



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:17 AM GMT

PDB ID : 3E33  
Title : Protein farnesyltransferase complexed with FPP and ethylenediamine scaffold inhibitor 7  
Authors : Hast, M.A.; Beese, L.S.  
Deposited on : 2008-08-06  
Resolution : 1.90 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](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.

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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

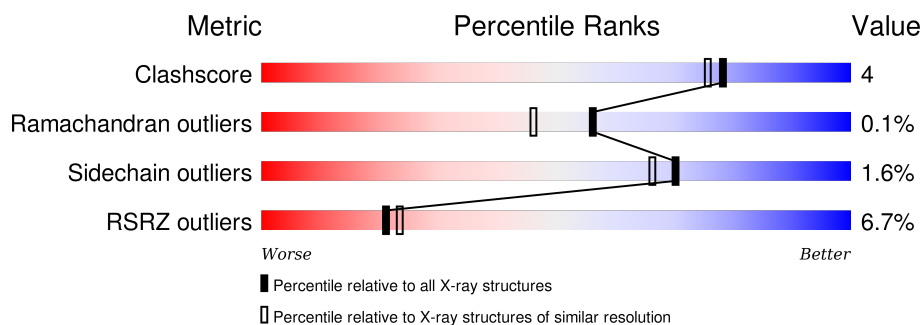
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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>7%</div> <div>79%</div> <div>6%</div> <div>14%</div> </div>
2	B	437	<div> <div>5%</div> <div>84%</div> <div>9%</div> <div>7%</div> </div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6239 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/geranylgeranyltransferase type-1 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2745	1746	481	513	5			

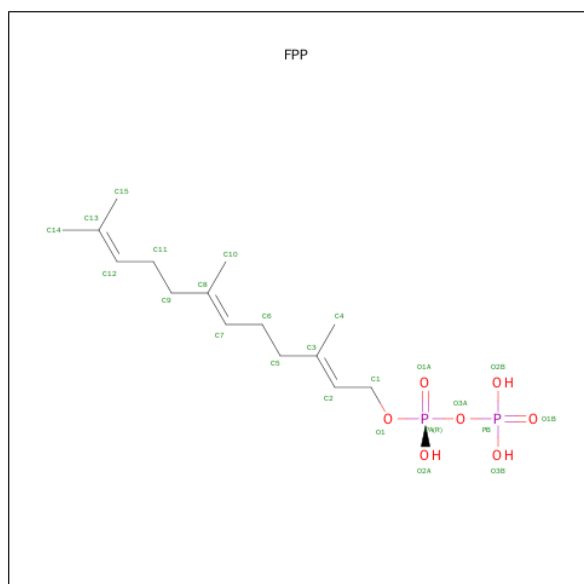
- Molecule 2 is a protein called Protein farnesyltransferase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	407	Total	C	N	O	S	0	0	0
			3203	2050	550	580	23			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

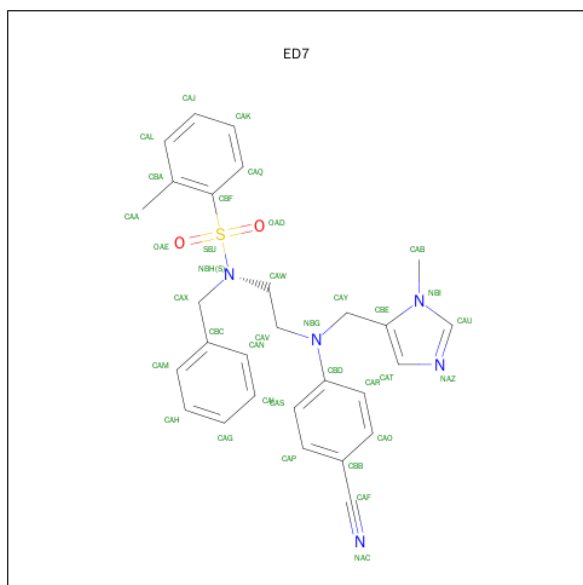
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		

- Molecule 4 is FARNESYL DIPHOSPHATE (three-letter code: FPP) (formula: C<sub>15</sub>H<sub>28</sub>O<sub>7</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	O	P	0	0
			24	15	7	2		

- Molecule 5 is N-BENZYL-N-(2-{(4-CYANOPHENYL)[(1-METHYL-1H-IMIDAZOL-5-YL)METHYL]AMINO}ETHYL)-2-METHYLBENZENESULFONAMIDE (three-letter code: ED7) (formula:  $C_{28}H_{29}N_5O_2S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			36	28	5	2	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	117	Total O 117 117	0	0
6	B	113	Total O 113 113	0	0



- Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	171.04 Å   171.04 Å   69.39 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	33.98 – 1.90 33.98 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (33.98-1.90) 99.2 (33.98-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.29 (at 1.89 Å)	Xtriage
Refinement program	REFMAC 5.4.0077	Depositor
R, $R_{free}$	0.201 ,   0.222 0.202 ,   (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	27.9	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 47.1	EDS
Estimated twinning fraction	0.022 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 90579 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6239	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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: ZN, ED7, 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	0/2812	0.51	0/3817
2	B	0.46	0/3292	0.55	1/4473 (0.0%)
All	All	0.46	0/6104	0.53	1/8290 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	308	LEU	CA-CB-CG	-6.80	99.66	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	2745	0	2666	22	0
2	B	3203	0	3130	22	0
3	B	1	0	0	0	0
4	B	24	0	25	2	0
5	B	36	0	29	1	0
6	A	117	0	0	1	0
6	B	113	0	0	1	0
All	All	6239	0	5850	43	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 4.

All (43) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:MET:O	1:A:156:ILE:HG23	1.71	0.90
1:A:302:LEU:C	1:A:304:PRO:CD	2.50	0.79
1:A:156:ILE:HG22	1:A:172:ARG:HH12	1.46	0.79
1:A:302:LEU:O	1:A:304:PRO:HD2	1.93	0.68
1:A:302:LEU:C	1:A:304:PRO:HD3	2.15	0.68
1:A:302:LEU:C	1:A:304:PRO:HD2	2.16	0.65
1:A:303:GLN:N	1:A:304:PRO:HD3	2.13	0.64
2:B:308:LEU:HD13	2:B:330:PHE:HB3	1.82	0.60
2:B:325:MET:SD	2:B:381:MET:HG3	2.42	0.59
1:A:152:MET:O	1:A:156:ILE:CG2	2.50	0.57
1:A:77:PRO:HG3	1:A:102:TYR:CZ	2.40	0.55
2:B:193:MET:SD	2:B:203:SER:HB3	2.46	0.55
4:B:1002:FPP:H102	5:B:1003:ED7:HAN	1.89	0.54
2:B:75:ARG:NH2	2:B:393:VAL:O	2.41	0.54
1:A:303:GLN:N	1:A:304:PRO:CD	2.69	0.53
1:A:156:ILE:HG22	1:A:172:ARG:NH1	2.19	0.53
2:B:239:ILE:HB	2:B:252:THR:HA	1.91	0.52
2:B:30:HIS:HE1	6:B:2824:HOH:O	1.92	0.51
2:B:422:GLY:O	2:B:423:PHE:HB2	2.12	0.50
2:B:202:ARG:HD2	4:B:1002:FPP:H142	1.92	0.50
2:B:51:VAL:O	2:B:55:ILE:HG12	2.13	0.49
2:B:192:LEU:HD23	2:B:199:VAL:CG2	2.42	0.48
2:B:185:LYS:HD3	2:B:191:PHE:CZ	2.48	0.48
2:B:28:PRO:HD2	2:B:29:GLU:OE1	2.14	0.48
1:A:361:ARG:HB3	2:B:322:ALA:HB1	1.96	0.47
1:A:208:TRP:NE1	1:A:212:GLU:HG3	2.30	0.46
1:A:302:LEU:O	1:A:304:PRO:CD	2.60	0.46
2:B:220:ASP:HA	2:B:223:GLU:HG2	1.97	0.46
1:A:156:ILE:HG21	6:A:2672:HOH:O	2.17	0.45
1:A:311:LEU:HD23	1:A:311:LEU:C	2.36	0.45
1:A:112:ARG:HA	1:A:140:LEU:CD2	2.46	0.45
1:A:294:ASN:O	1:A:298:GLN:HG3	2.15	0.45
2:B:192:LEU:HD23	2:B:199:VAL:HG23	2.00	0.43
2:B:408:VAL:O	2:B:412:THR:HG23	2.19	0.43
1:A:198:LYS:HD2	2:B:294:LYS:HE3	2.00	0.43
2:B:301:SER:O	2:B:305:ALA:HB3	2.17	0.43
2:B:333:GLN:HG3	2:B:387:MET:SD	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:ILE:CG2	1:A:172:ARG:HH12	2.24	0.42
2:B:253:PHE:HA	2:B:307:LEU:HD21	2.01	0.42
2:B:220:ASP:HA	2:B:223:GLU:CG	2.50	0.42
1:A:346:LYS:HE3	1:A:357:ARG:NH2	2.35	0.41
1:A:373:ILE:HA	1:A:374:PRO:HD3	1.97	0.41
2:B:276:TRP:O	2:B:280:ARG:HG2	2.22	0.40

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	321/377 (85%)	307 (96%)	13 (4%)	1 (0%)	46	35
2	B	405/437 (93%)	398 (98%)	7 (2%)	0	100	100
All	All	726/814 (89%)	705 (97%)	20 (3%)	1 (0%)	56	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	304	PRO

### 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	301/338 (89%)	294 (98%)	7 (2%)	58	51
2	B	344/371 (93%)	341 (99%)	3 (1%)	84	83
All	All	645/709 (91%)	635 (98%)	10 (2%)	70	66

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	PHE
1	A	85	SER
1	A	156	ILE
1	A	269	LEU
1	A	303	GLN
1	A	324	GLU
1	A	334	LEU
2	B	68	VAL
2	B	87	ARG
2	B	351	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	HIS
2	B	30	HIS
2	B	194	HIS

### 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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\# Z  > 2$
4	FPP	B	1002	-	21,23,23	2.26	3 (14%)	27,31,31	1.35	3 (11%)
5	ED7	B	1003	3	37,39,39	1.71	5 (13%)	50,54,54	1.72	7 (14%)

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
4	FPP	B	1002	-	-	0/25/25/25	0/0/0/0
5	ED7	B	1003	3	-	0/31/31/31	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1003	ED7	CBF-SBJ	-3.00	1.74	1.77
5	B	1003	ED7	CBE-NBI	-2.16	1.33	1.38
5	B	1003	ED7	SBJ-NBH	2.64	1.67	1.63
4	B	1002	FPP	PB-O3B	5.36	1.74	1.54
5	B	1003	ED7	OAD-SBJ	5.53	1.50	1.43
4	B	1002	FPP	PB-O2B	5.60	1.74	1.54
4	B	1002	FPP	PA-O2A	5.64	1.79	1.54
5	B	1003	ED7	OAE-SBJ	6.24	1.51	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1003	ED7	OAE-SBJ-OAD	-6.30	108.59	119.47
5	B	1003	ED7	CAX-NBH-SBJ	-4.11	107.75	117.45
5	B	1003	ED7	NAZ-CAU-NBI	-4.10	106.73	112.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1003	ED7	CAA-CBA-CBF	-3.18	120.79	124.09
4	B	1002	FPP	C6-C7-C8	-2.43	122.48	127.76
4	B	1002	FPP	PA-O3A-PB	-2.39	124.65	132.67
5	B	1003	ED7	CAL-CBA-CBF	2.36	119.11	116.21
5	B	1003	ED7	CBF-SBJ-NBH	2.72	112.15	106.70
4	B	1002	FPP	C10-C8-C9	3.06	120.09	115.41
5	B	1003	ED7	OAD-SBJ-NBH	4.92	111.55	106.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1002	FPP	2	0
5	B	1003	ED7	1	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	323/377 (85%)	0.35	25 (7%) 16 18	17, 31, 54, 62	0
2	B	407/437 (93%)	0.36	24 (5%) 26 29	18, 27, 45, 60	0
All	All	730/814 (89%)	0.36	49 (6%) 21 23	17, 28, 50, 62	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	19	TRP	8.5
2	B	380	ALA	8.1
2	B	64	PHE	6.3
1	A	55	PHE	6.0
2	B	17	PRO	5.6
1	A	375	ALA	4.9
1	A	305	SER	4.8
2	B	381	MET	4.8
1	A	326	GLN	4.7
1	A	373	ILE	4.4
2	B	423	PHE	4.4
2	B	422	GLY	4.0
1	A	371	SER	4.0
1	A	372	ASP	4.0
1	A	364	GLN	3.8
1	A	328	ASP	3.8
2	B	32	ARG	3.6
1	A	374	PRO	3.5
1	A	304	PRO	3.5
2	B	18	VAL	3.5
2	B	379	GLY	3.3
2	B	70	ARG	3.3
2	B	20	SER	3.3
1	A	286	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	319	GLY	3.1
1	A	327	CYS	3.0
1	A	217	ASP	2.9
2	B	121	ILE	2.6
2	B	266	ARG	2.6
1	A	84	PRO	2.5
1	A	339	GLU	2.5
1	A	377	VAL	2.5
2	B	321	PRO	2.5
1	A	302	LEU	2.4
2	B	120	GLN	2.4
1	A	324	GLU	2.4
1	A	306	HIS	2.4
1	A	367	HIS	2.3
2	B	303	TRP	2.3
2	B	151	ALA	2.3
1	A	333	ILE	2.2
2	B	21	GLU	2.2
1	A	330	LYS	2.2
2	B	277	VAL	2.2
1	A	368	SER	2.1
2	B	325	MET	2.1
2	B	253	PHE	2.0
1	A	376	SER	2.0
2	B	105	TYR	2.0

## 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, 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( $\text{\AA}^2$ )	Q<0.9
4	FPP	B	1002	24/24	0.93	0.18	1.31	22,30,35,38	0
5	ED7	B	1003	36/36	0.95	0.11	-0.58	19,31,39,41	0
3	ZN	B	1001	1/1	1.00	0.08	-	20,20,20,20	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.