



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:26 AM GMT

PDB ID : 1FT1
Title : CRYSTAL STRUCTURE OF PROTEIN FARNESYLTRANSFERASE AT
2.25 ANGSTROMS RESOLUTION
Authors : Beese, L.S.; Park, H.-W.
Deposited on : 1997-03-17
Resolution : 2.25 Å(reported)

This is a full wwPDB validation 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>

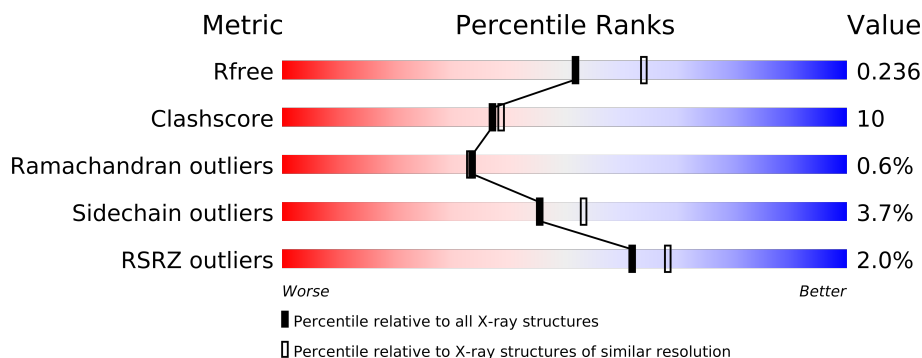
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.25 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	1108 (2.28-2.24)
Clashscore	79885	1326 (2.28-2.24)
Ramachandran outliers	78287	1291 (2.28-2.24)
Sidechain outliers	78261	1291 (2.28-2.24)
RSRZ outliers	66119	1110 (2.28-2.24)

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	377	
2	B	437	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6353 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 PROTEIN FARNESYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	0	0
			2688	1712	473	498	5			

- Molecule 2 is a protein called PROTEIN FARNESYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	416	Total	C	N	O	S	0	0	0
			3262	2078	558	602	24			

- 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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	155	Total	O	0	0
			155	155		
4	B	247	Total	O	0	0
			247	247		

4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	167.06Å 167.06Å 97.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.25 24.91 – 2.10	Depositor EDS
% Data completeness (in resolution range)	89.6 (6.00-2.25) 83.9 (24.91-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.10Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.210 , 0.260 0.194 , 0.236	Depositor DCC
R_{free} test set	3153 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 64.6	EDS
Estimated twinning fraction	0.035 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 76048 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6353	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% 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: ZN

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	0.48	0/2754	0.64	0/3738
2	B	0.52	0/3349	0.73	2/4549 (0.0%)
All	All	0.50	0/6103	0.69	2/8287 (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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	308	LEU	CA-CB-CG	-6.98	99.25	115.30
2	B	277	VAL	CB-CA-C	-5.20	101.52	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	93	TYR	Sidechain

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	2688	0	2614	61	0
2	B	3262	0	3173	61	0
3	B	1	0	0	0	0
4	A	155	0	0	2	0
4	B	247	0	0	7	0
All	All	6353	0	5787	118	0

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 10.

All (118) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:159:ILE:HG12	1:A:168:VAL:HG13	1.41	1.02
2:B:77:LYS:HA	2:B:77:LYS:HE2	1.56	0.87
1:A:96:PHE:HA	1:A:126:LEU:HD13	1.67	0.77
2:B:74:GLN:H	2:B:344:GLN:HE22	1.35	0.74
2:B:134:GLN:HE22	2:B:173:ASN:H	1.33	0.74
1:A:289:LEU:HD12	1:A:317:ASP:HB3	1.72	0.72
1:A:75:ILE:HD11	1:A:109:ARG:HD3	1.73	0.70
2:B:281:GLN:HG3	4:B:1391:HOH:O	1.92	0.70
2:B:74:GLN:H	2:B:344:GLN:NE2	1.91	0.69
1:A:159:ILE:HG12	1:A:168:VAL:CG1	2.21	0.68
2:B:51:VAL:O	2:B:55:ILE:HG12	1.96	0.66
2:B:338:TYR:CE2	2:B:343:CYS:SG	2.90	0.65
2:B:386:VAL:HG21	2:B:393:VAL:HG13	1.78	0.64
2:B:24:TYR:HE2	4:B:1250:HOH:O	1.80	0.64
2:B:301:SER:O	2:B:305:ALA:HB3	1.97	0.63
1:A:352:ARG:NH2	2:B:281:GLN:O	2.32	0.63
2:B:78:HIS:HD1	2:B:349:GLY:H	1.45	0.63
1:A:156:ILE:HD11	1:A:172:ARG:HH22	1.64	0.62
1:A:148:LEU:HB2	1:A:179:LEU:HD21	1.82	0.62
2:B:277:VAL:O	2:B:280:ARG:HB2	1.99	0.62
1:A:357:ARG:O	1:A:361:ARG:HB2	2.01	0.61
2:B:185:LYS:HE3	2:B:221:LEU:O	2.01	0.60
2:B:333:GLN:HG3	2:B:387:MET:CE	2.32	0.60
1:A:281:LYS:NZ	1:A:289:LEU:HD11	2.16	0.60
2:B:24:TYR:HA	2:B:27:ARG:HE	1.65	0.59
1:A:189:ILE:HD11	1:A:205:HIS:HD2	1.67	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:138:ARG:NH2	4:A:1056:HOH:O	2.35	0.58
2:B:390:PRO:O	2:B:393:VAL:HG22	2.04	0.58
2:B:239:ILE:HB	2:B:252:THR:HA	1.85	0.58
2:B:73:LEU:HA	2:B:344:GLN:HE22	1.69	0.56
1:A:266:MET:CE	1:A:266:MET:HA	2.34	0.56
1:A:239:GLN:HA	1:A:239:GLN:HE21	1.71	0.56
1:A:303:GLN:O	1:A:307:SER:HB2	2.06	0.56
1:A:173:ARG:HD2	2:B:198:GLU:OE2	2.07	0.55
1:A:307:SER:HA	1:A:311:LEU:HD13	1.87	0.55
2:B:333:GLN:HG3	2:B:387:MET:HE2	1.89	0.55
2:B:32:ARG:HH11	2:B:32:ARG:HG3	1.71	0.55
2:B:280:ARG:NH2	4:B:1009:HOH:O	2.40	0.55
1:A:101:ASP:HA	1:A:104:ARG:NH1	2.23	0.54
2:B:71:LEU:HD21	2:B:341:MET:HG3	1.90	0.53
2:B:280:ARG:HG3	2:B:304:GLN:NE2	2.23	0.53
2:B:386:VAL:CG2	2:B:393:VAL:HG13	2.38	0.53
2:B:177:LEU:HD21	2:B:210:VAL:CG1	2.39	0.53
2:B:32:ARG:NH1	2:B:32:ARG:HG3	2.23	0.52
2:B:370:LEU:O	2:B:374:GLN:HG3	2.08	0.52
1:A:366:LYS:HG3	1:A:367:HIS:CE1	2.44	0.52
2:B:23:LEU:HD13	2:B:341:MET:HE2	1.92	0.52
1:A:156:ILE:CD1	1:A:172:ARG:HH12	2.23	0.52
1:A:354:GLU:HG2	2:B:328:TRP:O	2.10	0.52
1:A:223:VAL:HG11	1:A:240:ARG:HB2	1.92	0.52
2:B:86:LEU:HB2	2:B:107:ILE:HG21	1.91	0.51
1:A:191:ASP:O	1:A:194:ASN:HB2	2.11	0.51
2:B:87:ARG:NH1	2:B:122:VAL:HG13	2.25	0.51
1:A:368:SER:C	1:A:369:ARG:HG3	2.31	0.51
2:B:68:VAL:HG22	4:B:1351:HOH:O	2.11	0.51
1:A:154:TYR:CZ	1:A:158:ILE:HD11	2.46	0.50
1:A:342:GLU:OE1	1:A:346:LYS:HG3	2.12	0.49
1:A:353:LYS:O	1:A:357:ARG:HG2	2.12	0.49
2:B:377:GLY:HA2	2:B:381:MET:O	2.12	0.49
1:A:289:LEU:CD1	1:A:317:ASP:HB3	2.42	0.49
2:B:202:ARG:HD2	4:B:1374:HOH:O	2.12	0.49
1:A:158:ILE:HG22	1:A:168:VAL:HG21	1.94	0.48
2:B:306:GLY:O	2:B:309:PRO:HD2	2.13	0.48
2:B:23:LEU:HB2	2:B:26:LEU:HD12	1.95	0.48
2:B:280:ARG:HH11	2:B:289:GLN:NE2	2.11	0.48
2:B:29:GLU:CD	2:B:29:GLU:H	2.17	0.48
2:B:328:TRP:CZ2	2:B:376:PHE:HA	2.48	0.48
1:A:211:GLN:HG3	1:A:242:PHE:HZ	1.78	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:328:ASP:O	1:A:329:ASN:HB2	2.15	0.47
2:B:64:PHE:HD1	2:B:65:ASN:HB2	1.78	0.47
1:A:312:ILE:O	1:A:316:VAL:HG23	2.14	0.47
2:B:74:GLN:N	2:B:344:GLN:HE22	2.08	0.47
1:A:207:GLN:HE21	1:A:239:GLN:NE2	2.12	0.47
2:B:41:GLU:HG2	4:B:1189:HOH:O	2.15	0.47
1:A:346:LYS:HG3	1:A:357:ARG:HH21	1.78	0.47
1:A:189:ILE:HD11	1:A:205:HIS:CD2	2.48	0.47
2:B:282:MET:HG3	2:B:296:VAL:HB	1.96	0.47
2:B:177:LEU:HD21	2:B:210:VAL:HG13	1.97	0.46
1:A:355:TYR:O	1:A:358:TYR:HB3	2.15	0.46
2:B:75:ARG:HD3	4:B:1216:HOH:O	2.15	0.46
1:A:161:GLU:C	1:A:163:PRO:HD3	2.36	0.46
2:B:375:HIS:CE1	2:B:394:LEU:O	2.69	0.46
1:A:79:PRO:HA	1:A:101:ASP:OD1	2.16	0.46
1:A:65:LEU:HD13	1:A:67:ARG:CZ	2.45	0.45
2:B:151:ALA:HB3	2:B:152:PRO:CD	2.47	0.45
2:B:308:LEU:HD13	2:B:330:PHE:HB3	1.99	0.45
1:A:152:MET:O	1:A:156:ILE:HG12	2.17	0.44
1:A:187:GLU:HG3	4:A:1301:HOH:O	2.16	0.44
1:A:332:ASP:O	1:A:336:LYS:HG3	2.18	0.44
2:B:180:TYR:CZ	2:B:184:LEU:HD11	2.53	0.44
2:B:149:HIS:HB3	2:B:152:PRO:CG	2.47	0.44
1:A:351:ILE:HG12	2:B:281:GLN:HG2	2.00	0.43
1:A:342:GLU:HA	1:A:342:GLU:OE1	2.16	0.43
1:A:231:VAL:O	1:A:231:VAL:HG22	2.19	0.43
1:A:357:ARG:HD3	1:A:357:ARG:HA	1.85	0.43
1:A:77:PRO:HB3	1:A:102:TYR:CE1	2.53	0.43
1:A:224:ASP:OD1	1:A:240:ARG:NH2	2.51	0.43
1:A:251:SER:HA	1:A:287:ARG:HH12	1.84	0.43
1:A:77:PRO:HB2	1:A:101:ASP:HB3	2.00	0.43
2:B:280:ARG:HA	2:B:280:ARG:HD3	1.76	0.43
2:B:375:HIS:HE1	2:B:394:LEU:O	2.01	0.43
1:A:320:GLU:O	1:A:324:GLU:HG2	2.18	0.43
2:B:282:MET:HG2	2:B:287:GLY:O	2.19	0.42
1:A:136:PHE:CE2	1:A:140:LEU:HD11	2.54	0.42
1:A:264:LEU:O	1:A:268:LYS:HG3	2.19	0.42
1:A:300:LEU:O	1:A:303:GLN:HB2	2.20	0.42
2:B:149:HIS:HB3	2:B:152:PRO:HG2	2.02	0.42
2:B:22:PRO:HG2	2:B:27:ARG:HG2	2.02	0.41
2:B:24:TYR:H	2:B:333:GLN:NE2	2.18	0.41
1:A:198:LYS:HE2	1:A:233:ASN:HA	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:156:ILE:CD1	1:A:172:ARG:HH22	2.32	0.41
2:B:71:LEU:CD2	2:B:341:MET:HG3	2.49	0.41
1:A:156:ILE:HD13	1:A:172:ARG:HH12	1.84	0.41
2:B:262:LEU:O	2:B:264:LYS:HG2	2.19	0.41
1:A:154:TYR:CE1	1:A:158:ILE:HD11	2.55	0.41
1:A:329:ASN:HB3	1:A:332:ASP:HB3	2.02	0.41
1:A:355:TYR:CE1	1:A:359:ILE:HD11	2.56	0.41
1:A:344:LEU:HD13	1:A:356:TRP:CZ2	2.55	0.40

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	313/377 (83%)	282 (90%)	30 (10%)	1 (0%)	50	54
2	B	414/437 (95%)	396 (96%)	15 (4%)	3 (1%)	30	29
All	All	727/814 (89%)	678 (93%)	45 (6%)	4 (1%)	33	33

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	304	PRO
2	B	432	SER
2	B	74	GLN
2	B	64	PHE

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	294/338 (87%)	281 (96%)	13 (4%)	39	43
2	B	351/371 (95%)	340 (97%)	11 (3%)	52	61
All	All	645/709 (91%)	621 (96%)	24 (4%)	45	53

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	106	VAL
1	A	109	ARG
1	A	121	ARG
1	A	168	VAL
1	A	177	GLU
1	A	226	LEU
1	A	239	GLN
1	A	266	MET
1	A	342	GLU
1	A	352	ARG
1	A	362	SER
1	A	369	ARG
2	B	29	GLU
2	B	65	ASN
2	B	66	HIS
2	B	67	LEU
2	B	87	ARG
2	B	88	GLN
2	B	101	PRO
2	B	122	VAL
2	B	277	VAL
2	B	280	ARG
2	B	393	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	HIS
1	A	211	GLN
1	A	239	GLN
1	A	246	ASN
1	A	261	GLN
1	A	294	ASN

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Mol	Chain	Res	Type
1	A	367	HIS
2	B	80	HIS
2	B	134	GLN
2	B	275	GLN
2	B	289	GLN
2	B	333	GLN
2	B	344	GLN

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 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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	315/377 (83%)	-0.25	6 (1%) 64 70	20, 34, 51, 68	0
2	B	416/437 (95%)	-0.39	9 (2%) 59 65	13, 26, 45, 65	0
All	All	731/814 (89%)	-0.33	15 (2%) 62 66	13, 30, 48, 68	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	64	PHE	7.9
2	B	65	ASN	4.8
1	A	369	ARG	4.1
2	B	380	ALA	3.8
1	A	326	GLN	3.6
2	B	22	PRO	3.3
2	B	66	HIS	3.2
2	B	381	MET	3.1
2	B	379	GLY	2.9
1	A	55	PHE	2.8
2	B	63	LYS	2.7
2	B	32	ARG	2.3
1	A	368	SER	2.3
1	A	328	ASP	2.1
1	A	329	ASN	2.1

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
3	ZN	B	1001	1/1	0.05	-1.77	27,27,27,27	0

6.5 Other polymers

There are no such residues in this entry.