



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:03 PM GMT

PDB ID : 1N4Q  
Title : Protein Geranylgeranyltransferase type-I Complexed with a GGPP Analog  
and a KKKSKTKCVIL Peptide  
Authors : Taylor, J.S.; Reid, T.S.; Casey, P.J.; Beese, L.S.  
Deposited on : 2002-11-01  
Resolution : 2.40 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](mailto: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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

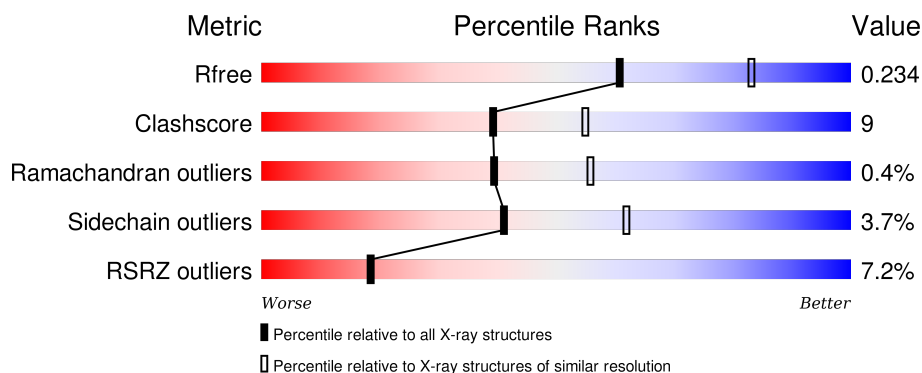
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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  $\geq 3$ , 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	377	<div> <div>4%</div> <div>67% 15% 17%</div> </div>
1	C	377	<div> <div>2%</div> <div>67% 15% 17%</div> </div>
1	E	377	<div> <div>3%</div> <div>64% 18% 17%</div> </div>
1	G	377	<div> <div>3%</div> <div>65% 18% 17%</div> </div>
1	I	377	<div> <div>4%</div> <div>67% 15% 17%</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	377	
2	B	377	
2	D	377	
2	F	377	
2	H	377	
2	J	377	
2	L	377	
3	M	11	
3	N	11	
3	O	11	
3	P	11	
3	Q	11	
3	R	11	

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
6	CL	C	1301	-	-	-	X
6	CL	G	1311	-	-	-	X
6	CL	K	1317	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 33546 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 protein farnesyltransferase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2611	1672	458	476	5			
1	C	314	Total	C	N	O	S	0	0	0
			2630	1683	457	485	5			
1	E	314	Total	C	N	O	S	0	0	0
			2639	1685	461	488	5			
1	G	314	Total	C	N	O	S	0	0	0
			2621	1677	455	484	5			
1	I	314	Total	C	N	O	S	0	0	0
			2645	1690	460	490	5			
1	K	314	Total	C	N	O	S	0	0	0
			2667	1700	466	496	5			

- Molecule 2 is a protein called geranyltransferase type-I beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	346	Total	C	N	O	S	0	0	0
			2689	1702	467	496	24			
2	D	346	Total	C	N	O	S	0	0	0
			2690	1705	463	498	24			
2	F	346	Total	C	N	O	S	0	0	0
			2700	1708	468	500	24			
2	H	346	Total	C	N	O	S	0	0	0
			2680	1698	460	498	24			
2	J	346	Total	C	N	O	S	0	0	0
			2706	1710	471	501	24			
2	L	346	Total	C	N	O	S	0	0	0
			2710	1713	471	502	24			

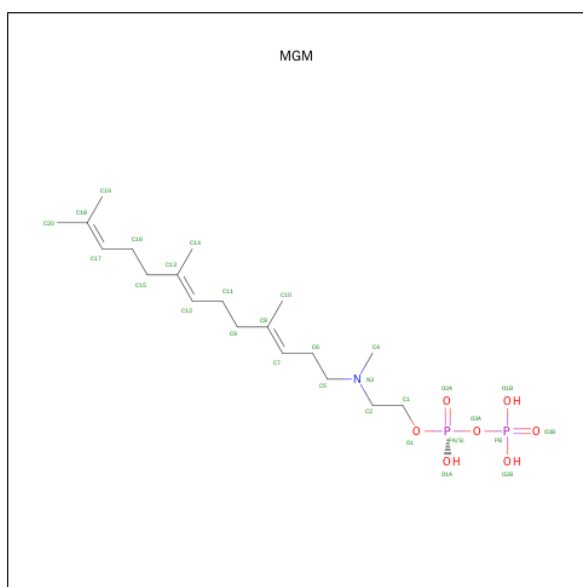
- Molecule 3 is a protein called Fusion protein consisting of transforming protein p21b and Ras related protein Rap-2b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	5	Total	C	N	O	S	0	0	0
			39	26	6	6	1			
3	N	5	Total	C	N	O	S	0	0	0
			39	26	6	6	1			
3	O	5	Total	C	N	O	S	0	0	0
			39	26	6	6	1			
3	P	5	Total	C	N	O	S	0	0	0
			39	26	6	6	1			
3	Q	5	Total	C	N	O	S	0	0	0
			39	26	6	6	1			
3	R	5	Total	C	N	O	S	0	0	0
			39	26	6	6	1			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	J	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		
4	H	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		
4	L	1	Total	Zn	0	0
			1	1		
4	F	1	Total	Zn	0	0
			1	1		

- Molecule 5 is 2-[METHYL-(5-GERANYL-4-METHYL-PENT-3-ENYL)-AMINO]-ETHYL-DIPHOSPHATE (three-letter code: MGM) (formula: C<sub>19</sub>H<sub>37</sub>NO<sub>7</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			29	19	1	7	2		
5	D	1	Total	C	N	O	P	0	0
			29	19	1	7	2		
5	F	1	Total	C	N	O	P	0	0
			29	19	1	7	2		
5	H	1	Total	C	N	O	P	0	0
			29	19	1	7	2		
5	J	1	Total	C	N	O	P	0	0
			29	19	1	7	2		
5	L	1	Total	C	N	O	P	0	0
			29	19	1	7	2		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

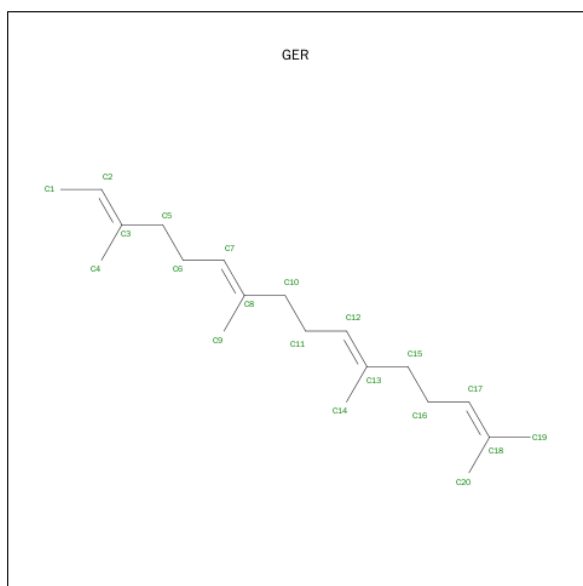
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	1	Total	Cl	0	0
			1	1		
6	J	1	Total	Cl	0	0
			1	1		
6	D	1	Total	Cl	0	0
			1	1		
6	K	1	Total	Cl	0	0
			1	1		
6	H	1	Total	Cl	0	0
			1	1		
6	C	1	Total	Cl	0	0
			1	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	1	Total Cl 1 1	0	0

- Molecule 7 is GERAN-8-YL GERAN (three-letter code: GER) (formula: C<sub>20</sub>H<sub>34</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	R	1	Total C 20 20	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	78	Total O 78 78	0	0
8	B	64	Total O 64 64	0	0
8	C	82	Total O 82 82	0	0
8	D	89	Total O 89 89	0	0
8	E	81	Total O 81 81	0	0
8	F	91	Total O 91 91	0	0
8	G	75	Total O 75 75	0	0

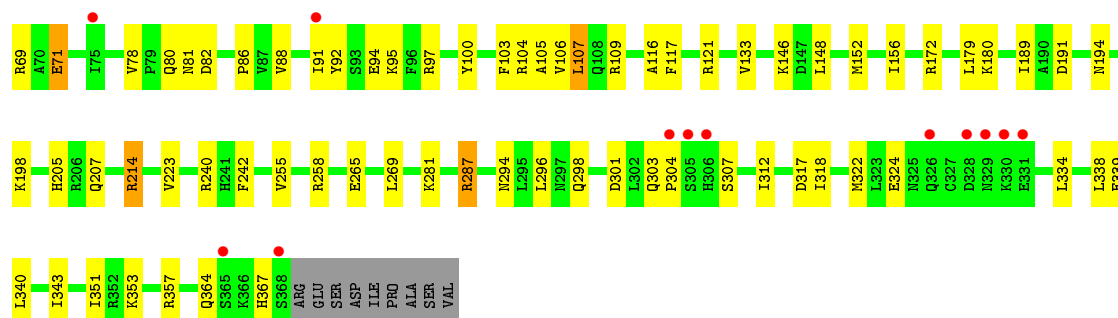
*Continued on next page...*

*Continued from previous page...*

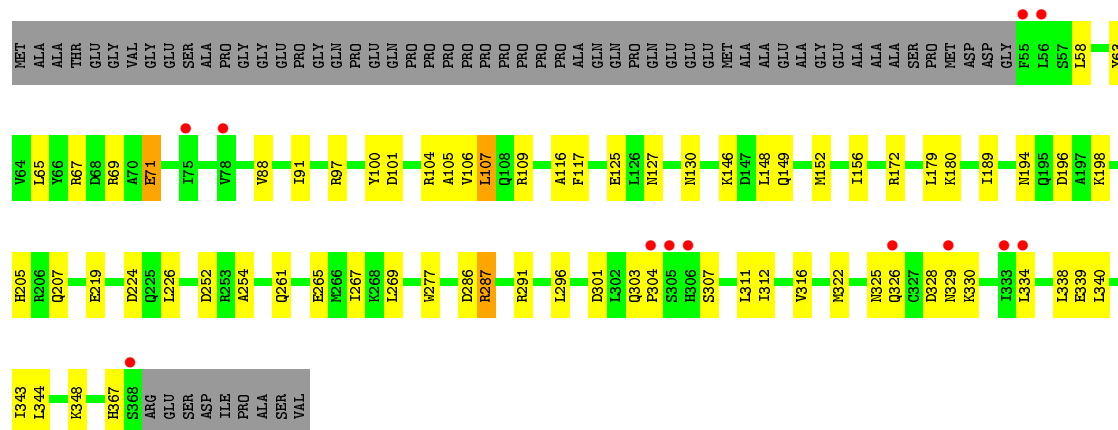
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	H	56	Total 56	O 56	0	0
8	I	104	Total 104	O 104	0	0
8	J	82	Total 82	O 82	0	0
8	K	169	Total 169	O 169	0	0
8	L	121	Total 121	O 121	0	0
8	M	7	Total 7	O 7	0	0
8	N	4	Total 4	O 4	0	0
8	O	4	Total 4	O 4	0	0
8	P	1	Total 1	O 1	0	0
8	Q	6	Total 6	O 6	0	0
8	R	3	Total 3	O 3	0	0



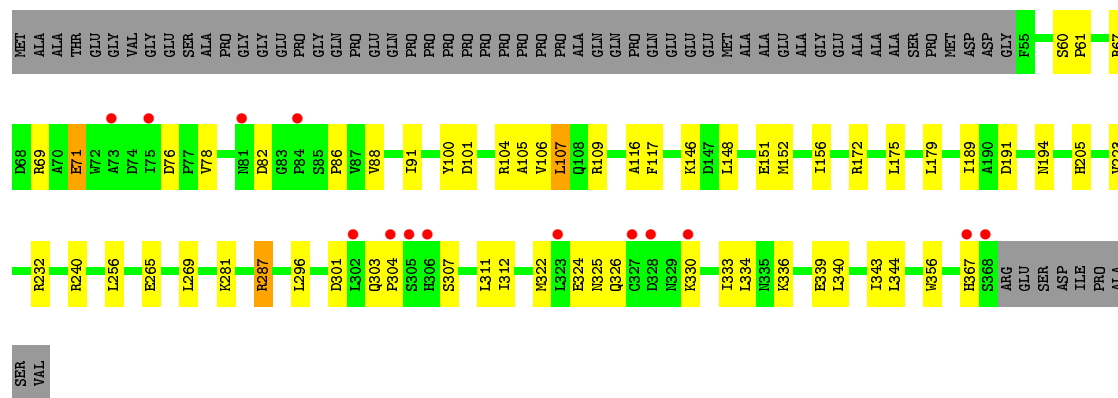




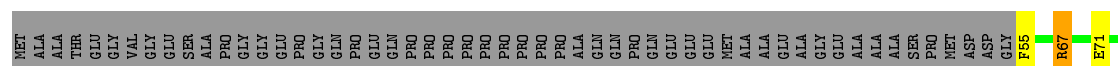
- Molecule 1: protein farnesyltransferase alpha subunit

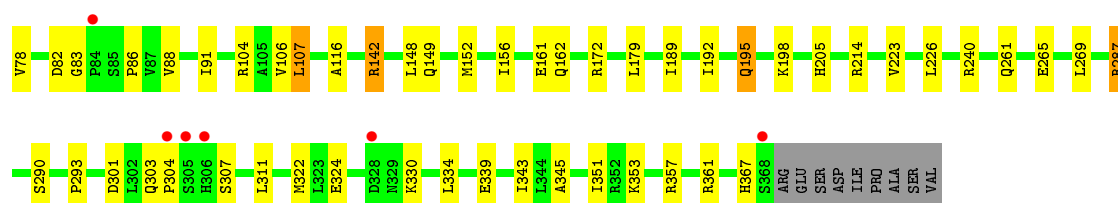


- Molecule 1: protein farnesyltransferase alpha subunit

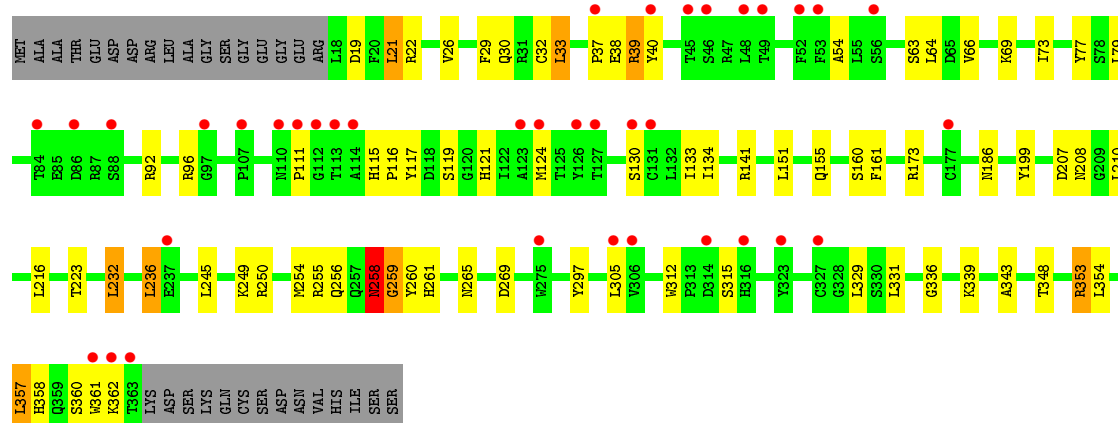


- Molecule 1: protein farnesyltransferase alpha subunit

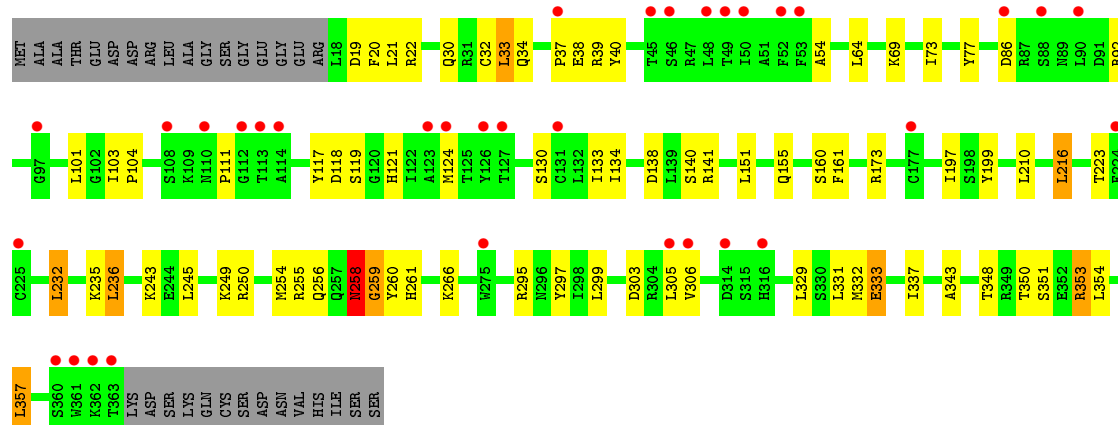




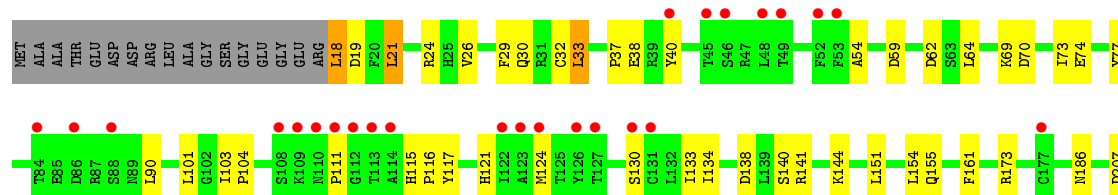
- Molecule 2: geranyltransferase type-I beta subunit



- Molecule 2: geranyltransferase type-I beta subunit



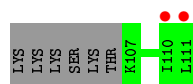
- Molecule 2: geranyltransferase type-I beta subunit



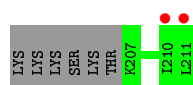




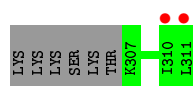
- Molecule 3: Fusion protein consisting of transforming protein p21b and Ras related protein Rap-2b



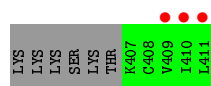
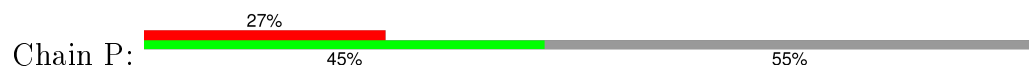
- Molecule 3: Fusion protein consisting of transforming protein p21b and Ras related protein Rap-2b



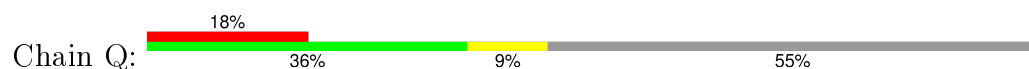
- Molecule 3: Fusion protein consisting of transforming protein p21b and Ras related protein Rap-2b



- Molecule 3: Fusion protein consisting of transforming protein p21b and Ras related protein Rap-2b



- Molecule 3: Fusion protein consisting of transforming protein p21b and Ras related protein Rap-2b



- Molecule 3: Fusion protein consisting of transforming protein p21b and Ras related protein Rap-2b



LYS	K607	
LYS	C608	
LYS	V609	
SER	I610	
LYS	L611	
THR		

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	271.06Å 268.03Å 184.97Å 90.00° 131.73° 90.00°	Depositor
Resolution (Å)	29.99 – 2.40 33.12 – 2.40	Depositor EDS
% Data completeness (in resolution range)	92.8 (29.99-2.40) 92.6 (33.12-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.89 (at 2.39Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.214 , 0.234 0.213 , 0.234	Depositor DCC
$R_{free}$ test set	17765 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.6	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 53.0	EDS
Estimated twinning fraction	0.087 for -h-2*k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 356310 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	33546	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GER, ZN, MGM, CL

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	0.32	0/2677	0.52	0/3645
1	C	0.35	0/2696	0.53	0/3668
1	E	0.33	0/2705	0.53	0/3680
1	G	0.34	0/2687	0.52	0/3658
1	I	0.35	0/2711	0.53	0/3686
1	K	0.39	0/2733	0.55	0/3713
2	B	0.35	0/2750	0.60	2/3720 (0.1%)
2	D	0.36	0/2751	0.60	2/3720 (0.1%)
2	F	0.37	0/2761	0.60	2/3733 (0.1%)
2	H	0.35	0/2741	0.59	2/3710 (0.1%)
2	J	0.36	0/2767	0.60	2/3741 (0.1%)
2	L	0.39	0/2771	0.62	2/3745 (0.1%)
3	M	0.56	0/38	0.52	0/48
3	N	0.53	0/38	0.54	0/48
3	O	0.57	0/38	0.54	0/48
3	P	0.53	0/38	0.51	0/48
3	Q	0.55	0/38	0.52	0/48
3	R	0.67	0/38	1.08	0/48
All	All	0.36	0/32978	0.57	12/44707 (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
2	B	0	1
2	D	0	1
2	F	0	1
All	All	0	3



There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	259	GLY	N-CA-C	-6.07	97.93	113.10
2	L	259	GLY	N-CA-C	-5.91	98.32	113.10
2	H	259	GLY	N-CA-C	-5.90	98.34	113.10
2	D	259	GLY	N-CA-C	-5.87	98.43	113.10
2	F	259	GLY	N-CA-C	-5.82	98.54	113.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	297	TYR	Sidechain
2	D	297	TYR	Sidechain
2	F	297	TYR	Sidechain

## 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	2611	0	2497	46	0
1	C	2630	0	2521	41	0
1	E	2639	0	2532	56	0
1	G	2621	0	2502	58	0
1	I	2645	0	2543	40	0
1	K	2667	0	2577	45	0
2	B	2689	0	2585	50	0
2	D	2690	0	2588	50	0
2	F	2700	0	2602	48	0
2	H	2680	0	2562	60	0
2	J	2706	0	2608	54	0
2	L	2710	0	2617	38	0
3	M	39	0	47	0	0
3	N	39	0	47	0	0
3	O	39	0	47	0	0
3	P	39	0	47	0	0
3	Q	39	0	47	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	R	39	0	47	6	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	H	1	0	0	0	0
4	J	1	0	0	0	0
4	L	1	0	0	0	0
5	B	29	0	34	3	0
5	D	29	0	34	3	0
5	F	29	0	34	2	0
5	H	29	0	34	2	0
5	J	29	0	34	3	0
5	L	29	0	34	4	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	1	0
6	H	1	0	0	0	0
6	J	1	0	0	0	0
6	K	1	0	0	1	0
7	R	20	0	33	7	0
8	A	78	0	0	3	0
8	B	64	0	0	1	0
8	C	82	0	0	2	0
8	D	89	0	0	1	0
8	E	81	0	0	0	0
8	F	91	0	0	3	0
8	G	75	0	0	5	0
8	H	56	0	0	1	0
8	I	104	0	0	1	0
8	J	82	0	0	3	0
8	K	169	0	0	7	0
8	L	121	0	0	3	0
8	M	7	0	0	0	0
8	N	4	0	0	0	0
8	O	4	0	0	0	0
8	P	1	0	0	0	0
8	Q	6	0	0	1	0
8	R	3	0	0	0	0
All	All	33546	0	31253	569	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 9.

The worst 5 of 569 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:K:156:ILE:HG12	1:K:172:ARG:HH12	1.03	1.15
1:E:156:ILE:HG12	1:E:172:ARG:HH12	1.08	1.13
1:A:156:ILE:HG12	1:A:172:ARG:HH12	1.13	1.12
1:C:156:ILE:HG12	1:C:172:ARG:HH12	1.14	1.07
1:I:156:ILE:HG12	1:I:172:ARG:HH12	1.14	1.05

There are no symmetry-related clashes.

## 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	312/377 (83%)	289 (93%)	23 (7%)	0	100	100
1	C	312/377 (83%)	292 (94%)	20 (6%)	0	100	100
1	E	312/377 (83%)	290 (93%)	22 (7%)	0	100	100
1	G	312/377 (83%)	291 (93%)	21 (7%)	0	100	100
1	I	312/377 (83%)	293 (94%)	19 (6%)	0	100	100
1	K	312/377 (83%)	294 (94%)	18 (6%)	0	100	100
2	B	344/377 (91%)	329 (96%)	12 (4%)	3 (1%)	21	30
2	D	344/377 (91%)	329 (96%)	12 (4%)	3 (1%)	21	30
2	F	344/377 (91%)	329 (96%)	13 (4%)	2 (1%)	30	43
2	H	344/377 (91%)	330 (96%)	12 (4%)	2 (1%)	30	43
2	J	344/377 (91%)	327 (95%)	14 (4%)	3 (1%)	21	30
2	L	344/377 (91%)	331 (96%)	11 (3%)	2 (1%)	30	43
3	M	3/11 (27%)	3 (100%)	0	0	100	100
3	N	3/11 (27%)	3 (100%)	0	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	O	3/11 (27%)	3 (100%)	0	0	100	100
3	P	3/11 (27%)	3 (100%)	0	0	100	100
3	Q	3/11 (27%)	3 (100%)	0	0	100	100
3	R	3/11 (27%)	3 (100%)	0	0	100	100
All	All	3954/4590 (86%)	3742 (95%)	197 (5%)	15 (0%)	39	56

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	258	ASN
2	H	258	ASN
2	B	362	LYS
2	D	258	ASN
2	F	258	ASN

### 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	275/338 (81%)	269 (98%)	6 (2%)	60	79
1	C	280/338 (83%)	272 (97%)	8 (3%)	50	71
1	E	283/338 (84%)	274 (97%)	9 (3%)	46	68
1	G	278/338 (82%)	273 (98%)	5 (2%)	66	84
1	I	284/338 (84%)	278 (98%)	6 (2%)	61	80
1	K	290/338 (86%)	281 (97%)	9 (3%)	47	69
2	B	286/326 (88%)	271 (95%)	15 (5%)	29	45
2	D	286/326 (88%)	272 (95%)	14 (5%)	31	48
2	F	289/326 (89%)	274 (95%)	15 (5%)	29	45
2	H	284/326 (87%)	270 (95%)	14 (5%)	31	48
2	J	290/326 (89%)	274 (94%)	16 (6%)	27	42
2	L	291/326 (89%)	279 (96%)	12 (4%)	37	57

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	M	5/11 (46%)	5 (100%)	0	100	100
3	N	5/11 (46%)	5 (100%)	0	100	100
3	O	5/11 (46%)	5 (100%)	0	100	100
3	P	5/11 (46%)	5 (100%)	0	100	100
3	Q	5/11 (46%)	5 (100%)	0	100	100
3	R	5/11 (46%)	5 (100%)	0	100	100
All	All	3446/4050 (85%)	3317 (96%)	129 (4%)	41	62

5 of 129 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	232	LEU
2	H	21	LEU
2	L	151	LEU
2	F	255	ARG
2	F	331	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	246	ASN
1	G	149	GLN
2	J	265	ASN
2	F	265	ASN
1	G	80	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 20 ligands modelled in this entry, 13 are monoatomic - leaving 7 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$
5	MGM	B	1401	-	26,28,28	0.90	2 (7%)	33,37,37	1.78	3 (9%)
5	MGM	D	1402	-	26,28,28	0.95	2 (7%)	33,37,37	1.78	3 (9%)
5	MGM	F	1403	-	26,28,28	0.91	1 (3%)	33,37,37	1.80	4 (12%)
5	MGM	H	1404	-	26,28,28	0.88	2 (7%)	33,37,37	1.76	3 (9%)
5	MGM	J	1405	-	26,28,28	0.90	2 (7%)	33,37,37	1.75	3 (9%)
5	MGM	L	1406	-	26,28,28	0.89	1 (3%)	33,37,37	1.73	4 (12%)
7	GER	R	1300	3	19,19,19	1.09	2 (10%)	22,22,22	0.75	0

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
5	MGM	B	1401	-	-	0/31/31/31	0/0/0/0
5	MGM	D	1402	-	-	0/31/31/31	0/0/0/0
5	MGM	F	1403	-	-	0/31/31/31	0/0/0/0
5	MGM	H	1404	-	-	0/31/31/31	0/0/0/0
5	MGM	J	1405	-	-	0/31/31/31	0/0/0/0
5	MGM	L	1406	-	-	0/31/31/31	0/0/0/0
7	GER	R	1300	3	-	0/20/20/20	0/0/0/0

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	1404	MGM	C12-C13	2.05	1.37	1.33
5	J	1405	MGM	C12-C13	2.10	1.37	1.33
5	H	1404	MGM	C7-C8	2.14	1.37	1.33
5	B	1401	MGM	C7-C8	2.15	1.37	1.33
5	B	1401	MGM	C12-C13	2.19	1.37	1.33

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1406	MGM	C10-C8-C9	-2.12	112.17	115.41
5	F	1403	MGM	C10-C8-C9	-2.09	112.22	115.41
5	D	1402	MGM	C2-N3-C5	2.48	121.92	111.70
5	F	1403	MGM	C2-N3-C5	2.48	121.94	111.70
5	B	1401	MGM	C2-N3-C5	2.49	121.97	111.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1401	MGM	3	0
5	D	1402	MGM	3	0
5	F	1403	MGM	2	0
5	H	1404	MGM	2	0
5	J	1405	MGM	3	0
5	L	1406	MGM	4	0
7	R	1300	GER	7	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	314/377 (83%)	0.06	14 (4%) 37 38	42, 63, 91, 106	0
1	C	314/377 (83%)	-0.04	7 (2%) 65 64	41, 59, 87, 138	0
1	E	314/377 (83%)	0.06	13 (4%) 41 42	40, 63, 86, 105	0
1	G	314/377 (83%)	0.10	12 (3%) 44 45	42, 62, 89, 140	0
1	I	314/377 (83%)	0.03	14 (4%) 37 38	35, 60, 88, 100	0
1	K	314/377 (83%)	-0.21	6 (1%) 70 69	30, 48, 71, 87	0
2	B	346/377 (91%)	0.41	37 (10%) 8 8	41, 57, 81, 103	0
2	D	346/377 (91%)	0.33	34 (9%) 10 9	37, 51, 84, 101	0
2	F	346/377 (91%)	0.38	33 (9%) 10 10	36, 51, 83, 105	0
2	H	346/377 (91%)	0.59	43 (12%) 5 5	43, 64, 90, 112	0
2	J	346/377 (91%)	0.37	33 (9%) 10 10	36, 55, 83, 103	0
2	L	346/377 (91%)	0.23	27 (7%) 16 15	32, 46, 72, 95	0
3	M	5/11 (45%)	1.67	2 (40%) 0 0	52, 53, 60, 71	0
3	N	5/11 (45%)	1.95	2 (40%) 0 0	51, 55, 60, 73	0
3	O	5/11 (45%)	2.06	2 (40%) 0 0	53, 56, 60, 74	0
3	P	5/11 (45%)	2.48	3 (60%) 0 0	62, 62, 73, 83	0
3	Q	5/11 (45%)	1.83	2 (40%) 0 0	51, 51, 67, 78	0
3	R	5/11 (45%)	2.17	2 (40%) 0 0	50, 52, 78, 79	0
All	All	3990/4590 (86%)	0.22	286 (7%) 18 18	30, 57, 86, 140	0

The worst 5 of 286 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	55	PHE	8.5
2	J	108	SER	6.7
2	B	363	THR	6.3

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	G	306	HIS	6.0
2	H	305	LEU	6.0

## 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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
6	CL	G	1311	1/1	0.96	0.22	8.65	59,59,59,59	0
6	CL	K	1317	1/1	0.96	0.17	7.79	61,61,61,61	0
6	CL	C	1301	1/1	0.96	0.25	5.58	65,65,65,65	0
5	MGM	H	1404	29/29	0.88	0.39	1.66	59,69,91,94	0
5	MGM	J	1405	29/29	0.90	0.35	1.59	41,58,81,82	0
5	MGM	B	1401	29/29	0.88	0.37	1.57	46,66,88,88	0
5	MGM	L	1406	29/29	0.90	0.34	1.51	39,54,79,80	0
5	MGM	F	1403	29/29	0.88	0.34	1.19	46,58,81,83	0
5	MGM	D	1402	29/29	0.89	0.33	1.15	43,59,80,80	0
7	GER	R	1300	20/20	0.78	0.30	1.02	66,71,80,81	0
6	CL	F	1309	1/1	0.99	0.12	-0.09	51,51,51,51	0
4	ZN	L	378	1/1	1.00	0.14	-0.50	36,36,36,36	0
4	ZN	F	378	1/1	1.00	0.12	-0.81	45,45,45,45	0
4	ZN	J	378	1/1	1.00	0.13	-0.81	42,42,42,42	0
4	ZN	B	378	1/1	1.00	0.12	-0.89	47,47,47,47	0
4	ZN	D	378	1/1	0.99	0.11	-1.07	39,39,39,39	0
4	ZN	H	378	1/1	0.98	0.12	-1.26	60,60,60,60	0
6	CL	D	1306	1/1	0.98	0.11	-1.27	45,45,45,45	0
6	CL	H	1312	1/1	0.97	0.10	-1.61	59,59,59,59	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	CL	J	1315	1/1	0.93	0.10	-2.08	60,60,60,60	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.