



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:02 PM UTC

PDB ID : 1FPP / pdb\_00001fpp  
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

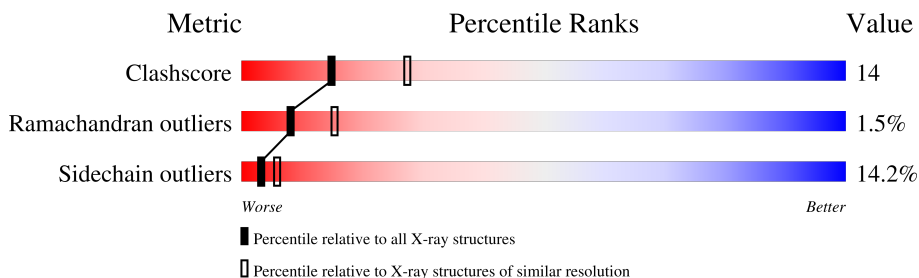
# 1 Overall quality at a glance

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	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$

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
			Total	C	N	O	S			
1	B	400	3145	2010	542	570	23	0	0	0

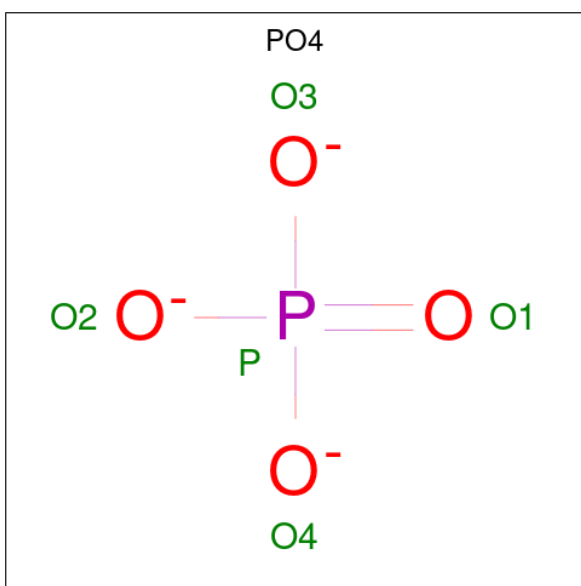
- Molecule 2 is a protein called PROTEIN FARNESYLTRANSFERASE.

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

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

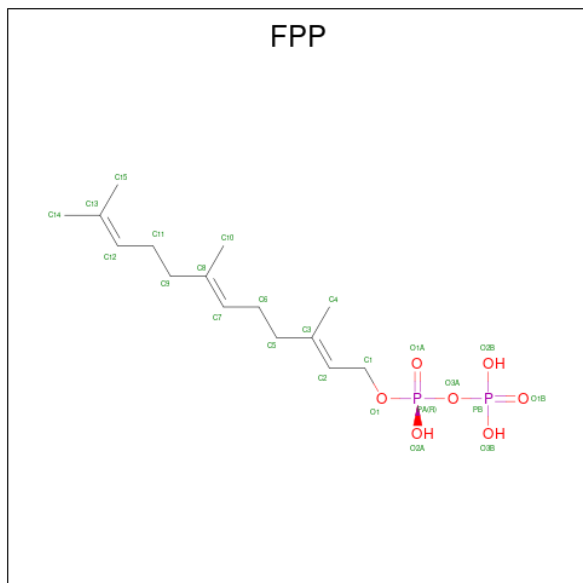
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O<sub>4</sub>P).



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

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



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

- Molecule 6 is water.

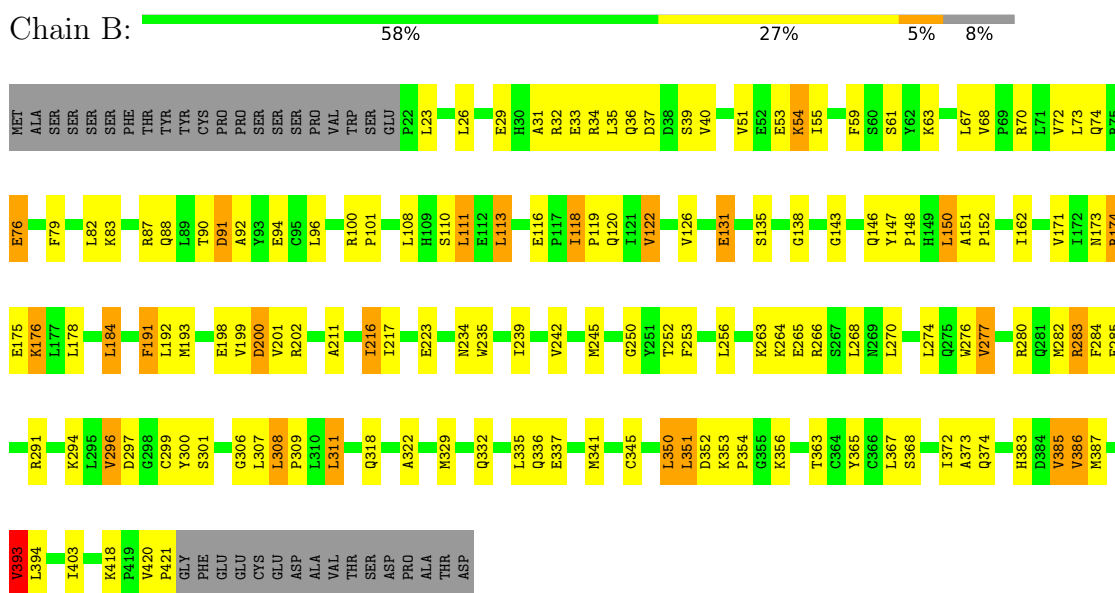
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	9	Total O 9 9	0	0
6	A	8	Total O 8 8	0	0

### 3 Residue-property plots [i](#)

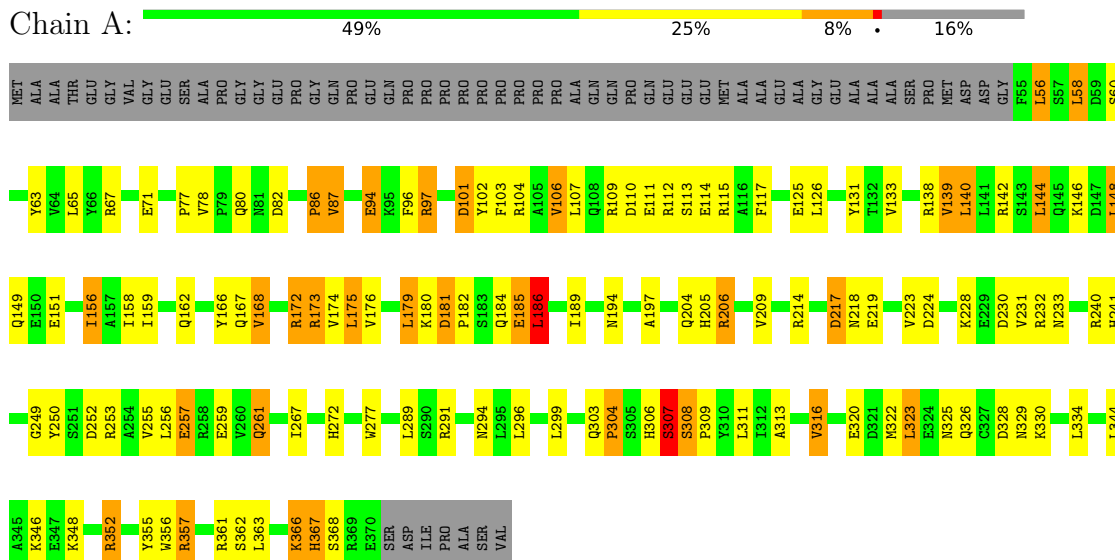
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

- Molecule 1: PROTEIN FARNESYLTRANSFERASE



- Molecule 2: PROTEIN FARNESYLTRANSFERASE



## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	170.00Å 170.00Å 68.86Å 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.	Xtrriage
Total number of atoms	5889	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

## 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: FPP, ZN, PO4

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	0.41	0/3230	1.26	21/4387 (0.5%)
2	A	0.40	0/2763	1.27	11/3750 (0.3%)
All	All	0.40	0/5993	1.27	32/8137 (0.4%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	206	ARG	CD-NE-CZ	19.83	152.17	124.40
2	A	86	PRO	N-CA-C	9.63	125.91	110.40
1	B	277	VAL	N-CA-CB	8.45	119.83	110.62
1	B	296	VAL	CB-CA-C	-7.86	98.40	111.29
1	B	200	ASP	CA-CB-CG	7.68	120.28	112.60
1	B	277	VAL	CB-CA-C	-7.46	102.49	111.81
2	A	173	ARG	CD-NE-CZ	7.46	134.84	124.40
1	B	393	VAL	N-CA-CB	7.45	120.11	110.13
1	B	291	ARG	CD-NE-CZ	7.34	134.67	124.40
1	B	216	ILE	N-CA-CB	-7.28	102.89	112.36
2	A	101	ASP	CA-CB-CG	6.63	119.23	112.60
1	B	67	LEU	CA-C-N	-6.22	117.32	123.04
1	B	67	LEU	C-N-CA	-6.22	117.32	123.04
2	A	352	ARG	CD-NE-CZ	6.21	133.10	124.40
2	A	194	ASN	CA-CB-CG	-6.03	106.58	112.60
2	A	181	ASP	CA-CB-CG	6.00	118.60	112.60
1	B	385	VAL	CA-C-N	-5.79	115.12	123.11
1	B	385	VAL	C-N-CA	-5.79	115.12	123.11
1	B	234	ASN	CA-C-N	5.76	128.58	120.28
1	B	234	ASN	C-N-CA	5.76	128.58	120.28
1	B	173	ASN	CA-CB-CG	5.66	118.26	112.60
2	A	367	HIS	CA-CB-CG	-5.56	108.24	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	393	VAL	CB-CA-C	-5.46	102.69	111.59
1	B	383	HIS	CA-CB-CG	-5.42	108.38	113.80
1	B	283	ARG	CD-NE-CZ	5.40	131.96	124.40
1	B	352	ASP	CA-CB-CG	5.36	117.96	112.60
1	B	191	PHE	CA-CB-CG	5.32	119.12	113.80
2	A	110	ASP	CA-CB-CG	5.18	117.78	112.60
2	A	307	SER	CA-C-O	5.18	127.92	120.51
2	A	139	VAL	N-CA-CB	5.16	117.56	110.54
1	B	37	ASP	CA-C-O	-5.06	115.97	121.44
1	B	174	ARG	N-CA-C	5.00	116.42	111.07

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	77	0
2	A	2697	0	2620	89	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	160	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 14.

All (160) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:ARG:HB3	1:B:216:ILE:HD11	1.62	0.81
1:B:329:MET:HE3	2:A:355:TYR:HA	1.64	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:O3B	5:B:440:FPP:H11	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
1:B:90:THR:C	1:B:92:ALA:H	2.07	0.61
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
1:B:54:LYS:N	1:B:54:LYS:HD2	2.18	0.58
2:A:303:GLN:N	2:A:304:PRO:HD2	2.19	0.58
2:A:140:LEU:O	2:A:144:LEU:HB2	2.03	0.58
1:B:76:GLU:H	1:B:76:GLU:CD	2.10	0.58
1:B:322:ALA:HB1	2:A:361:ARG:HB3	1.85	0.57
1:B:126:VAL:HA	2:A:87:VAL:HG21	1.87	0.57
1:B:329:MET:CE	2:A:355:TYR:HA	2.33	0.57
1:B:26:LEU:HD21	1:B:341:MET:HE1	1.87	0.57
1:B:151:ALA:N	1:B:152:PRO:HD2	2.19	0.57
1:B:193:MET:HE3	1:B:202:ARG:CZ	2.35	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:90:THR:C	1:B:92:ALA:N	2.64	0.54
1:B:350:LEU:HB2	1:B:363:THR:HA	1.89	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
1:B:337:GLU:OE2	1:B:387:MET:HE2	2.09	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: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
2:A:249:GLY:O	2:A:255:VAL:HG21	2.12	0.50
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
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
1:B:26:LEU:HD22	1:B:59:PHE:HB3	1.94	0.48
2:A:117:PHE:HA	2:A:140:LEU:HD23	1.96	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
2:A:114:GLU:OE1	2:A:146:LYS:NZ	2.42	0.47
1:B:386:VAL:HG11	1:B:393:VAL:HG13	1.96	0.47
1:B:245:MET:CE	2:A:204:GLN:HA	2.45	0.47
2:A:250:TYR:O	2:A:256:LEU:HD13	2.13	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
2:A:325:ASN:O	2:A:326:GLN:C	2.58	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:230:ASP:OD1	2:A:232:ARG:HB2	2.15	0.46
2:A:320:GLU:HG2	2:A:363:LEU:HD21	1.97	0.46
2:A:224:ASP:OD1	2:A:240:ARG:NH2	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:ARG:HD2	1:B:318:GLN:CD	2.40	0.46
2:A:151:GLU:HG3	2:A:175:LEU:HD21	1.97	0.46
1:B:51:VAL:O	1:B:55:ILE:HG12	2.15	0.46
1:B:274:LEU:HA	1:B:311:LEU:HD21	1.97	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:303:GLN:O	2:A:304:PRO:C	2.59	0.46
1:B:198:GLU:HB2	2:A:166:TYR:OH	2.16	0.46
2:A:159:ILE:CG1	2:A:168:VAL:HG13	2.36	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:94:GLU:C	1:B:96:LEU:H	2.23	0.45
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
2:A:67:ARG:HH22	2:A:94:GLU:CD	2.24	0.45
1:B:202:ARG:CG	5:B:440:FPP:H142	2.47	0.45
1:B:235:TRP:H	1:B:235:TRP:CD1	2.33	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:H41	5:B:440:FPP:H62	1.75	0.44
1:B:31:ALA:O	1:B:34:ARG:HG3	2.17	0.44
1:B:308:LEU:HD12	1:B:329:MET:HB2	1.98	0.44
1:B:351:LEU:HD22	1:B:356:LYS:O	2.17	0.44
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:272:HIS:CD2	2:A:308:SER:HB3	2.52	0.44
2:A:96:PHE:HA	2:A:126:LEU:HD13	2.00	0.43
2:A:197:ALA:HB1	2:A:233:ASN:HD21	1.81	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
1:B:274:LEU:HD21	1:B:329:MET:HE1	2.01	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:245:MET:HE3	2:A:204:GLN:HA	2.01	0.42
1:B:308:LEU:N	1:B:309:PRO:CD	2.81	0.42
2:A:185:GLU:O	2:A:186:LEU:C	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:218:ASN:HD22	2:A:218:ASN:HA	1.66	0.42
1:B:138:GLY:CA	1:B:176:LYS:HB3	2.50	0.42
2:A:94:GLU:HA	2:A:97:ARG:NH2	2.34	0.42
1:B:34:ARG:O	1:B:35:LEU:C	2.61	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:299:CYS:C	1:B:301:SER:N	2.78	0.41
2:A:184:GLN:HG2	6:A:379:HOH:O	2.20	0.41
2:A:296:LEU:CD2	2:A:322:MET:HE1	2.50	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
1:B:374:GLN:OE1	1:B:394:LEU:N	2.47	0.41
2:A:189:ILE:HD11	2:A:205:HIS:HD2	1.85	0.41
2:A:230:ASP:C	2:A:232:ARG:N	2.79	0.41
2:A:344:LEU:HD13	2:A:356:TRP:CZ2	2.56	0.41
1:B:264:LYS:O	1:B:265:GLU:C	2.63	0.41
1:B:100:ARG:N	1:B:101:PRO:CD	2.84	0.41
2:A:77:PRO:HB2	2:A:101:ASP:HB3	2.03	0.41
2:A:82:ASP:HB3	2:A:86:PRO:HB3	2.03	0.41
2:A:303:GLN:HA	2:A:307:SER:HB3	2.02	0.41
2:A:308:SER:CB	2:A:309:PRO:CD	2.92	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:252:ASP:O	2:A:253:ARG:C	2.64	0.40
2:A:303:GLN:HB3	2:A:304:PRO:CD	2.51	0.40
2:A:176:VAL:HG13	2:A:181:ASP:O	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
2:A:219:GLU:HA	2:A:219:GLU:OE1	2.21	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%)	16	30
2	A	314/377 (83%)	281 (90%)	25 (8%)	8 (2%)	4	8
All	All	712/814 (88%)	644 (90%)	57 (8%)	11 (2%)	8	15

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 [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	B	338/371 (91%)	291 (86%)	47 (14%)	3	6
2	A	295/338 (87%)	252 (85%)	43 (15%)	3	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	633/709 (89%)	543 (86%)	90 (14%)	<b>3</b> <b>6</b>

All (90) 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	63	LYS
1	B	68	VAL
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	113	LEU
1	B	118	ILE
1	B	122	VAL
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	192	LEU
1	B	201	VAL
1	B	223	GLU
1	B	242	VAL
1	B	263	LYS
1	B	268	LEU
1	B	270	LEU
1	B	277	VAL
1	B	294	LYS
1	B	296	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	308	LEU
1	B	311	LEU
1	B	350	LEU
1	B	351	LEU
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	94	GLU
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	144	LEU
2	A	148	LEU
2	A	149	GLN
2	A	156	ILE
2	A	162	GLN
2	A	168	VAL
2	A	172	ARG
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	223	VAL
2	A	228	LYS
2	A	231	VAL
2	A	257	GLU
2	A	261	GLN
2	A	289	LEU

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Mol	Chain	Res	Type
2	A	291	ARG
2	A	294	ASN
2	A	316	VAL
2	A	323	LEU
2	A	330	LYS
2	A	334	LEU
2	A	346	LYS
2	A	352	ARG
2	A	357	ARG
2	A	366	LYS
2	A	368	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	36	GLN
1	B	80	HIS
1	B	128	GLN
1	B	186	GLN
1	B	333	GLN
1	B	383	HIS
2	A	81	ASN
2	A	149	GLN
2	A	167	GLN
2	A	218	ASN
2	A	221	GLN
2	A	261	GLN
2	A	294	ASN
2	A	367	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 oligosaccharides 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	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	PO4	B	439	-	4,4,4	1.03	0	6,6,6	0.27	0
5	FPP	B	440	-	22,23,23	1.62	2 (9%)	27,31,31	1.68	6 (22%)

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	FPP	B	440	-	-	8/25/25/25	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	440	FPP	PA-O3A	-5.41	1.53	1.59
5	B	440	FPP	PA-O1A	2.08	1.58	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	440	FPP	O3A-PA-O1A	-4.20	98.07	110.70
5	B	440	FPP	O3B-PB-O1B	-3.37	97.71	110.83
5	B	440	FPP	C4-C3-C5	2.93	120.31	115.23
5	B	440	FPP	O3B-PB-O3A	2.80	114.02	104.64
5	B	440	FPP	C10-C8-C9	2.55	119.65	115.23
5	B	440	FPP	O2A-PA-O1A	2.06	122.01	112.44

There are no chirality outliers.

All (8) torsion outliers are listed below:

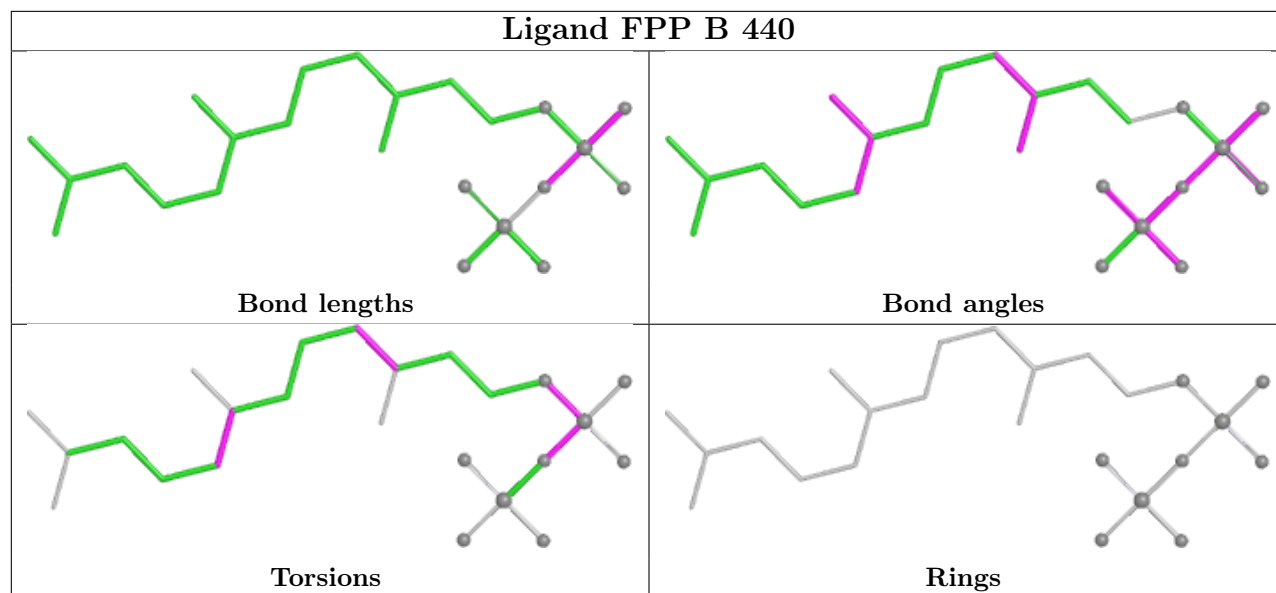
Mol	Chain	Res	Type	Atoms
5	B	440	FPP	C1-O1-PA-O1A
5	B	440	FPP	C1-O1-PA-O3A
5	B	440	FPP	C4-C3-C5-C6
5	B	440	FPP	C2-C3-C5-C6
5	B	440	FPP	PB-O3A-PA-O1A
5	B	440	FPP	PB-O3A-PA-O1
5	B	440	FPP	C10-C8-C9-C11
5	B	440	FPP	C7-C8-C9-C11

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

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 than 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](#)

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.