



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:27 PM GMT

PDB ID : 1FPP  
Title : PROTEIN FARNESYLTRANSFERASE COMPLEX WITH FARNESYL  
DIPHOSPHATE  
Authors : Dunten, P.; Kammlott, U.; Crowther, R.; Weber, D.; Palermo, R.; Birktoft, J.  
Deposited on : 1998-07-10  
Resolution : 2.75 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.

---

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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

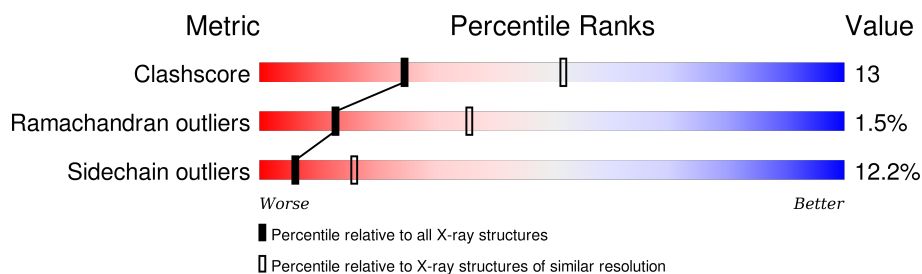
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	437	
2	A	377	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5889 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	400	Total	C	N	O	S	0	0	0
			3145	2010	542	570	23			

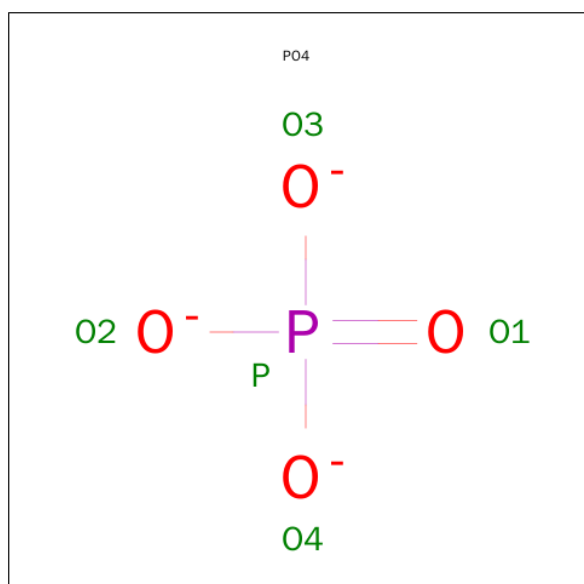
- Molecule 2 is a protein called PROTEIN FARNESYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	316	Total	C	N	O	S	0	0	0
			2697	1717	474	501	5			

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

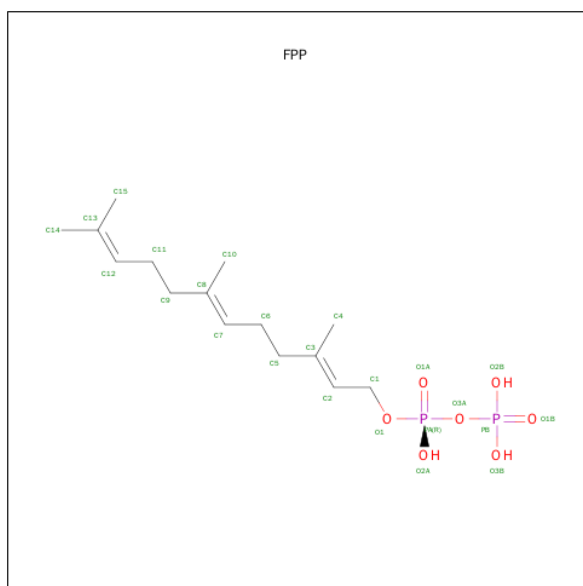
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is FARNESYL DIPHOSPHATE (three-letter code: FPP) (formula:  $C_{15}H_{28}O_7P_2$ ).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	8	Total	O	0	0
			8	8		
6	B	9	Total	O	0	0
			9	9		



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	170.00 Å   170.00 Å   68.86 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	12.00 – 2.75	Depositor
% Data completeness (in resolution range)	96.0 (12.00-2.75)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.230 , 0.300	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5889	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, PO4, 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	B	0.32	0/3230	0.91	6/4387 (0.1%)
2	A	0.33	0/2763	1.01	12/3750 (0.3%)
All	All	0.32	0/5993	0.96	18/8137 (0.2%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	206	ARG	CD-NE-CZ	20.41	152.17	123.60
2	A	206	ARG	NE-CZ-NH1	8.24	124.42	120.30
2	A	173	ARG	CD-NE-CZ	8.03	134.84	123.60
2	A	173	ARG	NE-CZ-NH1	8.01	124.30	120.30
1	B	291	ARG	CD-NE-CZ	7.91	134.67	123.60
1	B	296	VAL	CB-CA-C	-6.84	98.40	111.40
2	A	352	ARG	CD-NE-CZ	6.79	133.10	123.60
2	A	172	ARG	NE-CZ-NH2	-6.53	117.04	120.30
1	B	297	ASP	CB-CG-OD1	6.39	124.05	118.30
1	B	283	ARG	NE-CZ-NH1	6.27	123.43	120.30
2	A	173	ARG	NE-CZ-NH2	-6.16	117.22	120.30
2	A	352	ARG	NE-CZ-NH1	6.08	123.34	120.30
2	A	206	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	B	283	ARG	CD-NE-CZ	5.97	131.96	123.60
1	B	283	ARG	NE-CZ-NH2	-5.93	117.33	120.30
2	A	308	SER	N-CA-CB	-5.63	102.05	110.50
2	A	86	PRO	N-CA-C	5.31	125.91	112.10
2	A	361	ARG	NE-CZ-NH2	-5.25	117.67	120.30

There are no chirality outliers.

There are no planarity outliers.

## 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	B	3145	0	3081	69	0
2	A	2697	0	2620	84	0
3	B	1	0	0	0	0
4	B	5	0	0	0	0
5	B	24	0	25	6	0
6	A	8	0	0	1	0
6	B	9	0	0	0	0
All	All	5889	0	5726	148	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 13.

All (148) 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)
2:A:156:ILE:HG12	2:A:172:ARG:HH12	1.27	0.96
2:A:308:SER:HB2	2:A:309:PRO:HD2	1.47	0.94
2:A:159:ILE:HG12	2:A:168:VAL:HG13	1.55	0.88
1:B:174:ARG:HB3	1:B:216:ILE:HD11	1.62	0.81
1:B:329:MET:HE3	2:A:355:TYR:HA	1.63	0.80
2:A:156:ILE:HD11	2:A:172:ARG:HH22	1.51	0.75
1:B:306:GLY:O	1:B:309:PRO:HD2	1.90	0.72
1:B:250:GLY:CA	5:B:440:FPP:H91	2.23	0.68
1:B:350:LEU:HD23	1:B:363:THR:HG23	1.76	0.67
1:B:335:LEU:HD23	1:B:373:ALA:HB2	1.78	0.66
1:B:253:PHE:HA	1:B:307:LEU:HD21	1.78	0.66
2:A:206:ARG:HD3	2:A:219:GLU:OE2	1.96	0.66
1:B:178:LEU:HB2	1:B:216:ILE:HG23	1.77	0.65
2:A:156:ILE:HG12	2:A:172:ARG:NH1	2.06	0.64
1:B:150:LEU:HD22	1:B:184:LEU:HD23	1.79	0.64
1:B:29:GLU:O	1:B:32:ARG:HG2	1.98	0.64
2:A:308:SER:HB2	2:A:309:PRO:CD	2.23	0.64
5:B:440:FPP:H11	5:B:440:FPP:O3B	1.99	0.63
2:A:138:ARG:HD3	2:A:174:VAL:HG11	1.82	0.62
1:B:119:PRO:HG2	1:B:122:VAL:HG13	1.80	0.61

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:106:VAL:HG12	2:A:111:GLU:HB3	1.81	0.61
2:A:357:ARG:HB3	2:A:361:ARG:HH21	1.66	0.60
2:A:357:ARG:HB3	2:A:361:ARG:NH2	2.17	0.60
1:B:250:GLY:HA3	5:B:440:FPP:H91	1.82	0.59
1:B:198:GLU:OE2	2:A:173:ARG:HD2	2.02	0.59
2:A:131:TYR:HB3	2:A:167:GLN:NE2	2.17	0.59
1:B:79:PHE:CD1	1:B:116:GLU:HG3	2.38	0.58
2:A:303:GLN:N	2:A:304:PRO:HD2	2.19	0.58
1:B:54:LYS:N	1:B:54:LYS:HD2	2.18	0.58
2:A:140:LEU:O	2:A:144:LEU:HB2	2.03	0.58
1:B:322:ALA:HB1	2:A:361:ARG:HB3	1.85	0.57
1:B:329:MET:CE	2:A:355:TYR:HA	2.33	0.57
1:B:126:VAL:HA	2:A:87:VAL:HG21	1.87	0.57
1:B:151:ALA:N	1:B:152:PRO:HD2	2.19	0.57
1:B:353:LYS:HB2	1:B:354:PRO:HD2	1.87	0.56
2:A:156:ILE:CD1	2:A:172:ARG:HH22	2.16	0.56
1:B:113:LEU:HD21	1:B:368:SER:HA	1.87	0.56
1:B:90:THR:C	1:B:92:ALA:H	2.07	0.56
2:A:252:ASP:OD2	2:A:255:VAL:HG13	2.06	0.56
2:A:189:ILE:HD11	2:A:205:HIS:CD2	2.41	0.55
2:A:111:GLU:HG2	2:A:113:SER:HB3	1.88	0.55
2:A:197:ALA:HB1	2:A:233:ASN:ND2	2.22	0.55
2:A:101:ASP:HA	2:A:104:ARG:NH1	2.22	0.54
1:B:350:LEU:HB2	1:B:363:THR:HA	1.89	0.53
1:B:76:GLU:CD	1:B:76:GLU:H	2.10	0.53
1:B:118:ILE:HG23	1:B:122:VAL:CG2	2.39	0.53
1:B:191:PHE:O	1:B:199:VAL:HG12	2.09	0.53
2:A:205:HIS:O	2:A:209:VAL:HG23	2.09	0.52
2:A:323:LEU:HB2	2:A:367:HIS:CE1	2.44	0.52
2:A:328:ASP:O	2:A:329:ASN:HB2	2.08	0.52
1:B:297:ASP:HB3	1:B:300:TYR:HD2	1.75	0.52
2:A:65:LEU:HD21	2:A:94:GLU:HG2	1.91	0.52
2:A:94:GLU:HA	2:A:97:ARG:HH21	1.74	0.52
2:A:56:LEU:HG	2:A:63:TYR:HA	1.91	0.52
2:A:114:GLU:OE1	2:A:146:LYS:NZ	2.42	0.52
2:A:267:ILE:HD13	2:A:277:TRP:CE2	2.44	0.52
2:A:308:SER:CB	2:A:309:PRO:HD2	2.27	0.52
2:A:158:ILE:HG23	2:A:168:VAL:HG22	1.90	0.51
2:A:240:ARG:HD3	2:A:259:GLU:OE1	2.11	0.51
1:B:90:THR:C	1:B:92:ALA:N	2.64	0.50
2:A:249:GLY:O	2:A:255:VAL:HG21	2.12	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:103:PHE:CZ	2:A:133:VAL:HG22	2.46	0.50
2:A:102:TYR:O	2:A:106:VAL:HG22	2.12	0.49
1:B:131:GLU:HG3	1:B:171:VAL:HG13	1.94	0.49
1:B:337:GLU:OE2	1:B:387:MET:HE2	2.13	0.49
2:A:58:LEU:HD22	2:A:125:GLU:HB3	1.95	0.48
1:B:111:LEU:HD23	1:B:118:ILE:HD11	1.94	0.48
2:A:117:PHE:HA	2:A:140:LEU:HD23	1.96	0.48
1:B:26:LEU:HD22	1:B:59:PHE:HB3	1.94	0.48
2:A:148:LEU:HB3	2:A:179:LEU:CD2	2.44	0.48
1:B:282:MET:HB3	1:B:285:GLU:OE1	2.14	0.47
1:B:386:VAL:HG11	1:B:393:VAL:HG13	1.96	0.47
2:A:250:TYR:O	2:A:256:LEU:HD13	2.13	0.47
1:B:245:MET:CE	2:A:204:GLN:HA	2.45	0.47
1:B:23:LEU:HB2	1:B:26:LEU:HG	1.97	0.47
1:B:82:LEU:HB3	1:B:111:LEU:HD13	1.97	0.47
1:B:143:GLY:HA3	1:B:146:GLN:NE2	2.30	0.47
1:B:283:ARG:NH2	2:A:348:LYS:O	2.48	0.46
2:A:113:SER:OG	2:A:115:ARG:HG2	2.14	0.46
2:A:320:GLU:HG2	2:A:363:LEU:HD21	1.97	0.46
2:A:230:ASP:OD1	2:A:232:ARG:HB2	2.15	0.46
2:A:224:ASP:OD1	2:A:240:ARG:NH2	2.47	0.46
2:A:151:GLU:HG3	2:A:175:LEU:HD21	1.97	0.46
1:B:274:LEU:HA	1:B:311:LEU:HD21	1.97	0.46
1:B:51:VAL:O	1:B:55:ILE:HG12	2.15	0.46
1:B:332:GLN:O	1:B:336:GLN:HG3	2.15	0.46
1:B:147:TYR:HB3	1:B:148:PRO:HD2	1.98	0.46
1:B:365:TYR:HA	1:B:368:SER:HB2	1.97	0.46
2:A:159:ILE:CG1	2:A:168:VAL:HG13	2.36	0.46
1:B:198:GLU:HB2	2:A:166:TYR:OH	2.16	0.46
2:A:344:LEU:HD13	2:A:356:TRP:CE2	2.51	0.46
1:B:308:LEU:HD13	1:B:308:LEU:HA	1.87	0.46
1:B:239:ILE:HB	1:B:252:THR:HA	1.99	0.45
1:B:276:TRP:O	1:B:280:ARG:HG2	2.16	0.45
1:B:202:ARG:CG	5:B:440:FPP:H142	2.47	0.45
1:B:200:ASP:OD1	1:B:202:ARG:HB3	2.18	0.44
1:B:33:GLU:O	1:B:284:PHE:HB2	2.16	0.44
5:B:440:FPP:H62	5:B:440:FPP:H41	1.75	0.44
1:B:308:LEU:HD12	1:B:329:MET:HB2	1.98	0.44
1:B:31:ALA:O	1:B:34:ARG:HG3	2.17	0.44
1:B:351:LEU:HD22	1:B:356:LYS:O	2.17	0.44
2:A:272:HIS:CD2	2:A:308:SER:HB3	2.52	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:LEU:HD22	1:B:311:LEU:HD13	1.99	0.44
2:A:257:GLU:O	2:A:261:GLN:HB2	2.18	0.44
2:A:197:ALA:HB1	2:A:233:ASN:HD21	1.81	0.43
2:A:96:PHE:HA	2:A:126:LEU:HD13	2.00	0.43
2:A:313:ALA:HA	2:A:316:VAL:HG13	2.01	0.43
1:B:211:ALA:HB1	1:B:217:ILE:HG12	2.00	0.43
2:A:241:HIS:HA	2:A:250:TYR:OH	2.19	0.43
2:A:356:TRP:CE3	2:A:356:TRP:HA	2.53	0.43
2:A:344:LEU:HB3	2:A:356:TRP:CD1	2.54	0.43
1:B:91:ASP:O	1:B:94:GLU:HG3	2.19	0.43
1:B:308:LEU:N	1:B:309:PRO:CD	2.81	0.42
2:A:151:GLU:HA	2:A:151:GLU:OE1	2.20	0.42
2:A:80:GLN:HB2	2:A:104:ARG:NH2	2.34	0.42
2:A:218:ASN:HD22	2:A:218:ASN:HA	1.66	0.42
2:A:325:ASN:O	2:A:326:GLN:C	2.58	0.42
2:A:94:GLU:HA	2:A:97:ARG:NH2	2.34	0.42
1:B:138:GLY:CA	1:B:176:LYS:HB3	2.50	0.42
1:B:216:ILE:HD13	1:B:421:PRO:HD2	2.01	0.42
1:B:345:CYS:HB2	1:B:351:LEU:HD21	2.01	0.42
2:A:78:VAL:O	2:A:104:ARG:HD2	2.20	0.42
2:A:362:SER:O	2:A:366:LYS:HG3	2.20	0.42
1:B:162:ILE:HD11	1:B:403:ILE:HG22	2.02	0.41
1:B:266:ARG:HD2	1:B:318:GLN:CD	2.40	0.41
2:A:184:GLN:HG2	6:A:379:HOH:O	2.20	0.41
1:B:119:PRO:HG2	1:B:122:VAL:CG1	2.49	0.41
1:B:151:ALA:N	1:B:152:PRO:CD	2.84	0.41
1:B:113:LEU:HD23	1:B:367:LEU:HB3	2.03	0.41
2:A:189:ILE:HD11	2:A:205:HIS:HD2	1.85	0.41
1:B:374:GLN:OE1	1:B:394:LEU:N	2.47	0.41
2:A:303:GLN:O	2:A:304:PRO:C	2.59	0.41
2:A:344:LEU:HD13	2:A:356:TRP:CZ2	2.56	0.41
1:B:94:GLU:C	1:B:96:LEU:H	2.23	0.41
2:A:308:SER:CB	2:A:309:PRO:CD	2.92	0.41
2:A:303:GLN:HA	2:A:307:SER:HB3	2.02	0.41
2:A:77:PRO:HB2	2:A:101:ASP:HB3	2.03	0.41
1:B:100:ARG:N	1:B:101:PRO:CD	2.84	0.41
2:A:82:ASP:HB3	2:A:86:PRO:HB3	2.03	0.41
2:A:240:ARG:NH1	2:A:259:GLU:OE2	2.54	0.41
2:A:299:LEU:HB3	2:A:311:LEU:HD21	2.03	0.41
5:B:440:FPP:H52	5:B:440:FPP:H12A	1.88	0.40
2:A:303:GLN:HB3	2:A:304:PRO:CD	2.51	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:67:ARG:HH22	2:A:94:GLU:CD	2.24	0.40
2:A:176:VAL:HG13	2:A:181:ASP:O	2.21	0.40
2:A:219:GLU:OE1	2:A:219:GLU:HA	2.21	0.40
2:A:112:ARG:HA	2:A:140:LEU:HD11	2.03	0.40
2:A:146:LYS:HD3	2:A:146:LYS:HA	1.88	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	B	398/437 (91%)	363 (91%)	32 (8%)	3 (1%)	24	55
2	A	314/377 (83%)	281 (90%)	25 (8%)	8 (2%)	7	21
All	All	712/814 (88%)	644 (90%)	57 (8%)	11 (2%)	13	36

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	304	PRO
2	A	307	SER
1	B	74	GLN
2	A	217	ASP
2	A	185	GLU
2	A	308	SER
1	B	91	ASP
1	B	120	GLN
2	A	186	LEU
2	A	306	HIS
2	A	182	PRO

### 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	B	338/371 (91%)	296 (88%)	42 (12%)	6	15
2	A	295/338 (87%)	260 (88%)	35 (12%)	6	17
All	All	633/709 (89%)	556 (88%)	77 (12%)	6	16

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	36	GLN
1	B	39	SER
1	B	40	VAL
1	B	53	GLU
1	B	54	LYS
1	B	61	SER
1	B	70	ARG
1	B	72	VAL
1	B	73	LEU
1	B	76	GLU
1	B	83	LYS
1	B	87	ARG
1	B	88	GLN
1	B	108	LEU
1	B	110	SER
1	B	111	LEU
1	B	131	GLU
1	B	135	SER
1	B	150	LEU
1	B	175	GLU
1	B	176	LYS
1	B	184	LEU
1	B	185	LYS
1	B	223	GLU
1	B	231	ARG
1	B	242	VAL
1	B	266	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	268	LEU
1	B	270	LEU
1	B	271	LYS
1	B	277	VAL
1	B	294	LYS
1	B	296	VAL
1	B	311	LEU
1	B	351	LEU
1	B	353	LYS
1	B	372	ILE
1	B	385	VAL
1	B	386	VAL
1	B	393	VAL
1	B	418	LYS
1	B	420	VAL
2	A	56	LEU
2	A	58	LEU
2	A	60	SER
2	A	71	GLU
2	A	87	VAL
2	A	97	ARG
2	A	106	VAL
2	A	107	LEU
2	A	109	ARG
2	A	139	VAL
2	A	140	LEU
2	A	142	ARG
2	A	148	LEU
2	A	149	GLN
2	A	156	ILE
2	A	162	GLN
2	A	168	VAL
2	A	175	LEU
2	A	179	LEU
2	A	180	LYS
2	A	186	LEU
2	A	214	ARG
2	A	217	ASP
2	A	228	LYS
2	A	231	VAL
2	A	257	GLU
2	A	261	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	A	289	LEU
2	A	291	ARG
2	A	294	ASN
2	A	316	VAL
2	A	330	LYS
2	A	346	LYS
2	A	357	ARG
2	A	368	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	88	GLN
1	B	186	GLN
1	B	333	GLN
2	A	81	ASN
2	A	89	GLN
2	A	218	ASN
2	A	261	GLN
2	A	294	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 ⓘ

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	PO4	B	439	-	4,4,4	0.78	0	6,6,6	0.25	0
5	FPP	B	440	-	21,23,23	1.19	1 (4%)	27,31,31	2.33	5 (18%)

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	PO4	B	439	-	-	0/0/0/0	0/0/0/0
5	FPP	B	440	-	-	0/25/25/25	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	440	FPP	C7-C8	2.13	1.37	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	440	FPP	PA-O3A-PB	-4.04	119.14	132.67
5	B	440	FPP	O3B-PB-O1B	-4.00	97.71	110.58
5	B	440	FPP	C10-C8-C9	2.78	119.65	115.41
5	B	440	FPP	C4-C3-C5	3.21	120.31	115.41
5	B	440	FPP	O3A-PA-O1	8.22	124.73	102.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	440	FPP	6	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 ⓘ

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.