

Full wwPDB X-ray Structure Validation Report (i)

May 14, 2020 - 04:18 am BST

:	3E33
:	Protein farnesyltransferase complexed with FPP and ethylenediamine scaffold
	inhibitor 7
:	Hast, M.A.; Beese, L.S.
:	2008-08-06
:	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 A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

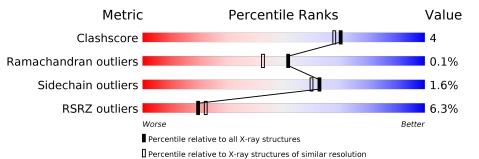
MolProbity		4.02b-467 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)		1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
$\operatorname{CCP4}$:	$7.0.044 (\mathrm{Gargrove})$
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain		
1	А	377	6% 79% 6%		14%
2	В	437	5%	9%	7%



 $\mathbf{2}$

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.

 $\bullet\,$ Molecule 1 is a protein called Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Λ	323	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	Л	020	2745	1746	481	513	5	0	0	0

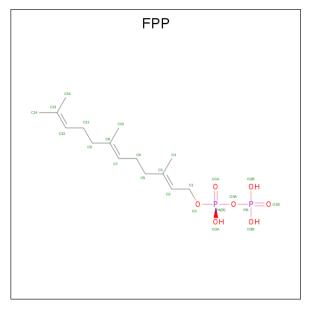
• Molecule 2 is a protein called Protein farmesyltransferase subunit beta.

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

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

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

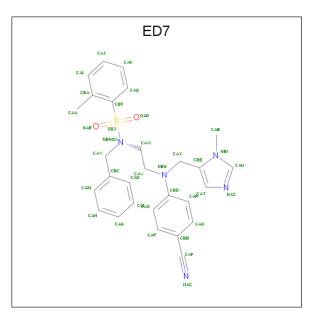
• Molecule 4 is FARNESYL DIPHOSPHATE (three-letter code: FPP) (formula: C₁₅H₂₈O₇P₂).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	В	1	Total			Р	0	0
	_	_	24	15	7	2	Ū	

• Molecule 5 is N-benzyl-N-(2-{(4-cyanophenyl)[(1-methyl-1H-imidazol-5-yl)methyl]amino}et hyl)-2-methylbenzenesulfonamide (three-letter code: ED7) (formula: $C_{28}H_{29}N_5O_2S$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
۲.	D	1	Total	С	Ν	Ο	S	0	0
0	D	1	36	28	5	2	1	0	0

• Molecule 6 is water.

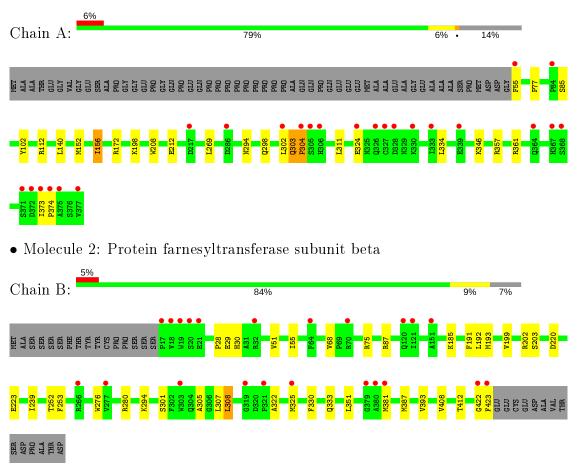
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	117	Total O 117 117	0	0
6	В	113	Total O 113 113	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
$\begin{array}{c} \text{Cell constants} \\ \text{a, b, c, } \alpha, \beta, \gamma \end{array}$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Depositor
$\begin{array}{c c} a, b, c, a, p, \gamma \\ \hline \\ Resolution (Å) \end{array}$	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	Depositor EDS
% Data completeness (in resolution range)	99.2 (33.98-1.90) 99.2 (33.98-1.90) 99.2 (33.98-1.90)	Depositor EDS
R _{merge}	(Not available)	Depositor
$\frac{\mathrm{R}_{sym}}{< I/\sigma(I) > 1}$	(Not available) 2.29 (at 1.89Å)	Depositor Xtriage
Refinement program	REFMAC 5.4.0077	Depositor
R, R_{free}	$\begin{array}{cccc} 0.201 & , & 0.222 \\ 0.202 & , & ({ m Not available}) \end{array}$	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor $(Å^2)$	27.9	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	$0.39\ ,\ 47.1$	EDS
L-test for twinning ²	$< L > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.022 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6239	wwPDB-VP
Average B, all atoms $(Å^2)$	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.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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			nd angles
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.45	0/2812	0.51	0/3817
2	В	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	Ζ	$Observed(^{o})$	$Ideal(^{o})$
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	А	2745	0	2666	22	0
2	В	3203	0	3130	22	0
3	В	1	0	0	0	0
4	В	24	0	25	2	0
5	В	36	0	29	1	0
6	А	117	0	0	1	0
6	В	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



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

Continued from previous page...

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	Perce	entiles
1	А	321/377~(85%)	307~(96%)	13 (4%)	1 (0%)	41	31
2	В	405/437~(93%)	398~(98%)	7(2%)	0	100	100
All	All	726/814~(89%)	705 (97%)	20 (3%)	1 (0%)	51	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type	
1	А	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	in Analysed Rotameric Outlie		Outliers	Percentiles
1	А	301/338~(89%)	294~(98%)	7(2%)	50 45
2	В	344/371~(93%)	341 (99%)	3 (1%)	78 79
All	All	645/709~(91%)	635~(98%)	10~(2%)	62 60

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

Mol	Chain	Res	Type
1	А	55	PHE
1	А	85	SER
1	А	156	ILE
1	А	269	LEU
1	А	303	GLN
1	А	324	GLU
1	А	334	LEU
2	В	68	VAL
2	В	87	ARG
2	В	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	А	135	HIS
2	В	30	HIS
2	В	194	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.



5.6 Ligand geometry (i)

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 Chair		Chain	Chain Res	Link	Bo	ond leng	\mathbf{ths}	В	ond ang	les
	туре	Chain	nes	LIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FPP	В	1002	-	21, 23, 23	2.10	5 (23%)	$27,\!31,\!31$	1.32	4 (14%)
5	ED7	В	1003	3	$36,\!39,\!39$	1.87	4 (11%)	$50,\!54,\!54$	1.78	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	В	1002	-	-	4/25/25/25	-
5	ED7	В	1003	3	-	$\frac{5/31/31/31}{31}$	0/4/4/4

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
5	В	1003	ED7	OAE-SBJ	7.15	1.51	1.43
5	В	1003	ED7	OAD-SBJ	6.34	1.50	1.43
4	В	1002	FPP	PB-O2B	5.19	1.74	1.54
4	В	1002	FPP	PA-O2A	5.05	1.79	1.55
4	В	1002	FPP	PB-O3B	4.96	1.74	1.54
5	В	1003	ED7	CBF-SBJ	-3.04	1.74	1.78
5	В	1003	ED7	SBJ-NBH	2.76	1.67	1.63
4	В	1002	FPP	PB-O1B	2.18	1.57	1.50
4	В	1002	FPP	PA-O1A	2.08	1.58	1.50

All (9) bond length outliers are listed below:

All (11) bond angle outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
5	В	1003	ED7	OAE-SBJ-OAD	-6.74	108.59	119.52
5	В	1003	ED7	OAD-SBJ-NBH	5.33	111.55	106.69



3E33

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	В	1003	ED7	CAX-NBH-SBJ	-4.11	107.75	117.35
5	В	1003	ED7	NAZ-CAU-NBI	-3.72	106.73	112.26
5	В	1003	ED7	CAA-CBA-CBF	-3.44	120.79	124.16
5	В	1003	ED7	CBF-SBJ-NBH	2.89	112.15	106.81
4	В	1002	FPP	C10-C8-C9	2.86	120.09	115.27
5	В	1003	ED7	CAL-CBA-CBF	2.56	119.11	116.27
4	В	1002	FPP	PA-O3A-PB	-2.38	124.65	132.83
4	В	1002	FPP	C15-C13-C14	2.24	119.55	114.60
4	В	1002	FPP	C6-C7-C8	-2.15	122.48	127.66

Continued from previous page...

There are no chirality outliers.

Mol	Chain	\mathbf{Res}	Type	Atoms
5	В	1003	ED7	CAX-NBH-SBJ-CBF
5	В	1003	ED7	CAW-NBH-SBJ-OAD
5	В	1003	ED7	CAW-NBH-SBJ-CBF
5	В	1003	ED7	CAX-NBH-SBJ-OAE
4	В	1002	FPP	C4-C3-C5-C6
4	В	1002	FPP	C2-C3-C5-C6
4	В	1002	FPP	C1-O1-PA-O3A
5	В	1003	ED7	CBC-CAX-NBH-SBJ
4	В	1002	FPP	O1-C1-C2-C3

All (9) torsion outliers are listed below:

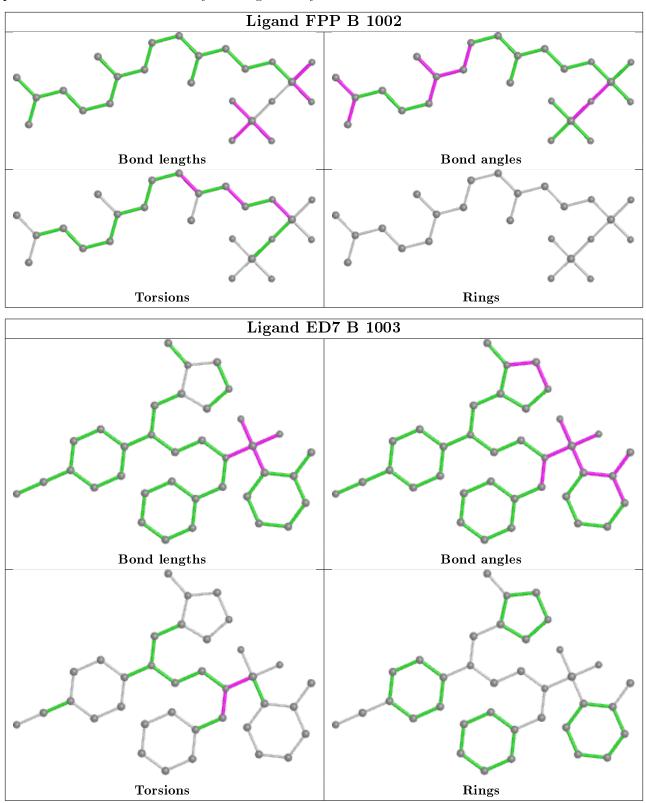
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	В	1002	FPP	2	0
5	В	1003	ED7	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient





equivalents in the CSD to analyse the geometry.



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	А	323/377~(85%)	0.31	24 (7%) 14 16	17, 31, 54, 62	0
2	В	407/437~(93%)	0.32	22 (5%) 25 29	18, 27, 45, 60	0
All	All	730/814~(89%)	0.32	46 (6%) 20 22	17, 28, 50, 62	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	19	TRP	8.4
2	В	380	ALA	7.9
2	В	64	PHE	6.1
1	А	55	PHE	5.8
2	В	17	PRO	5.5
1	А	375	ALA	4.8
2	В	381	MET	4.7
1	А	305	SER	4.7
1	А	326	GLN	4.7
1	А	373	ILE	4.3
2	В	423	PHE	4.3
2	В	422	GLY	3.9
1	А	371	SER	3.9
1	А	372	ASP	3.9
1	А	364	GLN	3.8
1	А	328	ASP	3.7
2	В	32	ARG	3.6
1	А	374	PRO	3.5
1	А	304	PRO	3.4
2	В	18	VAL	3.4
2	В	70	ARG	3.3
2	В	379	GLY	3.2
2	В	20	SER	3.2
1	A	286	ASP	3.0



3E33

Mol	Chain	Res	Type	RSRZ
2	В	319	GLY	3.0
1	А	327	CYS	3.0
1	А	217	ASP	2.8
2	В	121	ILE	2.6
2	В	266	ARG	2.5
1	А	339	GLU	2.5
1	А	84	PRO	2.5
1	А	377	VAL	2.4
2	В	321	PRO	2.4
2	В	120	GLN	2.4
1	А	302	LEU	2.4
1	А	324	GLU	2.3
1	А	306	HIS	2.3
1	А	367	HIS	2.3
2	В	151	ALA	2.2
2	В	303	TRP	2.2
1	А	333	ILE	2.1
2	В	21	GLU	2.1
1	А	330	LYS	2.1
1	А	368	SER	2.1
2	В	277	VAL	2.1
2	В	325	MET	2.0

Continued from previous page...

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. The B-factors column lists the minimum, median, 95^{th} 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.

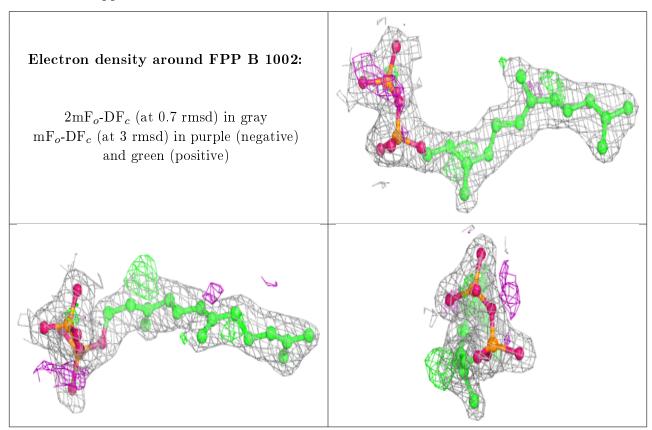
Mol	Type	Chain	\mathbf{Res}	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
4	FPP	В	1002	24/24	0.93	0.18	$22,\!30,\!35,\!38$	0



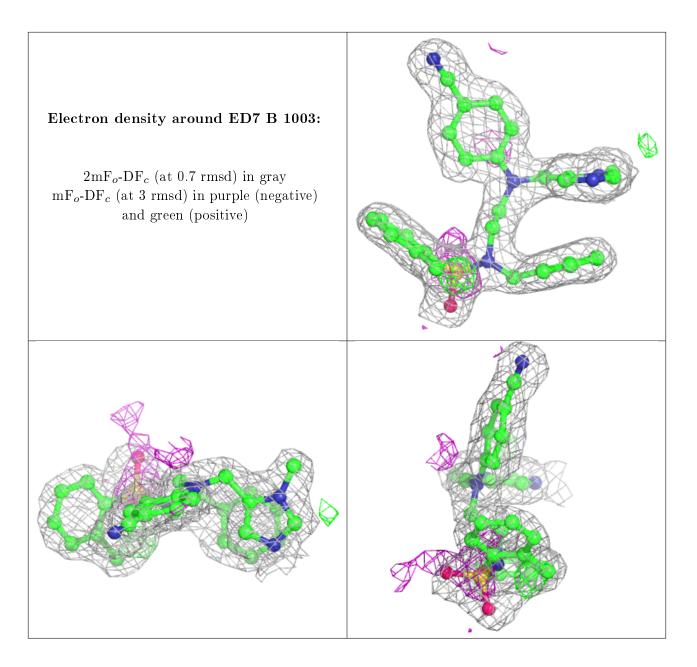
a 1	e		
Continued	from	previous	page

Mol	Type	Chain	\mathbf{Res}	Atoms	RSCC	RSR	$\mathbf{B} extsf{-}\mathbf{B} extsf{-}\mathbf{factors}(\mathbf{A}^2)$	Q<0.9
5	ED7	В	1003	36/36	0.95	0.11	$19,\!31,\!39,\!41$	0
3	ZN	В	1001	1/1	1.00	0.08	$20,\!20,\!20,\!20$	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.







6.5 Other polymers (i)

There are no such residues in this entry.

