



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 03:31 am GMT

PDB ID : 2F0Y  
Title : Crystal Structure Of Human Protein Farnesyltransferase Complexed With Farnesyl Diphosphate and hydantoin derivative  
Authors : Kim, K.H.; Lee, J.; Kim, J.  
Deposited on : 2005-11-14  
Resolution : 2.70 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.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

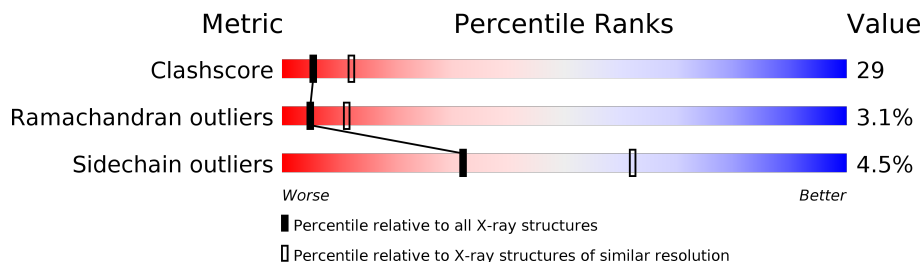
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)

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	A	379	
2	B	437	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6252 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/geranylgeranyltransferase type I alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2676	1707	466	498	5			

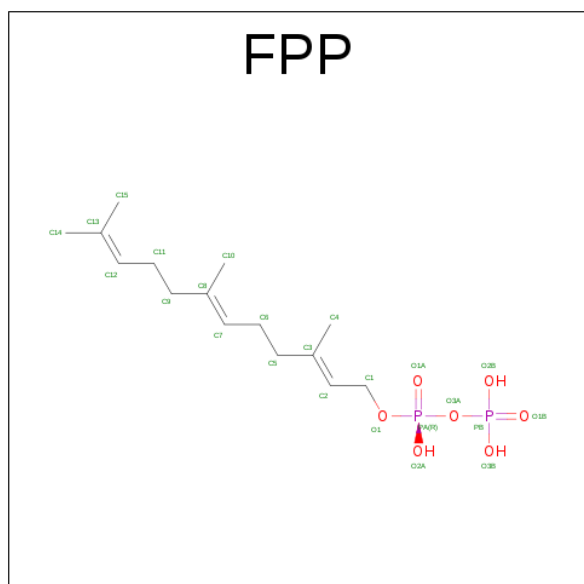
- Molecule 2 is a protein called Protein farnesyltransferase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	395	Total	C	N	O	S	0	0	0
			3107	1984	533	568	22			

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

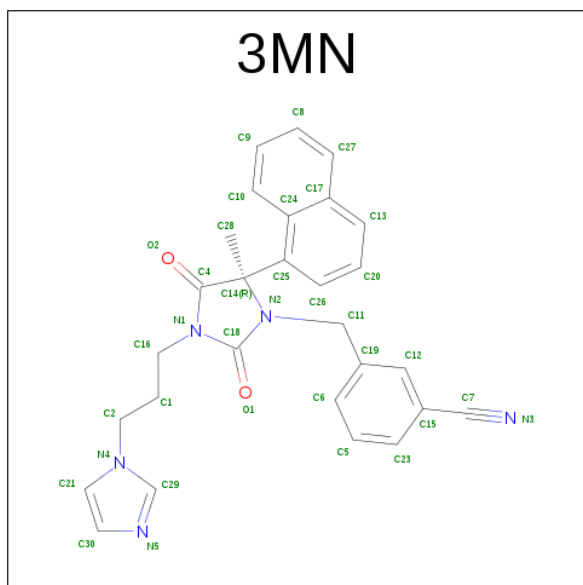
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		

- Molecule 4 is FARNESYL DIPHOSPHATE (three-letter code: FPP) (formula: C<sub>15</sub>H<sub>28</sub>O<sub>7</sub>P<sub>2</sub>).



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

- Molecule 5 is 3-(3-(3-(1H-IMIDAZOL-1-YL)PROPYL)-5-METHYL-5-(1-NAPHTHYL)-2,4-DIOXOIMIDAZOLIDIN-1-YL)METHYL)BENZONITRILE (three-letter code: 3MN) (formula: C<sub>28</sub>H<sub>25</sub>N<sub>5</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			35	28	5	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	201	Total O 201 201	0	0
6	B	208	Total O 208 208	0	0





PHE
GLU
GLU
LEU
LYS
ASP
GLU
THR
SER
ALA
GLU
PRO
ALA
THR
ASP

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	171.89Å 171.89Å 71.37Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-2.70)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.212 , 0.258	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6252	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	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: 3MN, ZN, 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	A	0.44	0/2743	0.61	0/3725
2	B	0.43	0/3188	0.63	0/4328
All	All	0.44	0/5931	0.62	0/8053

There are no bond length outliers.

There are no bond angle outliers.

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	A	2676	0	2594	150	0
2	B	3107	0	3038	185	0
3	B	1	0	0	0	0
4	B	24	0	25	2	0
5	B	35	0	25	3	0
6	A	201	0	0	20	0
6	B	208	0	0	21	0
All	All	6252	0	5682	329	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 29.



All (329) 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:B:127:CYS:HB3	2:B:171:ILE:HD11	1.54	0.89
1:A:75:ILE:HD11	1:A:115:ARG:HH22	1.38	0.87
2:B:389:VAL:HG23	2:B:391:GLU:H	1.40	0.86
1:A:303:GLN:HA	1:A:303:GLN:HE21	1.42	0.84
1:A:294:ASN:HB3	1:A:298:GLN:HE21	1.43	0.81
1:A:303:GLN:O	1:A:307:SER:HB2	1.83	0.79
1:A:312:ILE:HG23	1:A:340:LEU:HD22	1.66	0.78
2:B:140:PHE:O	2:B:148:PRO:HA	1.86	0.76
2:B:158:ASN:O	2:B:162:ILE:HG13	1.85	0.76
1:A:320:GLU:HG2	1:A:363:LEU:HD21	1.66	0.76
2:B:23:LEU:HD12	2:B:26:LEU:HD12	1.68	0.75
1:A:297:ASN:HA	1:A:300:LEU:HD11	1.69	0.75
1:A:332:ASP:O	1:A:336:LYS:HG3	1.86	0.75
1:A:223:VAL:HG13	1:A:236:VAL:HG12	1.68	0.75
2:B:336:GLN:NE2	2:B:374:GLN:HG2	2.01	0.75
2:B:166:GLU:HG3	2:B:170:ASP:OD2	1.87	0.74
2:B:27:ARG:HB3	2:B:29:GLU:OE1	1.87	0.74
2:B:328:TRP:H	2:B:332:GLN:NE2	1.86	0.74
2:B:308:LEU:HG	6:B:1139:HOH:O	1.86	0.73
1:A:67:ARG:HD3	6:A:499:HOH:O	1.89	0.73
2:B:328:TRP:HB2	2:B:332:GLN:HE21	1.52	0.72
2:B:325:MET:SD	2:B:381:MET:HG3	2.30	0.72
1:A:296:LEU:O	1:A:300:LEU:HG	1.89	0.71
2:B:420:VAL:H	2:B:421:PRO:HD2	1.55	0.70
1:A:362:SER:OG	1:A:366:LYS:HE2	1.91	0.70
2:B:176:LYS:HD3	2:B:179:GLN:OE1	1.93	0.69
1:A:141:LEU:HD11	1:A:151:GLU:OE2	1.93	0.69
1:A:342:GLU:O	1:A:346:LYS:HB2	1.93	0.69
1:A:353:LYS:O	1:A:357:ARG:HG3	1.93	0.69
2:B:100:ARG:HA	2:B:103:LEU:HD12	1.74	0.69
1:A:294:ASN:HB3	1:A:298:GLN:NE2	2.08	0.68
1:A:182:PRO:HG3	1:A:213:PHE:CG	2.29	0.68
2:B:101:PRO:HD3	2:B:142:GLY:O	1.92	0.68
2:B:185:LYS:HE3	2:B:189:GLY:HA2	1.75	0.68
2:B:389:VAL:HB	2:B:390:PRO:HD2	1.74	0.68
2:B:297:ASP:HB3	2:B:300:TYR:CD1	2.29	0.67
1:A:148:LEU:HB2	1:A:179:LEU:HD21	1.77	0.67
1:A:225:GLN:O	1:A:228:LYS:HB2	1.94	0.67
1:A:362:SER:O	1:A:366:LYS:HG2	1.94	0.66
1:A:297:ASN:HA	1:A:300:LEU:CD1	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:ASP:OD2	1:A:336:LYS:HD2	1.96	0.66
1:A:352:ARG:HH21	2:B:283:ARG:NH2	1.93	0.66
2:B:377:GLY:O	2:B:378:SER:HB2	1.96	0.66
2:B:398:HIS:CE1	2:B:400:VAL:HB	2.31	0.65
2:B:62:TYR:HD1	2:B:62:TYR:H	1.45	0.65
1:A:148:LEU:CB	1:A:179:LEU:HD21	2.25	0.65
2:B:82:LEU:HD21	2:B:110:SER:HB2	1.79	0.65
1:A:306:HIS:O	1:A:308:SER:N	2.30	0.65
2:B:226:ALA:HB2	2:B:264:ARG:HG3	1.79	0.65
1:A:366:LYS:HB3	1:A:366:LYS:NZ	2.12	0.64
2:B:308:LEU:HD22	2:B:330:PHE:HD2	1.62	0.64
2:B:311:LEU:HD12	6:B:1139:HOH:O	1.98	0.64
2:B:411:ALA:O	2:B:415:PHE:HD1	1.81	0.64
1:A:116:ALA:O	1:A:120:THR:HG23	1.98	0.63
1:A:256:LEU:O	1:A:260:VAL:HG23	1.98	0.63
1:A:303:GLN:HB2	1:A:304:PRO:HD3	1.80	0.63
1:A:199:ASN:HA	6:B:1142:HOH:O	1.97	0.63
2:B:71:LEU:HD12	2:B:387:LEU:CD2	2.28	0.62
1:A:303:GLN:NE2	1:A:307:SER:OG	2.31	0.62
1:A:239:GLN:O	1:A:243:VAL:HG23	1.99	0.62
2:B:198:GLU:CD	2:B:198:GLU:H	2.01	0.62
1:A:327:CYS:O	1:A:330:LYS:HG3	2.00	0.62
2:B:260:VAL:HG21	2:B:310:LEU:HD22	1.82	0.62
2:B:73:LEU:O	2:B:75:ARG:N	2.31	0.61
2:B:113:LEU:HD23	2:B:395:GLN:O	2.00	0.61
2:B:413:THR:O	2:B:417:GLN:HG3	2.00	0.61
2:B:102:TRP:CZ2	5:B:963:3MN:H27	2.36	0.61
2:B:23:LEU:CD1	2:B:26:LEU:HD12	2.30	0.61
1:A:219:GLU:O	1:A:223:VAL:HG23	2.00	0.61
1:A:322:MET:HB3	1:A:327:CYS:SG	2.40	0.61
2:B:390:PRO:HG2	2:B:391:GLU:OE2	2.00	0.61
2:B:175:GLU:O	2:B:179:GLN:HG3	2.00	0.60
1:A:301:ASP:O	1:A:302:LEU:HD23	2.01	0.60
1:A:351:ILE:HB	6:B:1029:HOH:O	2.01	0.60
1:A:184:GLN:HB3	6:A:503:HOH:O	2.02	0.60
2:B:62:TYR:CE2	2:B:341:MET:HG2	2.38	0.58
2:B:119:PRO:HB2	2:B:122:VAL:HG23	1.85	0.58
2:B:308:LEU:HD22	2:B:330:PHE:HB3	1.86	0.58
2:B:28:PRO:HD2	2:B:29:GLU:OE1	2.04	0.58
2:B:138:GLY:CA	2:B:176:LYS:HB3	2.34	0.58
2:B:308:LEU:H	2:B:308:LEU:HD12	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:121:ILE:HA	2:B:124:THR:HG22	1.86	0.58
2:B:71:LEU:HD12	2:B:387:LEU:HD23	1.85	0.57
1:A:320:GLU:HG2	1:A:363:LEU:CD2	2.34	0.57
1:A:154:TYR:CE1	1:A:158:ILE:HD11	2.40	0.57
2:B:253:PHE:HA	2:B:307:LEU:HD21	1.86	0.57
2:B:389:VAL:HG23	2:B:391:GLU:N	2.15	0.57
2:B:162:ILE:HA	2:B:407:LYS:HD2	1.86	0.57
1:A:223:VAL:HG13	1:A:236:VAL:CG1	2.33	0.57
1:A:314:PHE:O	1:A:317:ASP:HB2	2.05	0.57
2:B:308:LEU:CD2	2:B:330:PHE:HB3	2.35	0.56
2:B:192:LEU:HD22	2:B:197:GLY:O	2.05	0.56
1:A:75:ILE:HD11	1:A:115:ARG:NH2	2.15	0.56
2:B:415:PHE:O	2:B:418:LYS:HB2	2.05	0.56
2:B:202:ARG:HD2	4:B:1001:FPP:H142	1.86	0.56
2:B:282:MET:HG2	2:B:287:GLY:O	2.05	0.56
1:A:67:ARG:HA	1:A:102:TYR:OH	2.06	0.56
2:B:21:GLU:HB3	2:B:27:ARG:HG2	1.88	0.56
2:B:62:TYR:N	2:B:62:TYR:CD1	2.71	0.55
1:A:357:ARG:O	1:A:361:ARG:HD3	2.06	0.55
2:B:112:GLU:OE2	2:B:407:LYS:HG3	2.07	0.55
2:B:51:VAL:O	2:B:55:ILE:HG12	2.06	0.55
1:A:285:GLN:HG3	1:A:286:ASP:H	1.72	0.55
1:A:285:GLN:HG3	1:A:286:ASP:N	2.22	0.55
2:B:336:GLN:HG2	2:B:370:LEU:HD12	1.88	0.55
1:A:150:GLU:O	1:A:153:ASN:HB2	2.06	0.55
1:A:151:GLU:HG2	1:A:175:LEU:HD21	1.89	0.54
2:B:122:VAL:O	2:B:126:VAL:HG23	2.07	0.54
1:A:299:LEU:C	1:A:301:ASP:H	2.10	0.54
1:A:357:ARG:HH11	1:A:357:ARG:HG2	1.71	0.54
1:A:346:LYS:HE2	1:A:357:ARG:HH22	1.72	0.54
1:A:87:VAL:HG23	1:A:88:VAL:HG22	1.89	0.54
2:B:149:HIS:HB3	2:B:152:PRO:CG	2.38	0.54
1:A:287:ARG:HB2	6:A:559:HOH:O	2.06	0.54
2:B:99:SER:O	2:B:102:TRP:HB2	2.08	0.54
1:A:165:ASN:OD1	1:A:168:VAL:HG13	2.08	0.53
1:A:209:VAL:HG12	1:A:215:LEU:HD12	1.90	0.53
1:A:345:ALA:HB2	1:A:356:TRP:HB2	1.89	0.53
2:B:62:TYR:CD2	2:B:341:MET:HG2	2.44	0.53
1:A:364:GLN:O	1:A:365:SER:C	2.47	0.53
2:B:308:LEU:HD22	2:B:330:PHE:CD2	2.41	0.53
1:A:357:ARG:HB3	1:A:361:ARG:NH1	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:PRO:HB3	6:A:510:HOH:O	2.09	0.53
2:B:71:LEU:HD11	2:B:341:MET:CE	2.39	0.53
1:A:114:GLU:O	1:A:117:PHE:HB3	2.09	0.53
1:A:91:ILE:HD13	6:A:578:HOH:O	2.07	0.52
2:B:398:HIS:HE1	2:B:400:VAL:HB	1.73	0.52
1:A:137:ARG:HH11	1:A:137:ARG:HG3	1.73	0.52
2:B:188:ASP:N	2:B:188:ASP:OD2	2.28	0.52
2:B:389:VAL:CB	2:B:390:PRO:HD2	2.39	0.52
2:B:51:VAL:HG21	2:B:295:LEU:HD22	1.91	0.52
1:A:150:GLU:HG3	6:A:393:HOH:O	2.09	0.52
1:A:89:GLN:HA	2:B:100:ARG:NH2	2.25	0.52
2:B:289:GLN:NE2	2:B:294:LYS:H	2.07	0.52
2:B:62:TYR:HB3	6:B:1182:HOH:O	2.10	0.52
1:A:65:LEU:O	1:A:69:ARG:HG3	2.09	0.52
2:B:370:LEU:HD23	2:B:394:LEU:CD1	2.39	0.52
2:B:21:GLU:OE2	2:B:22:PRO:HD2	2.09	0.52
2:B:266:ARG:HB2	6:B:1032:HOH:O	2.10	0.52
1:A:59:ASP:HA	6:A:569:HOH:O	2.10	0.52
2:B:234:ASN:OD1	2:B:236:GLU:HB2	2.09	0.52
2:B:77:LYS:HG3	6:B:1088:HOH:O	2.10	0.52
1:A:97:ARG:HD2	6:A:432:HOH:O	2.10	0.52
2:B:328:TRP:CB	2:B:332:GLN:HE21	2.20	0.51
2:B:62:TYR:HD1	2:B:62:TYR:N	2.06	0.51
2:B:233:GLN:HA	2:B:238:GLY:O	2.09	0.51
1:A:253:ARG:NH1	6:A:402:HOH:O	2.35	0.51
1:A:59:ASP:OD2	1:A:59:ASP:N	2.43	0.51
2:B:150:LEU:HD12	2:B:192:LEU:O	2.10	0.51
2:B:202:ARG:HA	2:B:254:CYS:SG	2.51	0.51
2:B:376:PHE:O	2:B:382:LEU:HD23	2.10	0.51
2:B:154:TYR:O	2:B:158:ASN:HB2	2.10	0.51
1:A:104:ARG:O	1:A:108:GLN:HB2	2.11	0.51
2:B:89:LEU:HA	6:B:1140:HOH:O	2.09	0.51
1:A:147:ASP:OD2	1:A:149:HIS:HB2	2.11	0.51
2:B:120:GLN:O	2:B:124:THR:HG22	2.12	0.50
1:A:174:VAL:HA	1:A:177:GLU:OE2	2.11	0.50
1:A:352:ARG:NH2	2:B:283:ARG:NH2	2.58	0.50
1:A:65:LEU:HG	6:A:428:HOH:O	2.11	0.50
6:A:401:HOH:O	2:B:275:GLN:HG2	2.10	0.50
2:B:226:ALA:CB	2:B:264:ARG:HG3	2.41	0.50
1:A:77:PRO:HG3	1:A:102:TYR:CZ	2.46	0.50
2:B:48:GLN:O	2:B:52:GLU:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:ARG:HG3	6:A:399:HOH:O	2.12	0.50
2:B:280:ARG:NE	2:B:280:ARG:HA	2.27	0.49
2:B:299:CYS:HB3	2:B:362:HIS:CD2	2.46	0.49
2:B:53:GLU:HG2	6:B:1156:HOH:O	2.11	0.49
1:A:155:ILE:HD13	1:A:171:HIS:CD2	2.47	0.49
1:A:357:ARG:HB3	1:A:361:ARG:HH11	1.77	0.49
2:B:194:HIS:HE1	6:B:1136:HOH:O	1.96	0.49
2:B:370:LEU:HD23	2:B:394:LEU:HD12	1.94	0.49
2:B:200:ASP:OD1	2:B:202:ARG:HB2	2.12	0.49
2:B:149:HIS:ND1	2:B:152:PRO:HD2	2.27	0.49
2:B:416:LEU:C	2:B:418:LYS:H	2.16	0.49
2:B:34:ARG:HB3	6:B:1092:HOH:O	2.12	0.49
1:A:151:GLU:HG3	1:A:175:LEU:HD11	1.95	0.48
2:B:308:LEU:HB2	2:B:309:PRO:HD3	1.95	0.48
2:B:180:TYR:CZ	2:B:184:LEU:HD11	2.48	0.48
2:B:263:LYS:HA	2:B:265:GLU:OE2	2.13	0.48
1:A:312:ILE:O	1:A:315:LEU:HB2	2.13	0.48
1:A:155:ILE:HD13	1:A:171:HIS:HD2	1.78	0.48
2:B:283:ARG:CZ	2:B:283:ARG:HB3	2.43	0.48
2:B:326:SER:HB2	2:B:383:HIS:CD2	2.48	0.48
2:B:56:GLN:HA	2:B:56:GLN:NE2	2.27	0.48
1:A:323:LEU:HD22	1:A:367:HIS:CD2	2.48	0.47
2:B:338:TYR:CE2	2:B:343:CYS:SG	3.07	0.47
1:A:194:ASN:HA	6:A:451:HOH:O	2.13	0.47
2:B:115:ASP:HB2	2:B:395:GLN:CG	2.44	0.47
2:B:411:ALA:O	2:B:415:PHE:CD1	2.66	0.47
2:B:72:VAL:HG22	2:B:389:VAL:CG1	2.44	0.47
1:A:112:ARG:HA	1:A:140:LEU:CD2	2.44	0.47
1:A:180:ARG:HG2	6:A:530:HOH:O	2.13	0.47
1:A:302:LEU:O	1:A:306:HIS:N	2.47	0.47
2:B:102:TRP:CE2	5:B:963:3MN:H27	2.50	0.47
1:A:160:GLU:OE2	1:A:191:ASP:OD2	2.33	0.47
2:B:281:GLN:HB2	2:B:288:PHE:CZ	2.50	0.47
2:B:115:ASP:HB2	2:B:395:GLN:HG2	1.95	0.47
2:B:328:TRP:O	2:B:330:PHE:N	2.45	0.47
1:A:232:ARG:NH1	2:B:42:THR:OG1	2.48	0.47
1:A:189:ILE:HG21	1:A:206:ARG:HB2	1.97	0.46
1:A:102:TYR:O	1:A:105:ALA:HB3	2.16	0.46
1:A:303:GLN:NE2	1:A:307:SER:CB	2.78	0.46
1:A:188:PHE:CE1	1:A:192:ILE:HD11	2.50	0.46
2:B:71:LEU:HD11	2:B:341:MET:HE2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:LEU:HD22	1:A:338:LEU:HD11	1.97	0.46
1:A:339:GLU:O	1:A:343:ILE:HG13	2.16	0.46
1:A:71:GLU:N	1:A:71:GLU:OE1	2.49	0.46
2:B:91:ASP:O	2:B:94:GLU:HG3	2.15	0.46
1:A:103:PHE:C	1:A:105:ALA:N	2.68	0.46
1:A:322:MET:C	1:A:324:GLU:H	2.17	0.46
2:B:33:GLU:HB3	2:B:283:ARG:HG3	1.96	0.46
2:B:239:ILE:HB	2:B:252:THR:HA	1.96	0.46
2:B:73:LEU:HD12	2:B:344:GLN:OE1	2.16	0.46
5:B:963:3MN:C18	5:B:963:3MN:H10	2.46	0.46
1:A:103:PHE:C	1:A:105:ALA:H	2.19	0.46
1:A:295:LEU:O	1:A:299:LEU:HG	2.16	0.46
1:A:301:ASP:C	1:A:302:LEU:HD23	2.35	0.46
2:B:277:VAL:HG13	2:B:278:THR:N	2.31	0.46
2:B:304:GLN:O	2:B:307:LEU:HB2	2.16	0.46
2:B:350:LEU:HD13	2:B:367:LEU:HG	1.97	0.46
2:B:404:GLY:O	2:B:408:VAL:HG23	2.16	0.46
1:A:137:ARG:HD3	1:A:137:ARG:O	2.15	0.45
2:B:391:GLU:HA	6:B:1056:HOH:O	2.15	0.45
2:B:224:GLY:HA2	2:B:227:GLU:OE1	2.16	0.45
2:B:380:ALA:HB3	2:B:381:MET:CE	2.47	0.45
1:A:111:GLU:HG2	1:A:113:SER:OG	2.15	0.45
2:B:265:GLU:O	2:B:270:LEU:HD21	2.16	0.45
1:A:303:GLN:CB	1:A:304:PRO:HD3	2.46	0.45
2:B:71:LEU:HD13	2:B:340:LEU:HB2	1.97	0.45
1:A:136:PHE:CE2	1:A:140:LEU:HD11	2.51	0.45
2:B:340:LEU:HD11	6:B:1028:HOH:O	2.17	0.45
1:A:70:ALA:O	1:A:72:TRP:N	2.50	0.45
1:A:251:ASN:HB2	6:A:423:HOH:O	2.17	0.45
2:B:113:LEU:C	2:B:115:ASP:H	2.21	0.45
1:A:289:LEU:HG	6:A:418:HOH:O	2.16	0.44
1:A:303:GLN:HE21	1:A:303:GLN:CA	2.19	0.44
1:A:364:GLN:O	1:A:367:HIS:N	2.50	0.44
2:B:350:LEU:HD12	2:B:363:THR:HG23	1.99	0.44
2:B:113:LEU:HD22	2:B:371:SER:HB2	1.98	0.44
1:A:87:VAL:O	1:A:88:VAL:C	2.56	0.44
2:B:113:LEU:HD11	2:B:368:SER:HA	1.99	0.44
1:A:210:ILE:HA	1:A:215:LEU:HB2	2.00	0.44
1:A:241:TYR:HA	1:A:250:TYR:OH	2.17	0.44
1:A:244:ILE:HA	1:A:247:THR:OG1	2.17	0.44
1:A:71:GLU:HB2	6:A:464:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:418:LYS:HB3	2:B:419:PRO:HD2	2.00	0.44
2:B:151:ALA:HB3	2:B:152:PRO:CD	2.48	0.44
1:A:367:HIS:HD1	1:A:367:HIS:C	2.21	0.44
2:B:237:GLY:O	2:B:273:LEU:HA	2.18	0.44
2:B:420:VAL:HB	2:B:421:PRO:HD3	2.00	0.44
2:B:43:VAL:HG23	6:B:1057:HOH:O	2.17	0.44
1:A:91:ILE:HD11	2:B:88:GLN:HG2	1.99	0.44
1:A:75:ILE:CD1	1:A:115:ARG:HH22	2.20	0.44
2:B:127:CYS:HB3	2:B:171:ILE:CD1	2.37	0.44
1:A:328:ASP:O	1:A:329:ASN:HB2	2.18	0.44
2:B:78:HIS:ND1	2:B:349:GLY:N	2.62	0.44
1:A:161:GLU:HG3	1:A:162:GLN:HG3	2.00	0.44
2:B:46:ILE:HG22	2:B:50:LYS:HE3	2.00	0.44
2:B:254:CYS:SG	4:B:1001:FPP:H153	2.58	0.43
2:B:388:GLY:HA2	6:B:1119:HOH:O	2.18	0.43
2:B:161:CYS:O	2:B:407:LYS:HD3	2.18	0.43
2:B:412:THR:O	2:B:416:LEU:HG	2.18	0.43
6:A:389:HOH:O	2:B:271:LYS:HB2	2.17	0.43
1:A:342:GLU:OE2	1:A:346:LYS:HG2	2.18	0.43
2:B:266:ARG:HD3	6:B:1067:HOH:O	2.18	0.43
2:B:421:PRO:HG3	6:B:1002:HOH:O	2.17	0.43
2:B:121:ILE:HA	2:B:124:THR:CG2	2.48	0.43
2:B:280:ARG:O	2:B:289:GLN:HG2	2.18	0.43
2:B:362:HIS:O	2:B:366:CYS:HB2	2.17	0.43
2:B:90:THR:C	2:B:92:ALA:H	2.21	0.43
2:B:420:VAL:O	2:B:421:PRO:C	2.57	0.43
1:A:253:ARG:HG2	6:A:533:HOH:O	2.19	0.43
2:B:374:GLN:HA	2:B:385:VAL:O	2.18	0.42
1:A:136:PHE:CZ	1:A:140:LEU:HD21	2.54	0.42
2:B:121:ILE:CA	2:B:124:THR:HG22	2.49	0.42
1:A:169:TRP:CD1	1:A:201:HIS:HB3	2.55	0.42
1:A:312:ILE:CG2	1:A:344:LEU:HD21	2.48	0.42
2:B:174:ARG:HE	2:B:415:PHE:HD2	1.67	0.42
1:A:334:LEU:HD22	1:A:338:LEU:CD1	2.50	0.42
2:B:168:ALA:O	2:B:171:ILE:HG13	2.20	0.42
2:B:253:PHE:HB2	2:B:303:TRP:O	2.20	0.42
1:A:267:ILE:O	1:A:271:PRO:N	2.52	0.42
1:A:296:LEU:O	1:A:296:LEU:HD12	2.20	0.42
1:A:148:LEU:HB3	1:A:179:LEU:HD21	2.02	0.42
1:A:288:GLY:O	1:A:291:LYS:HB3	2.20	0.42
1:A:300:LEU:HA	1:A:303:GLN:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:139:GLY:C	2:B:140:PHE:CD1	2.93	0.42
2:B:227:GLU:OE2	2:B:264:ARG:NH2	2.50	0.42
1:A:287:ARG:HD2	1:A:287:ARG:HA	1.85	0.41
2:B:277:VAL:CG1	2:B:278:THR:N	2.83	0.41
2:B:336:GLN:HG2	2:B:370:LEU:CD1	2.49	0.41
2:B:26:LEU:HD21	2:B:59:PHE:C	2.40	0.41
1:A:255:VAL:HG13	1:A:258:ARG:NH2	2.35	0.41
1:A:333:ILE:O	1:A:336:LYS:N	2.53	0.41
2:B:192:LEU:HD23	2:B:199:VAL:HG22	2.02	0.41
2:B:275:GLN:HG3	6:B:1059:HOH:O	2.20	0.41
2:B:309:PRO:HA	2:B:328:TRP:CZ3	2.56	0.41
1:A:254:ALA:O	1:A:257:GLU:HB3	2.20	0.41
1:A:96:PHE:CE1	2:B:94:GLU:HB3	2.54	0.41
2:B:229:ILE:O	2:B:232:CYS:HB2	2.20	0.41
2:B:325:MET:CE	2:B:325:MET:HA	2.50	0.41
2:B:333:GLN:HB2	6:B:1009:HOH:O	2.21	0.41
1:A:241:TYR:O	1:A:245:SER:OG	2.31	0.41
2:B:343:CYS:O	2:B:350:LEU:HA	2.20	0.41
1:A:138:ARG:HA	1:A:141:LEU:HB2	2.01	0.41
1:A:165:ASN:O	1:A:168:VAL:HG22	2.20	0.41
2:B:377:GLY:O	2:B:378:SER:CB	2.66	0.41
2:B:75:ARG:HG2	2:B:114:LEU:HD22	2.02	0.41
2:B:82:LEU:HD21	2:B:110:SER:CB	2.48	0.41
1:A:159:ILE:HG12	1:A:168:VAL:HB	2.03	0.41
1:A:86:PRO:HG2	1:A:89:GLN:OE1	2.21	0.41
2:B:82:LEU:CD2	2:B:110:SER:HB2	2.47	0.41
1:A:185:GLU:O	1:A:186:LEU:C	2.59	0.41
1:A:303:GLN:HA	1:A:303:GLN:NE2	2.22	0.41
2:B:308:LEU:HD12	2:B:308:LEU:N	2.34	0.41
2:B:26:LEU:CD2	2:B:59:PHE:HB3	2.50	0.41
2:B:105:TYR:OH	2:B:402:ASN:HB3	2.21	0.41
2:B:225:THR:O	2:B:226:ALA:C	2.58	0.41
1:A:344:LEU:HD13	1:A:356:TRP:CE2	2.56	0.41
2:B:219:PRO:HB2	6:B:1053:HOH:O	2.19	0.41
1:A:78:VAL:HA	1:A:79:PRO:HD3	1.85	0.40
2:B:123:ALA:O	2:B:126:VAL:HB	2.21	0.40
1:A:197:ALA:HB1	1:A:233:ASN:HD21	1.86	0.40
1:A:359:ILE:O	1:A:363:LEU:HG	2.21	0.40
2:B:227:GLU:HG3	6:B:1207:HOH:O	2.20	0.40
1:A:135:HIS:HD1	2:B:147:TYR:HE1	1.69	0.40
2:B:113:LEU:CD2	2:B:371:SER:HB2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:PHE:HA	1:A:140:LEU:HD12	2.03	0.40
1:A:330:LYS:HD3	6:A:447:HOH:O	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	A	312/379 (82%)	257 (82%)	43 (14%)	12 (4%)	4	8
2	B	391/437 (90%)	351 (90%)	30 (8%)	10 (3%)	6	15
All	All	703/816 (86%)	608 (86%)	73 (10%)	22 (3%)	5	11

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	307	SER
2	B	74	GLN
2	B	378	SER
1	A	71	GLU
1	A	365	SER
2	B	329	MET
2	B	420	VAL
1	A	70	ALA
1	A	185	GLU
1	A	243	VAL
2	B	168	ALA
2	B	201	VAL
2	B	219	PRO
1	A	217	ASP
1	A	326	GLN
2	B	60	SER

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Mol	Chain	Res	Type
2	B	61	SER
1	A	58	LEU
1	A	209	VAL
2	B	419	PRO
1	A	84	PRO
1	A	86	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	A	293/341 (86%)	281 (96%)	12 (4%)	35	66
2	B	332/370 (90%)	316 (95%)	16 (5%)	30	59
All	All	625/711 (88%)	597 (96%)	28 (4%)	32	62

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	LEU
1	A	59	ASP
1	A	60	SER
1	A	71	GLU
1	A	85	ASN
1	A	137	ARG
1	A	268	LYS
1	A	269	LEU
1	A	301	ASP
1	A	303	GLN
1	A	334	LEU
1	A	366	LYS
2	B	29	GLU
2	B	53	GLU
2	B	62	TYR
2	B	88	GLN
2	B	121	ILE

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Mol	Chain	Res	Type
2	B	158	ASN
2	B	188	ASP
2	B	198	GLU
2	B	219	PRO
2	B	254	CYS
2	B	265	GLU
2	B	313	ARG
2	B	351	LEU
2	B	387	LEU
2	B	389	VAL
2	B	421	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	201	HIS
1	A	298	GLN
1	A	303	GLN
1	A	326	GLN
1	A	335	ASN
1	A	364	GLN
2	B	30	HIS
2	B	327	HIS
2	B	332	GLN
2	B	383	HIS

### 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	FPP	B	1001	-	22,23,23	0.95	2 (9%)	24,31,31	1.54	4 (16%)
5	3MN	B	963	3	35,39,39	1.93	7 (20%)	44,56,56	2.08	10 (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
4	FPP	B	1001	-	-	0/25/25/25	0/0/0/0
5	3MN	B	963	3	-	0/18/42/42	0/5/5/5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1001	FPP	PB-O3A	-2.25	1.56	1.60
4	B	1001	FPP	O1-C1	-2.01	1.41	1.43
5	B	963	3MN	C8-C27	2.29	1.42	1.36
5	B	963	3MN	C5-C6	2.41	1.43	1.38
5	B	963	3MN	C5-C23	2.47	1.43	1.38
5	B	963	3MN	C6-C19	2.48	1.44	1.38
5	B	963	3MN	C25-C24	2.50	1.49	1.43
5	B	963	3MN	C21-N4	4.98	1.46	1.37
5	B	963	3MN	C26-C25	5.91	1.44	1.37

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1001	FPP	C10-C8-C9	-3.37	109.44	115.29
5	B	963	3MN	O1-C18-N2	-3.34	122.21	125.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	963	3MN	C11-C19-C12	-2.85	114.59	120.23
5	B	963	3MN	C21-N4-C29	-2.59	105.67	108.22
5	B	963	3MN	C27-C17-C13	-2.18	118.02	123.18
5	B	963	3MN	C1-C16-N1	2.04	117.49	112.41
5	B	963	3MN	C16-N1-C18	2.07	125.82	123.63
4	B	1001	FPP	C10-C8-C7	2.41	130.14	123.69
5	B	963	3MN	C11-C19-C6	2.81	126.11	120.78
4	B	1001	FPP	C1-C2-C3	2.92	131.33	125.96
4	B	1001	FPP	C5-C6-C7	3.28	123.23	111.97
5	B	963	3MN	N2-C18-N1	3.78	109.84	107.46
5	B	963	3MN	C19-C11-N2	3.80	124.83	114.61
5	B	963	3MN	C14-C25-C24	9.10	125.34	120.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1001	FPP	2	0
5	B	963	3MN	3	0

## 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

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.