



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:35 AM UTC

PDB ID : 2F0Y / pdb_00002f0y
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

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>.

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)
Xtriage (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

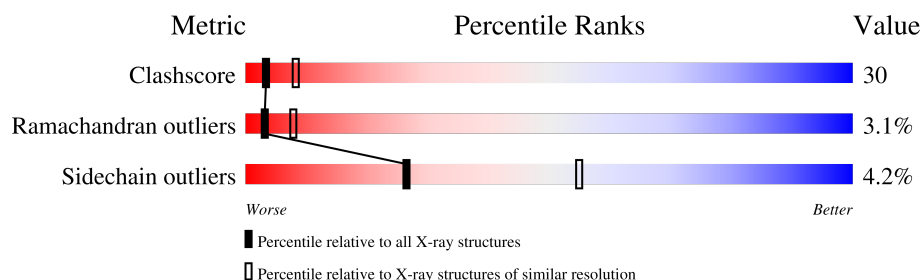
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	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			

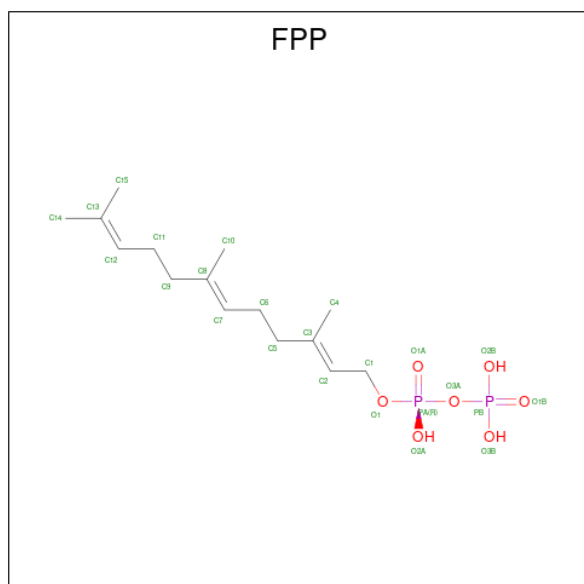
- Molecule 2 is a protein called Protein farnesyltransferase beta subunit.

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 (CCD ID: ZN) (formula: Zn).

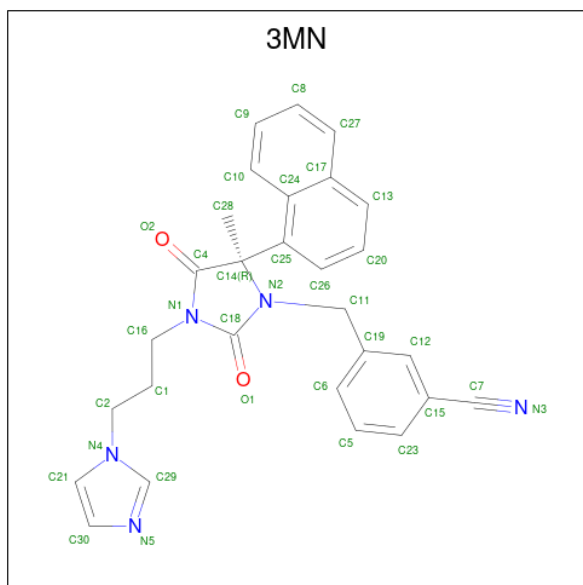
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		

- Molecule 4 is FARNESYL DIPHOSPHATE (CCD ID: FPP) (formula: C₁₅H₂₈O₇P₂).



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

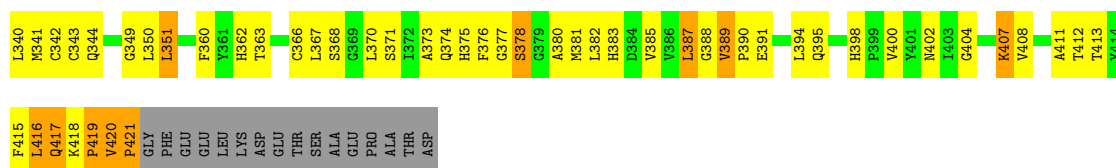
- Molecule 5 is 3-({3-[3-(1H-IMIDAZOL-1-YL)PROPYL]-5-METHYL-5-(1-NAPHTHYL)-2,4-DIOXOIMIDAZOLIDIN-1-YL}METHYL)BENZONITRILE (CCD ID: 3MN) (formula: C₂₈H₂₅N₅O₂).



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



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, α , β , γ	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 ²)	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: FPP, 3MN, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.53	0/2743	0.99	15/3725 (0.4%)
2	B	0.53	0/3188	1.01	14/4328 (0.3%)
All	All	0.53	0/5931	1.00	29/8053 (0.4%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	163	ILE	N-CA-C	-6.92	103.59	110.30
2	B	351	LEU	N-CA-C	6.56	118.50	109.18
2	B	26	LEU	N-CA-C	6.37	121.20	113.17
2	B	360	PHE	N-CA-C	6.31	118.97	111.71
1	A	237	TRP	N-CA-C	-6.17	104.66	111.82
1	A	292	TYR	CA-C-N	6.02	125.23	118.97
1	A	292	TYR	C-N-CA	6.02	125.23	118.97
2	B	416	LEU	N-CA-C	-5.93	104.89	111.36
1	A	85	ASN	CA-C-N	5.74	127.01	119.84
1	A	85	ASN	C-N-CA	5.74	127.01	119.84
1	A	307	SER	N-CA-C	5.69	122.92	110.80
2	B	327	HIS	N-CA-C	5.67	118.32	109.52
1	A	150	GLU	N-CA-C	-5.60	105.57	112.90
2	B	342	CYS	N-CA-C	5.57	120.96	113.72
2	B	218	THR	CA-C-N	5.55	126.77	119.84
2	B	218	THR	C-N-CA	5.55	126.77	119.84
1	A	78	VAL	CA-C-N	5.52	125.50	120.03
1	A	78	VAL	C-N-CA	5.52	125.50	120.03
2	B	375	HIS	N-CA-C	5.50	117.93	109.07
1	A	306	HIS	N-CA-C	5.46	120.85	114.62
1	A	76	ASP	CA-C-N	5.36	125.52	119.90
1	A	76	ASP	C-N-CA	5.36	125.52	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	417	GLN	N-CA-C	-5.32	105.97	113.20
1	A	285	GLN	N-CA-C	5.30	120.06	111.37
1	A	183	SER	N-CA-C	5.21	118.42	111.75
1	A	167	GLN	N-CA-C	5.21	117.70	111.71
2	B	122	VAL	N-CA-C	-5.15	105.30	110.30
2	B	295	LEU	N-CA-C	5.15	118.46	110.17
2	B	35	LEU	N-CA-C	5.09	117.42	110.24

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	161	0
2	B	3107	0	3038	195	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	349	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 30.

All (349) 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
2:B:324:SER:O	2:B:325:MET:HE2	1.76	0.85
1:A:303:GLN:HE21	1:A:303:GLN:HA	1.42	0.84
1:A:294:ASN:HB3	1:A:298:GLN:HE21	1.43	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:71:LEU:HD11	2:B:341:MET:HE2	1.71	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
2:B:381:MET:HE2	2:B:381:MET:N	2.10	0.67
1:A:225:GLN:O	1:A:228:LYS:HB2	1.94	0.67
2:B:198:GLU:CD	2:B:198:GLU:H	2.01	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:62:TYR:HD1	2:B:62:TYR:H	1.45	0.65
2:B:398:HIS:CE1	2:B:400:VAL:HB	2.31	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:NZ	1:A:366:LYS:HB3	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
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:23:LEU:CD1	2:B:26:LEU:HD12	2.30	0.61
2:B:102:TRP:CZ2	5:B:963:3MN:H27	2.36	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
1:A:299:LEU:C	1:A:301:ASP:H	2.10	0.59
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
2:B:121:ILE:HA	2:B:124:THR:HG22	1.86	0.58
1:A:364:GLN:O	1:A:365:SER:C	2.47	0.57
2:B:71:LEU:HD12	2:B:387:LEU:HD23	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:346:LYS:HE2	1:A:357:ARG:HH22	1.72	0.54
1:A:357:ARG:HH11	1:A:357:ARG:HG2	1.71	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
2:B:416:LEU:C	2:B:418:LYS:H	2.16	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
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
1:A:77:PRO:HB3	6:A:510:HOH:O	2.09	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:398:HIS:HE1	2:B:400:VAL:HB	1.73	0.52
1:A:137:ARG:HG3	1:A:137:ARG:HH11	1.73	0.52
2:B:188:ASP:OD2	2:B:188:ASP:N	2.28	0.52
2:B:51:VAL:HG21	2:B:295:LEU:HD22	1.91	0.52
2:B:389:VAL:CB	2:B:390:PRO:HD2	2.39	0.52
1:A:89:GLN:HA	2:B:100:ARG:NH2	2.25	0.52
1:A:150:GLU:HG3	6:A:393:HOH:O	2.09	0.52
2:B:62:TYR:HB3	6:B:1182:HOH:O	2.10	0.52
2:B:289:GLN:NE2	2:B:294:LYS:H	2.07	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:77:LYS:HG3	6:B:1088:HOH:O	2.10	0.52
2:B:234:ASN:OD1	2:B:236:GLU:HB2	2.09	0.52
1:A:97:ARG:HD2	6:A:432:HOH:O	2.10	0.52
1:A:152:MET:HE1	1:A:172:ARG:CZ	2.40	0.52
2:B:62:TYR:HD1	2:B:62:TYR:N	2.06	0.51
2:B:328:TRP:CB	2:B:332:GLN:HE21	2.20	0.51
2:B:233:GLN:HA	2:B:238:GLY:O	2.09	0.51
1:A:59:ASP:OD2	1:A:59:ASP:N	2.43	0.51
1:A:253:ARG:NH1	6:A:402:HOH:O	2.35	0.51
1:A:301:ASP:C	1:A:302:LEU:HD23	2.35	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:103:PHE:C	1:A:105:ALA:N	2.68	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:65:LEU:HG	6:A:428:HOH:O	2.11	0.50
1:A:103:PHE:C	1:A:105:ALA:H	2.19	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:322:MET:C	1:A:324:GLU:H	2.17	0.50
6:A:401:HOH:O	2:B:275:GLN:HG2	2.10	0.50
2:B:380:ALA:C	2:B:381:MET:HE2	2.37	0.50
2:B:226:ALA:CB	2:B:264:ARG:HG3	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:287:ARG:HG3	6:A:399:HOH:O	2.12	0.50
2:B:53:GLU:HG2	6:B:1156:HOH:O	2.11	0.49
2:B:280:ARG:HA	2:B:280:ARG:NE	2.27	0.49
2:B:299:CYS:HB3	2:B:362:HIS:CD2	2.46	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:113:LEU:C	2:B:115:ASP:H	2.21	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
1:A:87:VAL:O	1:A:88:VAL:C	2.56	0.49
1:A:367:HIS:C	1:A:367:HIS:HD1	2.21	0.49
2:B:90:THR:C	2:B:92:ALA:H	2.21	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: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:71:LEU:HD11	2:B:341:MET:CE	2.39	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
2:B:420:VAL:O	2:B:421:PRO:C	2.57	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:325:MET:HE2	2:B:325:MET:HA	1.96	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
2:B:26:LEU:HD21	2:B:59:PHE:C	2.40	0.47
1:A:160:GLU:OE2	1:A:191:ASP:OD2	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:ASP:HB2	2:B:395:GLN:HG2	1.95	0.47
2:B:281:GLN:HB2	2:B:288:PHE:CZ	2.50	0.47
1:A:232:ARG:NH1	2:B:42:THR:OG1	2.48	0.47
2:B:328:TRP:O	2:B:330:PHE:N	2.45	0.47
2:B:139:GLY:C	2:B:140:PHE:CD1	2.93	0.46
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
1:A:71:GLU:N	1:A:71:GLU:OE1	2.49	0.46
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
2:B:91:ASP:O	2:B:94:GLU:HG3	2.15	0.46
2:B:33:GLU:HB3	2:B:283:ARG:HG3	1.96	0.46
2:B:73:LEU:HD12	2:B:344:GLN:OE1	2.16	0.46
2:B:239:ILE:HB	2:B:252:THR:HA	1.96	0.46
5:B:963:3MN:C18	5:B:963:3MN:H10	2.46	0.46
1:A:295:LEU:O	1:A:299:LEU:HG	2.16	0.46
2:B:277:VAL:HG13	2:B:278:THR:N	2.31	0.46
1:A:185:GLU:O	1:A:186:LEU:C	2.59	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:O	1:A:137:ARG:HD3	2.15	0.45
2:B:225:THR:O	2:B:226:ALA:C	2.58	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
1:A:366:LYS:HB3	1:A:366:LYS:HZ3	1.81	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:C	1:A:72:TRP:H	2.25	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:LEU:HD22	2:B:371:SER:HB2	1.98	0.44
2:B:350:LEU:HD12	2:B:363:THR:HG23	1.99	0.44
2:B:113:LEU:HD11	2:B:368:SER:HA	1.99	0.44
1:A:71:GLU:HB2	6:A:464:HOH:O	2.17	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
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
2:B:237:GLY:O	2:B:273:LEU:HA	2.18	0.44
1:A:91:ILE:HD11	2:B:88:GLN:HG2	1.99	0.44
1:A:230:ASP:CG	2:B:42:THR:HB	2.43	0.44
2:B:43:VAL:HG23	6:B:1057:HOH:O	2.17	0.44
2:B:420:VAL:HB	2:B:421:PRO:HD3	2.00	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:161:CYS:O	2:B:407:LYS:HD3	2.18	0.43
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: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:60:SER:O	2:B:61:SER:C	2.61	0.43
1:A:181:ASP:OD1	1:A:181:ASP:C	2.60	0.43
2:B:362:HIS:O	2:B:366:CYS:HB2	2.17	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
2:B:21:GLU:HG2	2:B:26:LEU:C	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:167:GLN:H	1:A:167:GLN:CD	2.28	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
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:30:His:C	2:B:32:ARG:H	2.28	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:336:GLN:HE21	2:B:373:ALA:C	2.28	0.41
1:A:255:VAL:HG13	1:A:258:ARG:NH2	2.35	0.41
1:A:299:LEU:C	1:A:301:ASP:N	2.78	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:311:LEU:O	2:B:312:His:C	2.62	0.41
2:B:309:PRO:HA	2:B:328:TRP:CZ3	2.56	0.41
1:A:96:PHE:CE1	2:B:94:GLU:HB3	2.54	0.41
1:A:254:ALA:O	1:A:257:GLU:HB3	2.20	0.41
2:B:229:ILE:O	2:B:232:CYS:HB2	2.20	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
1:A:322:MET:C	1:A:324:GLU:N	2.76	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
2:B:377:GLY:O	2:B:378:SER:CB	2.66	0.41
1:A:86:PRO:HG2	1:A:89:GLN:OE1	2.21	0.41
1:A:159:ILE:HG12	1:A:168:VAL:HB	2.03	0.41
2:B:82:LEU:CD2	2:B:110:SER:HB2	2.47	0.41
2:B:380:ALA:HB3	2:B:381:MET:HE2	2.02	0.41
1:A:303:GLN:HA	1:A:303:GLN:NE2	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:308:LEU:HD12	2:B:308:LEU:N	2.34	0.41
1:A:216:TRP:CD1	1:A:216:TRP:H	2.37	0.41
1:A:344:LEU:HD13	1:A:356:TRP:CE2	2.56	0.41
1:A:367:HIS:C	1:A:367:HIS:ND1	2.76	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:297:ASN:C	1:A:299:LEU:N	2.80	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
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

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	312/379 (82%)	257 (82%)	43 (14%)	12 (4%)		
2	B	391/437 (90%)	351 (90%)	30 (8%)	10 (3%)		
All	All	703/816 (86%)	608 (86%)	73 (10%)	22 (3%)		

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	307	SER
2	B	74	GLN
2	B	378	SER

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Mol	Chain	Res	Type
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
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 [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	A	293/341 (86%)	280 (96%)	13 (4%)	25	53
2	B	332/370 (90%)	319 (96%)	13 (4%)	28	57
All	All	625/711 (88%)	599 (96%)	26 (4%)	26	55

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	VAL
1	A	58	LEU
1	A	59	ASP
1	A	60	SER

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Mol	Chain	Res	Type
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	121	ILE
2	B	158	ASN
2	B	188	ASP
2	B	219	PRO
2	B	254	CYS
2	B	265	GLU
2	B	351	LEU
2	B	387	LEU
2	B	389	VAL
2	B	407	LYS
2	B	421	PRO

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

Mol	Chain	Res	Type
1	A	108	GLN
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	120	GLN
2	B	128	GLN
2	B	327	HIS
2	B	332	GLN
2	B	383	HIS
2	B	410	GLN

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 oligosaccharides 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
5	3MN	B	963	3	38,39,39	1.97	11 (28%)	49,56,56	1.95	9 (18%)
4	FPP	B	1001	-	22,23,23	1.01	1 (4%)	27,31,31	1.52	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	3MN	B	963	3	-	1/18/42/42	0/5/5/5
4	FPP	B	1001	-	-	8/25/25/25	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	963	3MN	C26-C25	4.93	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	963	3MN	C21-N4	4.20	1.46	1.37
5	B	963	3MN	C14-C25	3.62	1.56	1.53
5	B	963	3MN	C14-C4	3.14	1.57	1.53
5	B	963	3MN	C25-C24	2.84	1.49	1.43
5	B	963	3MN	C5-C23	2.75	1.43	1.38
5	B	963	3MN	C5-C6	2.68	1.43	1.38
5	B	963	3MN	C30-N5	2.62	1.46	1.37
5	B	963	3MN	C6-C19	2.57	1.44	1.38
5	B	963	3MN	C8-C27	2.52	1.42	1.36
4	B	1001	FPP	PA-O3A	-2.49	1.56	1.59
5	B	963	3MN	C20-C13	2.10	1.41	1.36

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	963	3MN	C14-C25-C24	8.38	125.34	120.47
5	B	963	3MN	C19-C11-N2	4.71	124.83	114.58
5	B	963	3MN	N2-C18-N1	3.56	109.84	107.41
4	B	1001	FPP	C10-C8-C9	-3.34	109.44	115.23
5	B	963	3MN	O1-C18-N2	-3.16	122.21	125.70
4	B	1001	FPP	C1-C2-C3	3.13	131.33	126.20
5	B	963	3MN	C11-C19-C12	-3.01	114.59	120.27
5	B	963	3MN	C11-C19-C6	2.91	126.11	120.75
4	B	1001	FPP	C10-C8-C7	2.53	130.14	123.63
4	B	1001	FPP	O2A-PA-O3A	-2.50	100.51	107.27
4	B	1001	FPP	C5-C6-C7	2.27	123.23	112.02
5	B	963	3MN	C16-C1-C2	2.21	120.40	112.91
5	B	963	3MN	C27-C17-C13	-2.19	118.02	123.01
5	B	963	3MN	C1-C16-N1	2.17	117.49	112.36
4	B	1001	FPP	C11-C12-C13	2.12	134.71	127.64

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1001	FPP	C1-O1-PA-O1A
4	B	1001	FPP	C1-O1-PA-O2A
4	B	1001	FPP	C1-O1-PA-O3A
4	B	1001	FPP	C10-C8-C9-C11
4	B	1001	FPP	C7-C8-C9-C11
4	B	1001	FPP	C4-C3-C5-C6
4	B	1001	FPP	C2-C3-C5-C6

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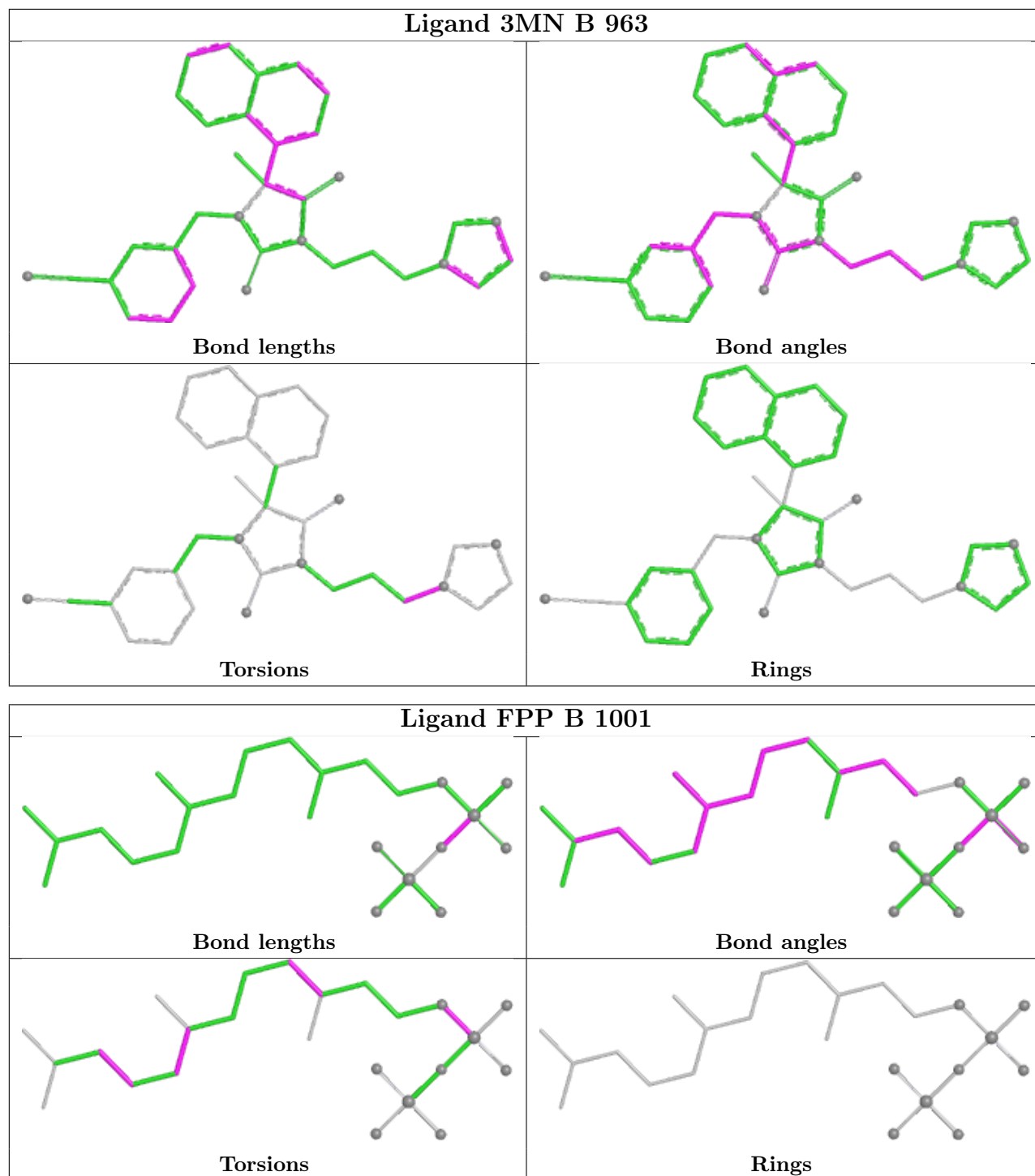
Mol	Chain	Res	Type	Atoms
5	B	963	3MN	C1-C2-N4-C21
4	B	1001	FPP	C9-C11-C12-C13

There are no ring outliers.

2 monomers are involved in 5 short contacts:

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

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.