



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 02:05 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 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>

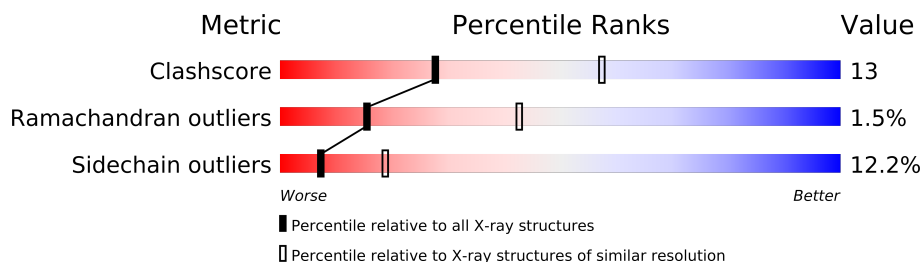
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
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 2.75 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	79885	2995 (2.80-2.72)
Ramachandran outliers	78287	2941 (2.80-2.72)
Sidechain outliers	78261	2944 (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 ≥ 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.

Note EDS was not executed.

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

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5889 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	B	400	Total	C	N	O	S	0	0	0
			3145	2010	542	570	23			

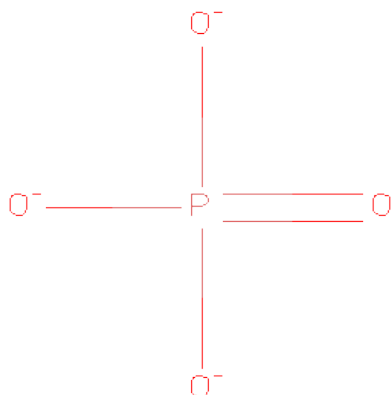
- Molecule 2 is a protein called PROTEIN FARNESYLTRANSFERASE.

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).

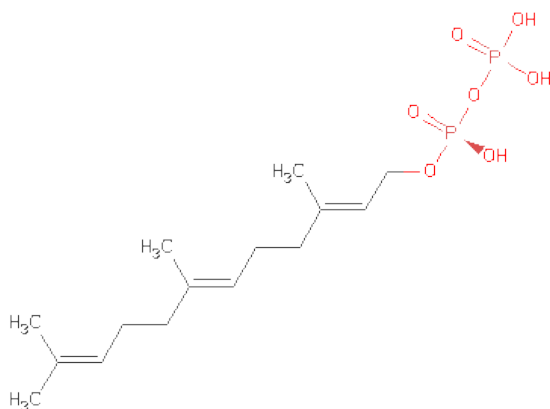
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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		

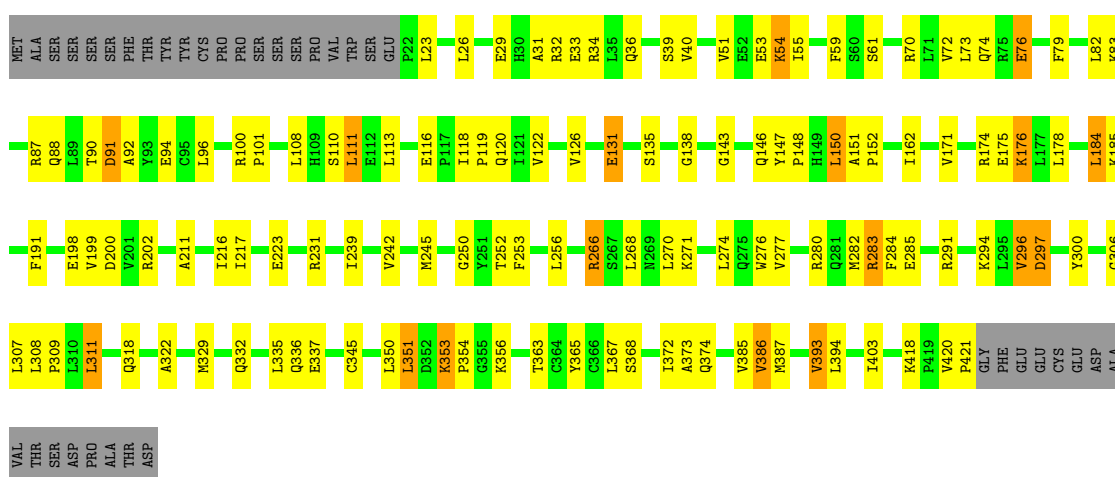
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

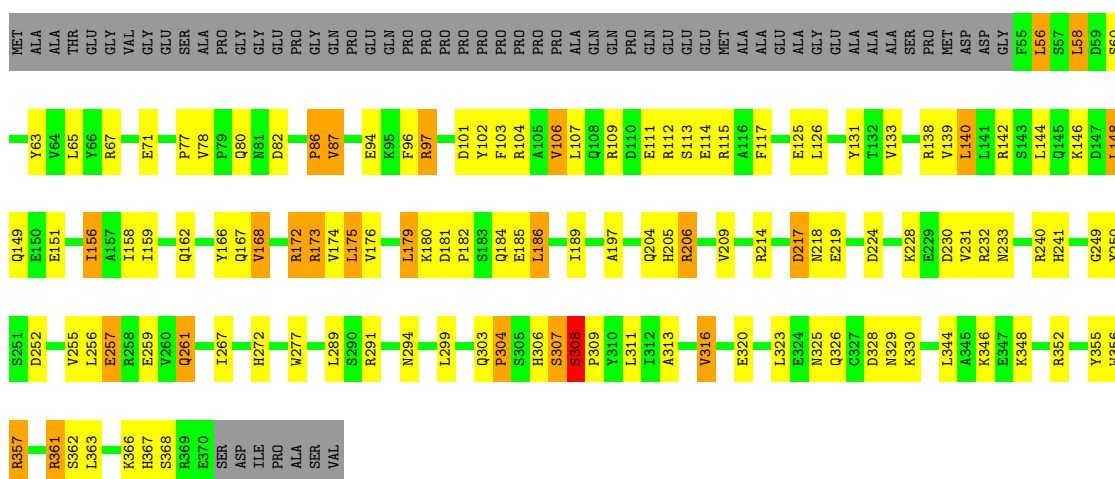
• Molecule 1: PROTEIN FARNESYLTRANSFERASE

Chain B:



• Molecule 2: PROTEIN FARNESYLTRANSFERASE

Chain A:



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, α , β , γ	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.	Xtriage
Total number of atoms	5889	wwPDB-VP
Average B, all atoms (Å ²)	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 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	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

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 13.

All (148) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

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Atom-1	Atom-2	Distance(Å)	Clash(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
2:A:103:PHE:CZ	2:A:133:VAL:HG22	2.46	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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

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	B	398/437 (91%)	363 (91%)	32 (8%)	3 (1%)	27	63
2	A	314/377 (83%)	281 (90%)	25 (8%)	8 (2%)	9	25
All	All	712/814 (88%)	644 (90%)	57 (8%)	11 (2%)	15	43

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%)	7	18
2	A	295/338 (87%)	260 (88%)	35 (12%)	8	20
All	All	633/709 (89%)	556 (88%)	77 (12%)	7	19

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
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

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Mol	Chain	Res	Type
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
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 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 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	0.71	0	6,6,6	0.29	0
5	FPP	B	440	-	23,23,23	1.48	3 (13%)	31,31,31	1.87	5 (16%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	440	FPP	PA-O3A	-3.43	1.53	1.59
5	B	440	FPP	PB-O3A	-3.37	1.54	1.60
5	B	440	FPP	C7-C8	2.08	1.37	1.32

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	440	FPP	O3A-PA-O1	4.77	124.73	103.41
5	B	440	FPP	PA-O3A-PB	-4.28	119.14	131.68
5	B	440	FPP	O3B-PB-O1B	-3.90	97.71	110.44
5	B	440	FPP	C4-C3-C5	3.24	120.31	115.39
5	B	440	FPP	C10-C8-C9	2.80	119.65	115.39

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 ⓘ

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.