



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 14, 2016 – 02:22 PM EDT

PDB ID : 5HN7
Title : Crystal structure of Plasmodium vivax geranylgeranylpyrophosphate synthase complexed with BPH-1158
Authors : Liu, Y.-L.; Zhang, Y.; Oldfield, E.
Deposited on : 2016-01-18
Resolution : 2.15 Å(reported)

This is a wwPDB X-ray Structure 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/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

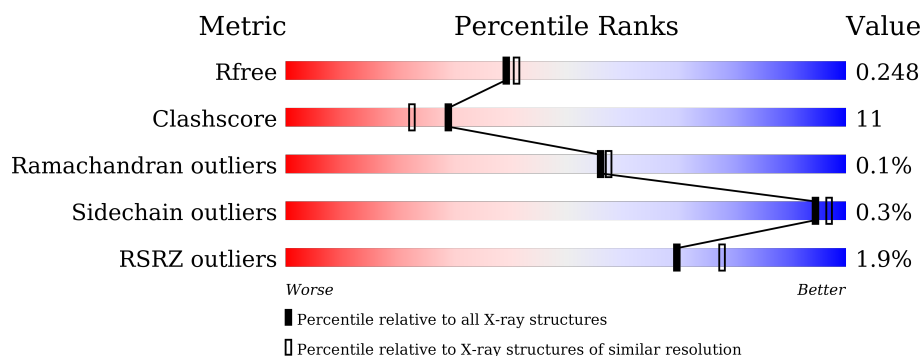
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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. 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	375	<div> <div>0%</div> <div> <div></div> <div>76%</div> <div>17%</div> <div>7%</div> </div> </div>
1	B	375	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>15%</div> <div>7%</div> </div> </div>
1	C	375	<div> <div>0%</div> <div> <div></div> <div>81%</div> <div>14%</div> <div>5%</div> </div> </div>
1	D	375	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>19%</div> <div>7%</div> </div> </div>
1	E	375	<div> <div>0%</div> <div> <div></div> <div>82%</div> <div>13%</div> <div>5%</div> </div> </div>
1	F	375	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>16%</div> <div>8%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	375	
1	H	375	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	04M	A	401	-	-	X	X
2	04M	B	401	-	-	-	X
2	04M	C	401	-	-	-	X
2	04M	D	401	-	-	-	X
2	04M	E	401	-	-	-	X
2	04M	F	401	-	-	-	X
2	04M	G	401	-	-	-	X
2	04M	H	401	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23721 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 Farnesyl pyrophosphate synthase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	0	0	0
			2778	1805	442	516	15			
1	B	348	Total	C	N	O	S	0	0	0
			2785	1812	443	515	15			
1	C	357	Total	C	N	O	S	0	0	0
			2851	1850	459	527	15			
1	D	347	Total	C	N	O	S	0	0	0
			2763	1795	441	512	15			
1	E	358	Total	C	N	O	S	0	0	0
			2862	1858	459	530	15			
1	F	345	Total	C	N	O	S	0	0	0
			2766	1797	440	514	15			
1	G	346	Total	C	N	O	S	0	0	0
			2774	1803	441	515	15			
1	H	348	Total	C	N	O	S	0	0	0
			2792	1817	443	517	15			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	134	MET	THR	SEE REMARK 999	UNP A5K4U6
A	227	ASP	ASN	SEE REMARK 999	UNP A5K4U6
B	134	MET	THR	SEE REMARK 999	UNP A5K4U6
B	227	ASP	ASN	SEE REMARK 999	UNP A5K4U6
C	134	MET	THR	SEE REMARK 999	UNP A5K4U6
C	227	ASP	ASN	SEE REMARK 999	UNP A5K4U6
D	134	MET	THR	SEE REMARK 999	UNP A5K4U6
D	227	ASP	ASN	SEE REMARK 999	UNP A5K4U6
E	134	MET	THR	SEE REMARK 999	UNP A5K4U6
E	227	ASP	ASN	SEE REMARK 999	UNP A5K4U6
F	134	MET	THR	SEE REMARK 999	UNP A5K4U6
F	227	ASP	ASN	SEE REMARK 999	UNP A5K4U6
G	134	MET	THR	SEE REMARK 999	UNP A5K4U6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	227	ASP	ASN	SEE REMARK 999	UNP A5K4U6
H	134	MET	THR	SEE REMARK 999	UNP A5K4U6
H	227	ASP	ASN	SEE REMARK 999	UNP A5K4U6

- # 04M

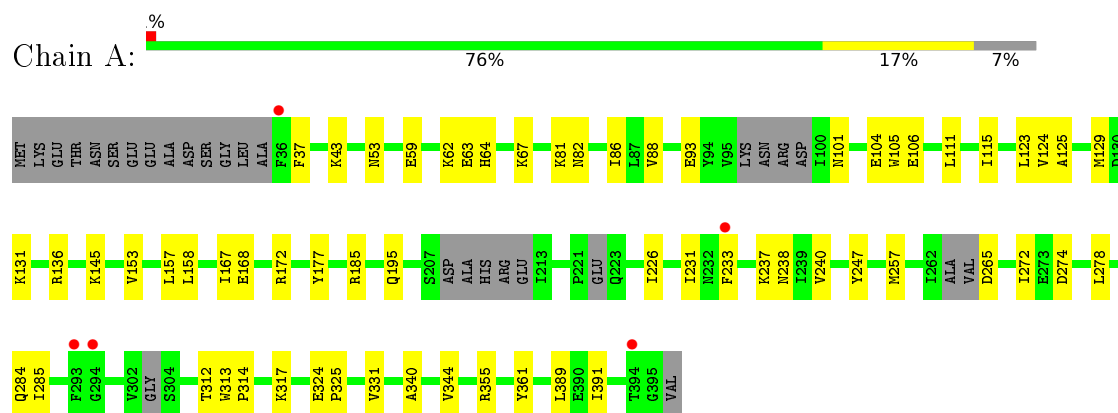
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	149	Total 149	O 149	0	0
3	B	145	Total 145	O 145	0	0
3	C	165	Total 165	O 165	0	0
3	D	129	Total 129	O 129	0	0
3	E	150	Total 150	O 150	0	0
3	F	97	Total 97	O 97	0	0
3	G	109	Total 109	O 109	0	0
3	H	126	Total 126	O 126	0	0

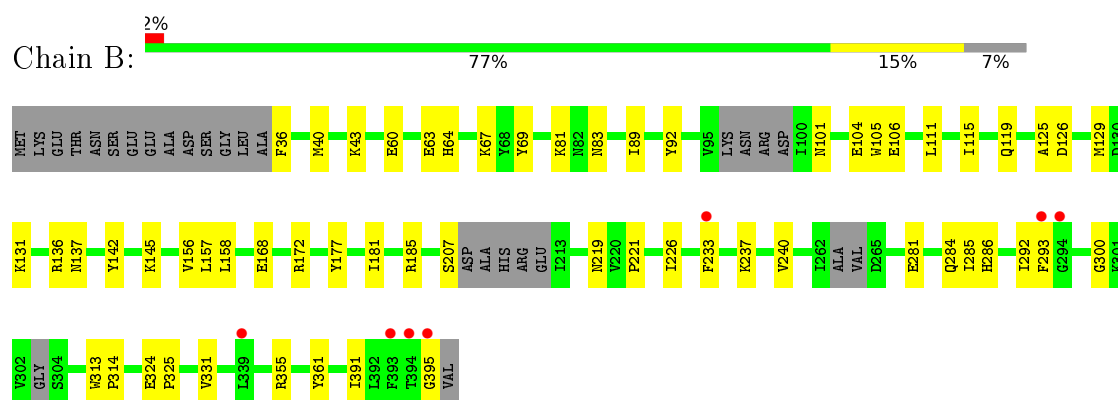
3 Residue-property plots

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.

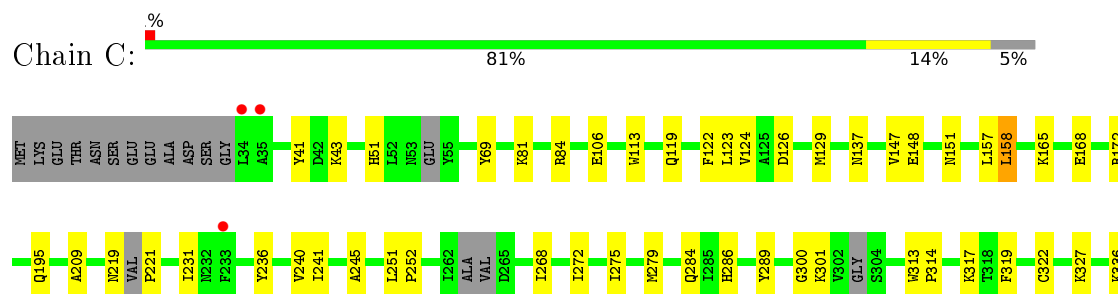
- Molecule 1: Farnesyl pyrophosphate synthase, putative

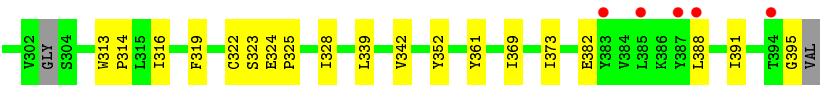


- Molecule 1: Farnesyl pyrophosphate synthase, putative

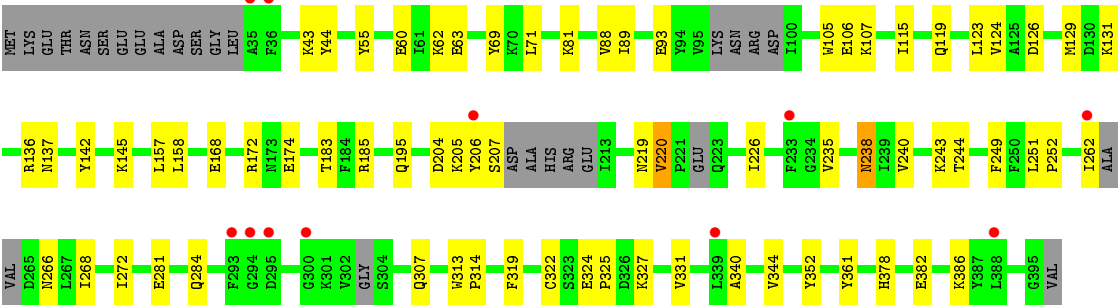
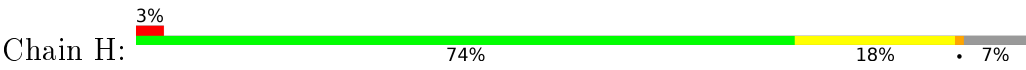


- Molecule 1: Farnesyl pyrophosphate synthase, putative





● Molecule 1: Farnesyl pyrophosphate synthase, putative



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	107.78Å 108.38Å 140.04Å 90.00° 90.43° 90.00°	Depositor
Resolution (Å)	36.81 – 2.15 36.81 – 2.15	Depositor EDS
% Data completeness (in resolution range)	96.8 (36.81-2.15) 94.9 (36.81-2.15)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.198 , 0.249 0.200 , 0.248	Depositor DCC
R_{free} test set	8481 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 21.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.017 for -k,-h,-l 0.016 for k,h,-l 0.439 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23721	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: 04M

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	0.33	0/2834	0.45	0/3838
1	B	0.32	0/2843	0.45	0/3852
1	C	0.34	0/2910	0.46	1/3941 (0.0%)
1	D	0.30	0/2819	0.44	0/3820
1	E	0.33	0/2921	0.46	0/3955
1	F	0.30	0/2821	0.44	0/3818
1	G	0.30	0/2830	0.43	0/3830
1	H	0.31	0/2849	0.45	0/3858
All	All	0.32	0/22827	0.45	1/30912 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	158	LEU	CA-CB-CG	-5.63	102.36	115.30

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	2778	0	2641	85	0
1	B	2785	0	2647	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2851	0	2705	55	0
1	D	2763	0	2616	73	0
1	E	2862	0	2719	55	0
1	F	2766	0	2636	58	0
1	G	2774	0	2636	57	0
1	H	2792	0	2662	71	0
2	A	35	0	0	29	0
2	B	35	0	0	14	0
2	C	35	0	0	11	0
2	D	35	0	0	10	0
2	E	35	0	0	10	0
2	F	35	0	0	8	0
2	G	35	0	0	10	0
2	H	35	0	0	11	0
3	A	149	0	0	9	0
3	B	145	0	0	4	0
3	C	165	0	0	4	0
3	D	129	0	0	4	0
3	E	150	0	0	4	0
3	F	97	0	0	1	0
3	G	109	0	0	5	0
3	H	126	0	0	2	0
All	All	23721	0	21262	499	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 11.

The worst 5 of 499 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:H:119:GLN:HE21	2:H:401:04M:CAW	1.22	1.50
1:G:119:GLN:HE21	2:G:401:04M:CAW	1.32	1.41
1:A:195:GLN:HG2	2:A:401:04M:CAO	1.53	1.37
1:D:157:LEU:HD13	2:G:401:04M:CAN	1.53	1.36
1:H:119:GLN:NE2	2:H:401:04M:CAW	1.90	1.34

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	335/375 (89%)	328 (98%)	7 (2%)	0	100	100
1	B	338/375 (90%)	330 (98%)	8 (2%)	0	100	100
1	C	347/375 (92%)	335 (96%)	12 (4%)	0	100	100
1	D	335/375 (89%)	324 (97%)	10 (3%)	1 (0%)	46	42
1	E	348/375 (93%)	339 (97%)	9 (3%)	0	100	100
1	F	333/375 (89%)	325 (98%)	7 (2%)	1 (0%)	46	42
1	G	334/375 (89%)	325 (97%)	9 (3%)	0	100	100
1	H	336/375 (90%)	322 (96%)	12 (4%)	2 (1%)	30	21
All	All	2706/3000 (90%)	2628 (97%)	74 (3%)	4 (0%)	56	57

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	220	VAL
1	H	220	VAL
1	F	205	LYS
1	H	205	LYS

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	282/339 (83%)	281 (100%)	1 (0%)	93	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	282/339 (83%)	282 (100%)	0	100	100
1	C	287/339 (85%)	287 (100%)	0	100	100
1	D	278/339 (82%)	277 (100%)	1 (0%)	93	96
1	E	289/339 (85%)	286 (99%)	3 (1%)	82	87
1	F	281/339 (83%)	281 (100%)	0	100	100
1	G	281/339 (83%)	280 (100%)	1 (0%)	93	96
1	H	284/339 (84%)	283 (100%)	1 (0%)	93	96
All	All	2264/2712 (84%)	2257 (100%)	7 (0%)	94	97

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	240	VAL
1	H	238	ASN
1	E	307	GLN
1	D	247	TYR
1	G	319	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	137	ASN
1	D	286	HIS
1	H	119	GLN
1	D	238	ASN
1	D	337	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	04M	A	401	-	34,37,37	1.71	3 (8%)	44,49,49	2.42	12 (27%)
2	04M	B	401	-	34,37,37	1.61	4 (11%)	44,49,49	2.95	10 (22%)
2	04M	C	401	-	34,37,37	1.75	4 (11%)	44,49,49	3.22	18 (40%)
2	04M	D	401	-	34,37,37	1.72	4 (11%)	44,49,49	2.59	16 (36%)
2	04M	E	401	-	34,37,37	1.75	3 (8%)	44,49,49	3.01	18 (40%)
2	04M	F	401	-	34,37,37	1.72	4 (11%)	44,49,49	2.83	18 (40%)
2	04M	G	401	-	34,37,37	1.64	3 (8%)	44,49,49	2.87	16 (36%)
2	04M	H	401	-	34,37,37	1.69	3 (8%)	44,49,49	3.05	18 (40%)

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
2	04M	A	401	-	-	0/26/38/38	0/3/3/3
2	04M	B	401	-	-	0/26/38/38	0/3/3/3
2	04M	C	401	-	-	0/26/38/38	0/3/3/3
2	04M	D	401	-	-	0/26/38/38	0/3/3/3
2	04M	E	401	-	-	0/26/38/38	0/3/3/3
2	04M	F	401	-	-	0/26/38/38	0/3/3/3
2	04M	G	401	-	-	0/26/38/38	0/3/3/3
2	04M	H	401	-	-	0/26/38/38	0/3/3/3

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	401	04M	CAV-CBC	-5.33	1.38	1.50
2	A	401	04M	CAV-CBC	-5.26	1.38	1.50
2	E	401	04M	CAV-CBC	-5.10	1.38	1.50
2	D	401	04M	CAV-CBC	-4.98	1.39	1.50
2	G	401	04M	CAV-CBC	-4.96	1.39	1.50

The worst 5 of 126 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	04M	OAY-CAT-CAW	-11.93	84.27	111.83
2	E	401	04M	OAY-CAU-CAX	-11.05	86.31	111.83
2	G	401	04M	OAY-CAU-CAX	-10.83	86.81	111.83
2	H	401	04M	OAY-CAU-CAX	-10.06	88.60	111.83
2	A	401	04M	OAY-CAT-CAW	-9.64	89.57	111.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 103 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	04M	29	0
2	B	401	04M	14	0
2	C	401	04M	11	0
2	D	401	04M	10	0
2	E	401	04M	10	0
2	F	401	04M	8	0
2	G	401	04M	10	0
2	H	401	04M	11	0

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	347/375 (92%)	0.13	5 (1%) 78 83	11, 25, 41, 51	0
1	B	348/375 (92%)	0.15	7 (2%) 68 75	11, 24, 40, 57	0
1	C	357/375 (95%)	0.06	3 (0%) 87 90	10, 24, 42, 53	0
1	D	347/375 (92%)	0.26	9 (2%) 59 68	16, 29, 48, 58	0
1	E	358/375 (95%)	0.10	2 (0%) 90 92	10, 24, 43, 57	0
1	F	345/375 (92%)	0.29	8 (2%) 64 72	15, 31, 50, 60	0
1	G	346/375 (92%)	0.31	9 (2%) 59 68	15, 31, 49, 62	0
1	H	348/375 (92%)	0.23	11 (3%) 51 61	15, 29, 49, 60	0
All	All	2796/3000 (93%)	0.19	54 (1%) 70 78	10, 27, 46, 62	0

The worst 5 of 54 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	294	GLY	6.3
1	C	35	ALA	5.1
1	F	388	LEU	4.7
1	E	396	VAL	4.5
1	B	395	GLY	4.5

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 [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. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	04M	A	401	35/35	0.81	0.38	12.67	13,61,78,80	0
2	04M	C	401	35/35	0.86	0.32	10.62	5,48,74,76	0
2	04M	B	401	35/35	0.84	0.30	10.54	8,41,56,61	0
2	04M	D	401	35/35	0.79	0.36	9.59	26,55,67,68	0
2	04M	E	401	35/35	0.87	0.29	7.84	6,48,60,66	0
2	04M	G	401	35/35	0.86	0.29	7.15	18,41,66,71	0
2	04M	H	401	35/35	0.81	0.32	6.68	16,53,70,71	0
2	04M	F	401	35/35	0.84	0.27	6.11	20,45,68,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.