distribution of residues by quality. The bar is primarily green, indicating good quality, with a small yellow segment and a very small orange segment at the end.



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	115.96Å 115.96Å 385.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.65 29.83 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.6 (30.00-2.65) 98.7 (29.83-2.65)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.64Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.222 , 0.274 0.251 , 0.282	Depositor DCC
R_{free} test set	4164 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	69.0	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 31.8	EDS
Estimated twinning fraction	0.944 for H, K, L 0.056 for -H-K, K, -L 0.047 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.944 for H, K, L 0.056 for -H-K, K, -L	Depositor
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 83457 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	20426	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PPV, MG, PEG, ISY, FPP

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	0.45	0/2516	0.64	2/3399 (0.1%)
1	B	0.61	0/2421	0.70	1/3269 (0.0%)
1	C	0.56	1/2524 (0.0%)	0.68	2/3412 (0.1%)
1	D	0.53	0/2414	0.67	0/3260
1	E	0.47	1/2506 (0.0%)	0.66	1/3388 (0.0%)
1	F	0.49	0/2394	0.67	3/3232 (0.1%)
1	G	0.61	0/2427	0.71	1/3278 (0.0%)
1	H	0.42	0/2499	0.62	0/3378
All	All	0.52	2/19701 (0.0%)	0.67	10/26616 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	2
1	F	0	1
1	G	0	1
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	217	VAL	CB-CG1	-6.83	1.38	1.52
1	E	217	VAL	CB-CG2	-6.45	1.39	1.52

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	LEU	CA-CB-CG	6.40	130.03	115.30
1	G	149	LEU	CA-CB-CG	6.23	129.63	115.30
1	E	217	VAL	CG1-CB-CG2	-6.13	101.09	110.90
1	F	32	GLU	CB-CA-C	-6.09	98.22	110.40
1	F	127	GLY	N-CA-C	5.83	127.67	113.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	35	LYS	Peptide
1	D	31	ALA	Peptide
1	D	32	GLU	Peptide
1	F	32	GLU	Peptide
1	G	35	LYS	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2488	0	0	26	2
1	B	2394	0	0	45	0
1	C	2496	0	0	30	0
1	D	2388	0	0	44	0
1	E	2478	0	0	21	0
1	F	2368	0	0	37	0
1	G	2400	0	0	50	0
1	H	2471	0	0	25	2
2	A	2	0	0	0	0
2	C	2	0	0	0	0
2	E	2	0	0	0	0
2	H	2	0	0	0	0
3	A	24	0	25	2	0
3	B	24	0	25	0	0
3	C	24	0	25	5	0
3	E	24	0	25	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	24	0	25	1	0
3	H	24	0	25	2	0
4	A	14	0	9	2	0
4	H	14	0	9	2	0
5	B	9	0	0	2	0
5	C	9	0	0	0	0
5	D	9	0	0	0	0
5	E	9	0	0	0	0
5	F	9	0	0	0	0
5	G	9	0	0	0	0
6	B	7	0	10	0	0
6	D	7	0	10	0	0
7	A	83	0	0	4	0
7	B	98	0	0	6	0
7	C	116	0	0	2	0
7	D	100	0	0	2	0
7	E	67	0	0	0	0
7	F	78	0	0	3	0
7	G	77	0	0	3	0
7	H	76	0	0	0	0
All	All	20426	0	188	251	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

The worst 5 of 251 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:274:ARG:NH2	1:F:30:LEU:CD1	2.06	1.18
1:B:256:HIS:CE1	7:B:551:HOH:O	2.02	1.10
1:G:46:ARG:CD	1:G:49:GLN:CA	2.30	1.10
1:B:48:VAL:CG1	1:B:49:GLN:CA	2.29	1.09
1:B:48:VAL:CG2	1:B:49:GLN:C	2.28	1.00

All (2) 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	Distance(Å)	Clash(Å)
1:A:15:ALA:O	1:H:46:ARG:NH1[1.665]	1.98	0.22
1:A:46:ARG:NH1	1:H:15:ALA:O[1.665]	2.19	0.01

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	322/348 (92%)	312 (97%)	9 (3%)	1 (0%)	50	80
1	B	307/348 (88%)	289 (94%)	15 (5%)	3 (1%)	22	48
1	C	323/348 (93%)	311 (96%)	11 (3%)	1 (0%)	50	80
1	D	304/348 (87%)	280 (92%)	14 (5%)	10 (3%)	6	12
1	E	321/348 (92%)	308 (96%)	12 (4%)	1 (0%)	50	80
1	F	302/348 (87%)	282 (93%)	14 (5%)	6 (2%)	11	25
1	G	308/348 (88%)	291 (94%)	16 (5%)	1 (0%)	50	80
1	H	320/348 (92%)	308 (96%)	11 (3%)	1 (0%)	50	80
All	All	2507/2784 (90%)	2381 (95%)	102 (4%)	24 (1%)	22	48

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	46	ARG
1	B	48	VAL
1	C	112	ASP
1	D	30	LEU
1	D	31	ALA

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	266/285 (93%)	231 (87%)	35 (13%)	6	13
1	B	256/285 (90%)	218 (85%)	38 (15%)	4	10
1	C	267/285 (94%)	226 (85%)	41 (15%)	4	9

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	256/285 (90%)	225 (88%)	31 (12%)	7	15
1	E	265/285 (93%)	230 (87%)	35 (13%)	6	13
1	F	253/285 (89%)	217 (86%)	36 (14%)	5	11
1	G	257/285 (90%)	221 (86%)	36 (14%)	5	11
1	H	264/285 (93%)	225 (85%)	39 (15%)	4	10
All	All	2084/2280 (91%)	1793 (86%)	291 (14%)	5	11

5 of 291 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	126	MET
1	E	174	THR
1	H	103	SER
1	D	175	SER
1	E	14	VAL

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

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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
3	FPP	A	1002	2	23,23,23	2.00	7 (30%)	31,31,31	1.25	4 (12%)
4	ISY	A	1003	-	13,13,13	4.76	6 (46%)	17,19,19	3.05	5 (29%)
5	PPV	B	1000	-	8,8,8	2.16	4 (50%)	13,13,13	1.43	2 (15%)
3	FPP	B	1001	-	23,23,23	2.09	10 (43%)	31,31,31	1.16	2 (6%)
6	PEG	B	1002	-	6,6,6	0.40	0	5,5,5	0.79	0
3	FPP	C	1002	2	23,23,23	2.02	9 (39%)	31,31,31	1.34	5 (16%)
5	PPV	C	1003	-	8,8,8	2.05	2 (25%)	13,13,13	1.13	1 (7%)
5	PPV	D	1000	-	8,8,8	2.22	4 (50%)	13,13,13	1.58	1 (7%)
6	PEG	D	1002	-	6,6,6	0.86	0	5,5,5	0.63	0
3	FPP	E	1002	2	23,23,23	2.06	8 (34%)	31,31,31	1.20	4 (12%)
5	PPV	E	1003	-	8,8,8	2.05	3 (37%)	13,13,13	1.41	2 (15%)
5	PPV	F	1000	-	8,8,8	2.23	3 (37%)	13,13,13	1.40	1 (7%)
5	PPV	G	1000	-	8,8,8	2.29	5 (62%)	13,13,13	1.51	1 (7%)
3	FPP	G	1001	-	23,23,23	2.02	8 (34%)	31,31,31	1.57	3 (9%)
3	FPP	H	1002	2	23,23,23	2.09	9 (39%)	31,31,31	1.37	3 (9%)
4	ISY	H	1003	-	13,13,13	3.93	5 (38%)	17,19,19	3.21	5 (29%)

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
3	FPP	A	1002	2	-	0/25/25/25	0/0/0/0
4	ISY	A	1003	-	-	1/11/13/13	0/0/0/0
5	PPV	B	1000	-	-	0/6/6/6	0/0/0/0
3	FPP	B	1001	-	-	0/25/25/25	0/0/0/0
6	PEG	B	1002	-	-	0/4/4/4	0/0/0/0
3	FPP	C	1002	2	-	0/25/25/25	0/0/0/0
5	PPV	C	1003	-	-	0/6/6/6	0/0/0/0
5	PPV	D	1000	-	-	0/6/6/6	0/0/0/0
6	PEG	D	1002	-	-	0/4/4/4	0/0/0/0
3	FPP	E	1002	2	-	0/25/25/25	0/0/0/0
5	PPV	E	1003	-	-	0/6/6/6	0/0/0/0
5	PPV	F	1000	-	-	0/6/6/6	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PPV	G	1000	-	-	0/6/6/6	0/0/0/0
3	FPP	G	1001	-	-	0/25/25/25	0/0/0/0
3	FPP	H	1002	2	-	0/25/25/25	0/0/0/0
4	ISY	H	1003	-	-	1/11/13/13	0/0/0/0

The worst 5 of 83 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1003	ISY	P3-S9	-14.56	1.69	2.08
4	H	1003	ISY	P3-S9	-10.87	1.79	2.08
4	H	1003	ISY	C14-C12	5.57	1.51	1.33
4	A	1003	ISY	C14-C12	5.39	1.51	1.33
4	A	1003	ISY	C11-C12	-4.94	1.40	1.51

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1003	ISY	C10-C11-C12	11.61	130.92	113.17
4	A	1003	ISY	C10-C11-C12	10.83	129.74	113.17
3	G	1001	FPP	PA-O3A-PB	-4.77	117.71	131.68
3	H	1002	FPP	PA-O3A-PB	-4.47	118.57	131.68
3	A	1002	FPP	PA-O3A-PB	-4.26	119.20	131.68

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1003	ISY	O7-P3-S9-C10
4	H	1003	ISY	O7-P3-S9-C10

There are no ring outliers.

5.7 Other polymers ⓘ

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	326/348 (93%)	0.38	17 (5%) 26 27	53, 82, 121, 153	0
1	B	313/348 (89%)	0.48	19 (6%) 21 21	49, 69, 125, 175	0
1	C	327/348 (93%)	0.35	25 (7%) 14 14	46, 69, 110, 141	0
1	D	312/348 (89%)	0.32	18 (5%) 22 23	49, 70, 109, 142	0
1	E	325/348 (93%)	0.40	32 (9%) 8 7	54, 79, 117, 144	0
1	F	310/348 (89%)	0.37	22 (7%) 16 16	52, 76, 108, 141	0
1	G	314/348 (90%)	0.31	14 (4%) 32 34	46, 66, 119, 166	0
1	H	324/348 (93%)	0.38	23 (7%) 16 16	57, 85, 121, 147	0
All	All	2551/2784 (91%)	0.37	170 (6%) 18 18	46, 75, 118, 175	0

The worst 5 of 170 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	244	ALA	7.3
1	A	244	ALA	6.9
1	G	30	LEU	6.7
1	H	243	SER	6.5
1	E	244	ALA	6.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	PEG	D	1002	7/7	0.36	2.81	3,4,5,8	0
2	MG	C	1000	1/1	0.29	2.60	53,53,53,53	0
6	PEG	B	1002	7/7	0.41	2.33	22,23,24,27	0
5	PPV	D	1000	9/9	0.21	0.53	109,109,110,110	0
2	MG	A	1001	1/1	0.16	-0.29	63,63,63,63	0
5	PPV	F	1000	9/9	0.17	-0.31	131,131,131,132	0
3	FPP	G	1001	24/24	0.21	-0.35	51,56,62,63	0
3	FPP	B	1001	24/24	0.21	-0.38	65,67,68,69	0
2	MG	E	1000	1/1	0.17	-0.42	62,62,62,62	0
2	MG	A	1000	1/1	0.13	-0.65	46,46,46,46	0
3	FPP	H	1002	24/24	0.15	-0.89	20,40,42,43	0
3	FPP	A	1002	24/24	0.15	-0.98	25,37,44,45	0
5	PPV	B	1000	9/9	0.13	-0.99	57,59,62,62	0
4	ISY	H	1003	14/14	0.14	-1.14	38,41,44,45	0
5	PPV	G	1000	9/9	0.12	-1.17	69,70,70,71	0
4	ISY	A	1003	14/14	0.15	-1.22	33,40,44,45	0
2	MG	H	1000	1/1	0.14	-1.25	42,42,42,42	0
2	MG	H	1001	1/1	0.12	-1.40	61,61,61,61	0
5	PPV	C	1003	9/9	0.12	-1.41	25,29,32,33	0
3	FPP	E	1002	24/24	0.13	-1.42	40,42,45,45	0
3	FPP	C	1002	24/24	0.12	-1.57	26,35,40,40	0
5	PPV	E	1003	9/9	0.11	-1.59	31,33,35,36	0
2	MG	C	1001	1/1	0.09	-2.65	36,36,36,36	0
2	MG	E	1001	1/1	0.11	-3.62	47,47,47,47	0

6.5 Other polymers ⓘ

There are no such residues in this entry.