



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2021 – 02:46 PM EDT

PDB ID : 1EZP
Title : CRYSTAL STRUCTURE OF HUMAN SQUALENE SYNTHASE
Authors : Pandit, J.; Danley, D.E.; Schulte, G.K.; Mazzalupo, S.M.; Pauly, T.A.; Hayward, C.M.; Hamanaka, E.S.; Thompson, J.F.; Harwood, H.J.
Deposited on : 2000-05-10
Resolution : 2.15 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.23.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

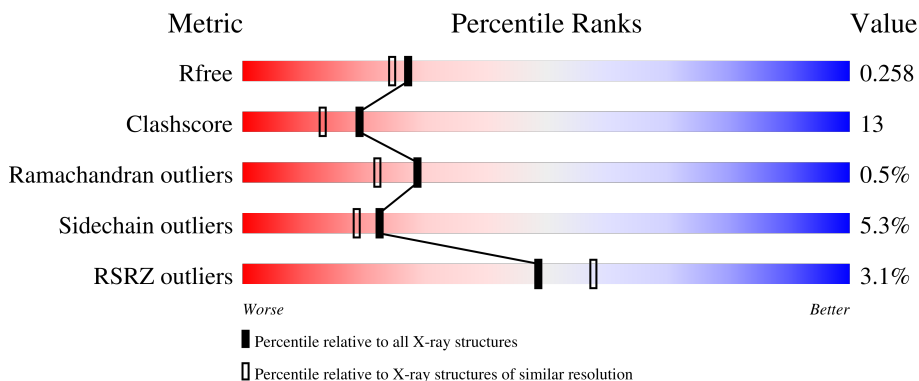
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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))
R_{free}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	340	
1	B	340	
1	C	340	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8364 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.

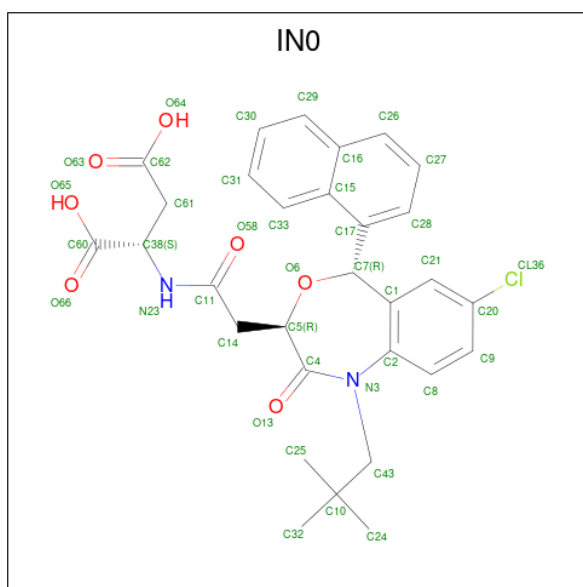
- Molecule 1 is a protein called FARNESYL-DIPHOSPHATE FARNESYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	323	Total 2620	C 1666	N 446	O 492	S 16	0	0	0
1	B	324	Total 2621	C 1664	N 447	O 494	S 16	0	0	0
1	C	320	Total 2593	C 1648	N 442	O 487	S 16	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	ARG	GLN	engineered mutation	UNP P37268
A	34	ASN	ASP	engineered mutation	UNP P37268
A	38	ASN	SER	engineered mutation	UNP P37268
B	33	ARG	GLN	engineered mutation	UNP P37268
B	34	ASN	ASP	engineered mutation	UNP P37268
B	38	ASN	SER	engineered mutation	UNP P37268
C	33	ARG	GLN	engineered mutation	UNP P37268
C	34	ASN	ASP	engineered mutation	UNP P37268
C	38	ASN	SER	engineered mutation	UNP P37268

- Molecule 2 is N-{2-[TRANS-7-CHLORO-1-(2,2-DIMETHYL-PROPYL) -5-NAPHTHALE N-1-YL-2-OXO-1,2,3,5-TETRAHYDRO-BENZO[E] [1,4]OXAZEPIN-3-YL]-ACETYL}-ASPARTIC ACID (three-letter code: IN0) (formula: C₃₀H₃₁ClN₂O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Cl	N			O
2	A	1	Total	C	Cl	N	O	0	0
			40	30	1	2	7		
2	B	1	Total	C	Cl	N	O	0	0
			40	30	1	2	7		
2	C	1	Total	C	Cl	N	O	0	0
			40	30	1	2	7		

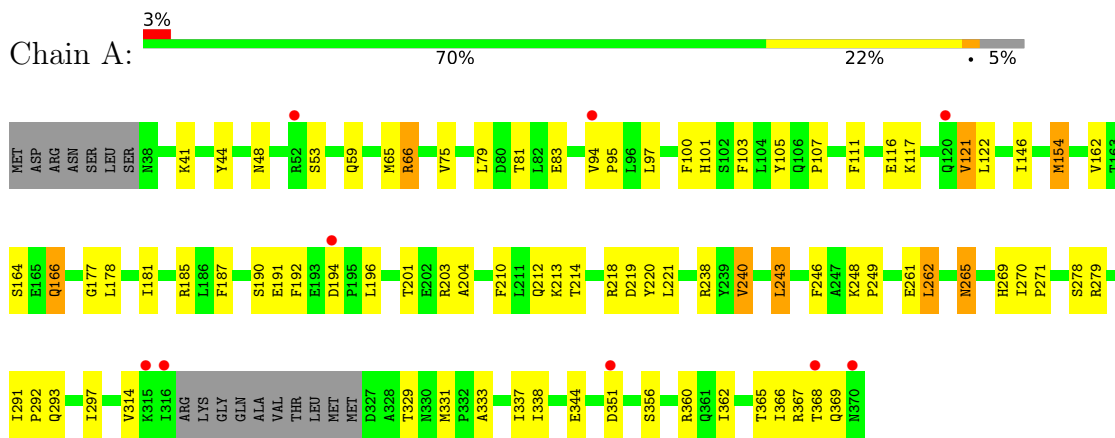
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	125	Total	O	0	0
			125	125		
3	B	152	Total	O	0	0
			152	152		
3	C	133	Total	O	0	0
			133	133		

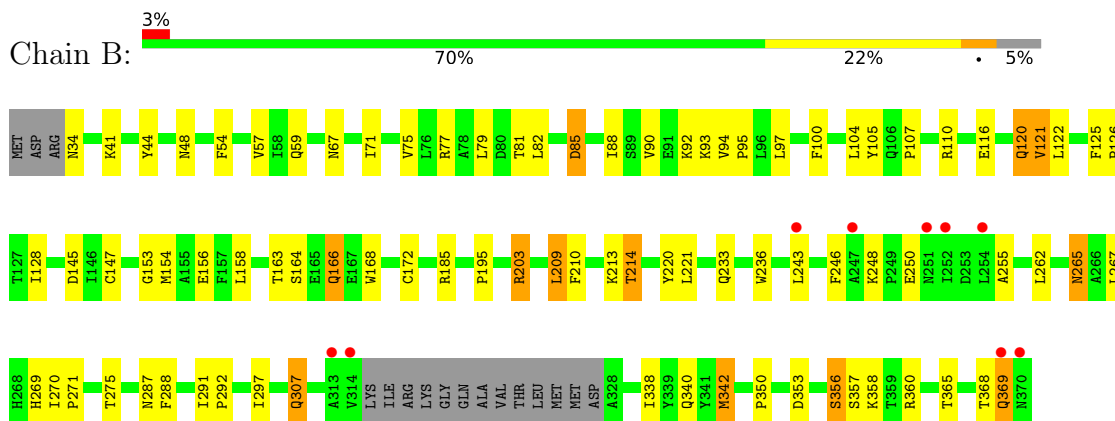
3 Residue-property plots i

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 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.

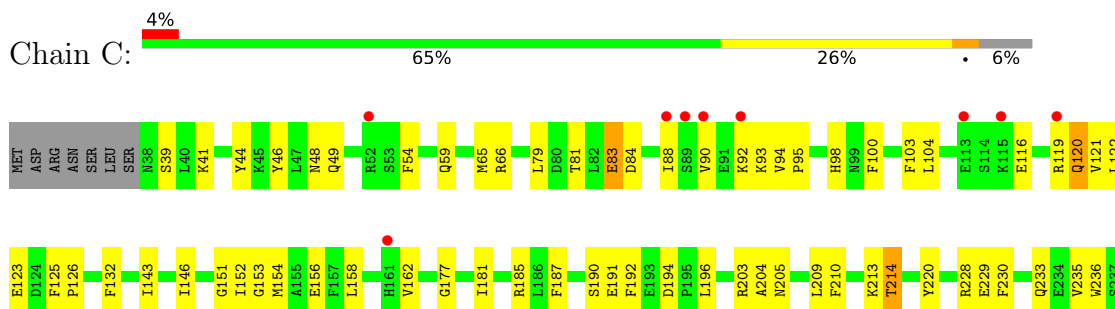
• Molecule 1: FARNESYL-DIPHOSPHATE FARNESYLTRANSFERASE

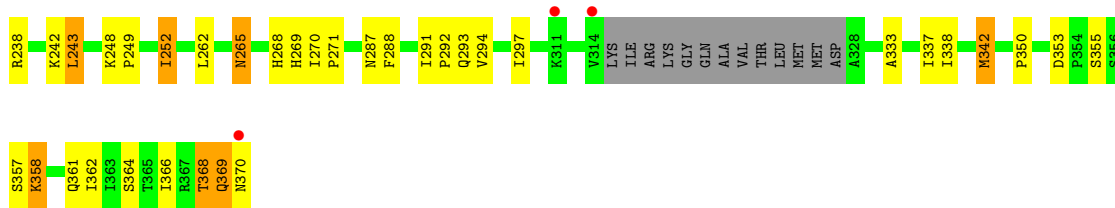


• Molecule 1: FARNESYL-DIPHOSPHATE FARNESYLTRANSFERASE



• Molecule 1: FARNESYL-DIPHOSPHATE FARNESYLTRANSFERASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.76Å 87.92Å 154.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.15 37.24 – 2.15	Depositor EDS
% Data completeness (in resolution range)	96.0 (40.00-2.15) 96.0 (37.24-2.15)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.53 (at 2.16Å)	Xtrriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.213 , 0.262 0.206 , 0.258	Depositor DCC
R_{free} test set	3340 reflections (6.05%)	wwPDB-VP
Wilson B-factor (Å ²)	23.2	Xtrriage
Anisotropy	0.373	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 64.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8364	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: INO

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	0.38	0/2674	0.57	1/3616 (0.0%)
1	B	0.37	0/2675	0.56	0/3618
1	C	0.38	0/2647	0.57	0/3580
All	All	0.38	0/7996	0.57	1/10814 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	162	VAL	N-CA-C	-5.82	95.29	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2620	0	2583	64	0
1	B	2621	0	2575	69	0
1	C	2593	0	2548	77	0
2	A	40	0	29	3	0
2	B	40	0	29	1	0
2	C	40	0	29	1	0
3	A	125	0	0	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	152	0	0	8	0
3	C	133	0	0	0	0
All	All	8364	0	7793	203	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (203) 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)
1:A:41:LYS:HA	1:B:368:THR:HG21	1.47	0.97
1:B:350:PRO:HG2	1:B:353:ASP:HB2	1.47	0.94
1:A:83:GLU:HB2	1:A:154:MET:HE3	1.53	0.91
1:A:65:MET:HE3	1:A:192:PHE:HB2	1.53	0.87
1:B:41:LYS:HA	1:C:368:THR:HG21	1.62	0.80
1:C:210:PHE:O	1:C:214:THR:HG23	1.82	0.80
1:A:210:PHE:O	1:A:214:THR:HG23	1.85	0.77
1:B:369:GLN:HB3	3:B:1048:HOH:O	1.85	0.77
1:A:297:ILE:HD12	1:A:338:ILE:HG12	1.68	0.76
1:A:65:MET:HE2	1:A:187:PHE:HA	1.70	0.72
1:B:365:THR:O	1:B:369:GLN:HB2	1.90	0.71
1:A:368:THR:HG21	1:C:41:LYS:HA	1.73	0.71
1:C:333:ALA:O	1:C:337:ILE:HG12	1.93	0.69
1:C:235:VAL:HG22	1:C:238:ARG:HH12	1.56	0.69
1:A:83:GLU:HB2	1:A:154:MET:CE	2.23	0.68
1:B:48:ASN:HD21	1:B:59:GLN:HE22	1.42	0.68
1:B:110:ARG:HD3	3:B:1066:HOH:O	1.93	0.67
1:B:44:TYR:CD2	1:C:368:THR:HB	2.29	0.67
1:B:210:PHE:O	1:B:214:THR:HG23	1.95	0.66
1:C:65:MET:HE3	1:C:192:PHE:HB2	1.79	0.65
1:B:163:THR:HA	1:B:233:GLN:HB2	1.79	0.65
1:B:172:CYS:HB3	1:B:209:LEU:HD22	1.79	0.64
1:B:287:ASN:O	1:B:291:ILE:HG12	1.98	0.63
1:C:291:ILE:HB	1:C:292:PRO:HD3	1.79	0.63
1:A:44:TYR:HB2	1:B:368:THR:HG22	1.80	0.63
1:C:297:ILE:HD12	1:C:338:ILE:HA	1.79	0.63
1:A:48:ASN:HD21	1:A:59:GLN:HE22	1.46	0.62
1:B:213:LYS:NZ	1:B:269:HIS:HE1	1.97	0.62
1:B:48:ASN:HD21	1:B:59:GLN:NE2	1.97	0.61
1:A:59:GLN:O	1:A:66:ARG:HD2	2.01	0.61
1:C:93:LYS:HD3	1:C:158:LEU:HD11	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:LEU:HD22	1:B:154:MET:CE	2.31	0.60
1:A:79:LEU:HG	1:A:154:MET:CE	2.31	0.60
1:C:213:LYS:NZ	1:C:265:ASN:HD21	2.00	0.60
1:C:287:ASN:O	1:C:291:ILE:HG12	2.02	0.60
1:A:213:LYS:NZ	1:A:265:ASN:HD21	2.00	0.59
1:C:229:GLU:HB3	1:C:243:LEU:HD12	1.83	0.59
1:B:185:ARG:HD2	3:B:1039:HOH:O	2.01	0.59
1:C:235:VAL:HA	1:C:238:ARG:NH1	2.17	0.59
1:A:41:LYS:HA	1:B:368:THR:CG2	2.27	0.58
1:A:293:GLN:O	1:A:297:ILE:HG13	2.03	0.58
1:B:213:LYS:NZ	1:B:265:ASN:HD21	2.02	0.57
1:B:291:ILE:HB	1:B:292:PRO:HD3	1.86	0.57
1:C:93:LYS:HB3	1:C:158:LEU:HD21	1.87	0.57
1:A:368:THR:HG22	1:C:44:TYR:CD1	2.40	0.57
1:C:48:ASN:HD21	1:C:59:GLN:HE22	1.53	0.57
1:B:75:VAL:HG13	1:B:100:PHE:HE2	1.69	0.57
1:B:121:VAL:HG12	1:B:122:LEU:HD22	1.87	0.57
1:A:79:LEU:HG	1:A:154:MET:HE2	1.86	0.56
1:C:362:ILE:O	1:C:366:ILE:HG12	2.05	0.56
1:C:90:VAL:O	1:C:94:VAL:HG23	2.05	0.56
1:C:265:ASN:C	1:C:265:ASN:HD22	2.08	0.56
1:C:357:SER:HB3	1:C:358:LYS:HE3	1.86	0.56
1:A:278:SER:HA	1:A:331:MET:HG3	1.88	0.56
1:C:213:LYS:NZ	1:C:269:HIS:HE1	2.04	0.56
1:B:358:LYS:HG3	3:B:1131:HOH:O	2.06	0.56
1:B:220:TYR:OH	1:B:246:PHE:HB2	2.07	0.55
1:B:248:LYS:HG2	1:B:250:GLU:HG2	1.88	0.55
1:C:65:MET:HE2	1:C:187:PHE:HA	1.88	0.55
1:A:181:ILE:HG22	1:A:185:ARG:HE	1.72	0.55
1:A:213:LYS:NZ	1:A:269:HIS:HE1	2.04	0.54
1:B:81:THR:HG23	1:B:116:GLU:HB3	1.89	0.54
1:C:46:TYR:HA	1:C:49:GLN:HG2	1.88	0.54
1:C:177:GLY:O	1:C:181:ILE:HG12	2.08	0.54
1:A:100:PHE:HA	1:A:103:PHE:CD2	2.43	0.53
1:C:181:ILE:HD13	1:C:204:ALA:HB3	1.90	0.53
1:C:151:GLY:HA2	1:C:154:MET:HE2	1.89	0.53
1:A:48:ASN:HD21	1:A:59:GLN:NE2	2.07	0.53
1:C:48:ASN:HD21	1:C:59:GLN:NE2	2.07	0.53
1:C:88:ILE:HB	1:C:93:LYS:HE3	1.89	0.53
1:A:220:TYR:HE1	1:A:243:LEU:HD22	1.74	0.53
1:A:181:ILE:O	1:A:185:ARG:HG3	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:LEU:HD21	1:C:154:MET:HE1	1.91	0.52
1:A:181:ILE:HD13	1:A:204:ALA:HB3	1.91	0.52
1:B:267:LEU:HD22	1:B:342:MET:HE1	1.91	0.52
1:A:362:ILE:O	1:A:366:ILE:HG12	2.09	0.52
1:C:220:TYR:HE1	1:C:243:LEU:HD22	1.75	0.52
1:A:365:THR:O	1:A:369:GLN:HB2	2.10	0.51
1:C:235:VAL:HA	1:C:238:ARG:HH11	1.73	0.51
1:C:210:PHE:CZ	1:C:270:ILE:HD11	2.46	0.51
1:C:294:VAL:O	1:C:297:ILE:HG12	2.10	0.51
1:A:213:LYS:HZ2	1:A:265:ASN:HD21	1.58	0.51
1:B:94:VAL:HB	1:B:95:PRO:HD3	1.93	0.51
1:C:364:SER:O	1:C:368:THR:HG23	2.12	0.50
1:A:121:VAL:HG12	1:A:122:LEU:HD22	1.92	0.50
1:B:164:SER:HB2	1:B:166:GLN:OE1	2.10	0.50
1:A:196:LEU:HD21	1:A:279:ARG:HD3	1.93	0.50
1:B:82:LEU:O	1:B:93:LYS:HE2	2.11	0.50
1:C:350:PRO:HG2	1:C:353:ASP:HB2	1.93	0.50
1:B:210:PHE:CZ	1:B:270:ILE:HD11	2.47	0.49
1:C:177:GLY:HA3	1:C:205:ASN:OD1	2.11	0.49
1:C:235:VAL:HG22	1:C:238:ARG:NH1	2.25	0.49
1:C:213:LYS:HZ3	1:C:265:ASN:HD21	1.58	0.49
1:A:181:ILE:HG23	1:A:201:THR:HG22	1.94	0.49
1:B:79:LEU:HG	1:B:154:MET:HE1	1.94	0.49
1:C:120:GLN:HE21	1:C:120:GLN:HA	1.77	0.49
1:B:145:ASP:HB3	1:B:185:ARG:HH22	1.76	0.49
1:B:236:TRP:CE2	1:B:243:LEU:HB2	2.47	0.49
1:B:356:SER:O	1:B:360:ARG:HG3	2.12	0.49
1:A:94:VAL:HB	1:A:95:PRO:HD3	1.93	0.49
1:C:94:VAL:HB	1:C:95:PRO:HD3	1.95	0.49
1:A:97:LEU:HD13	1:A:154:MET:HB2	1.94	0.49
1:A:105:TYR:O	1:A:107:PRO:HD3	2.12	0.49
1:B:97:LEU:HD22	1:B:154:MET:HE3	1.95	0.48
1:A:333:ALA:O	1:A:337:ILE:HG12	2.13	0.48
1:B:79:LEU:HG	1:B:154:MET:CE	2.43	0.48
1:C:98:HIS:CD2	1:C:152:ILE:HD13	2.49	0.48
1:A:146:ILE:HG23	1:A:178:LEU:HB3	1.96	0.48
1:B:120:GLN:NE2	1:B:120:GLN:HA	2.29	0.48
1:B:41:LYS:HG2	1:C:368:THR:HG21	1.96	0.47
1:A:81:THR:HG23	1:A:116:GLU:HG2	1.96	0.47
1:B:120:GLN:HA	1:B:120:GLN:HE21	1.80	0.47
1:A:262:LEU:O	1:A:265:ASN:HB3	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:357:SER:HB3	1:C:358:LYS:CE	2.44	0.47
1:C:153:GLY:O	1:C:156:GLU:HB3	2.16	0.46
1:A:53:SER:HA	1:B:340:GLN:HE22	1.81	0.46
1:B:342:MET:HA	1:B:342:MET:HE2	1.98	0.46
1:A:270:ILE:HB	1:A:271:PRO:HD3	1.97	0.46
1:C:233:GLN:HA	1:C:236:TRP:NE1	2.31	0.46
1:B:172:CYS:CB	1:B:209:LEU:HD22	2.45	0.46
1:C:119:ARG:O	1:C:123:GLU:HG3	2.15	0.46
1:A:177:GLY:O	1:A:181:ILE:HG12	2.16	0.46
1:B:54:PHE:CZ	2:B:992:IN0:H28	2.51	0.45
1:A:166:GLN:H	1:A:166:GLN:CD	2.19	0.45
1:A:164:SER:OG	1:A:166:GLN:HG2	2.16	0.45
1:C:297:ILE:HD13	1:C:338:ILE:HG12	1.98	0.45
1:B:271:PRO:HG3	1:B:369:GLN:HE22	1.82	0.45
1:B:92:LYS:O	1:B:95:PRO:HD2	2.16	0.45
1:A:331:MET:HB3	3:A:1061:HOH:O	2.16	0.45
1:C:355:SER:HA	1:C:358:LYS:HD2	1.99	0.45
1:A:248:LYS:HA	1:A:249:PRO:HD3	1.88	0.45
1:B:75:VAL:CG1	1:B:147:CYS:SG	3.05	0.45
1:C:100:PHE:HA	1:C:103:PHE:CD2	2.51	0.44
2:A:991:IN0:H242	2:A:991:IN0:H33	1.99	0.44
1:B:67:ASN:O	1:B:71:ILE:HG12	2.17	0.44
1:B:153:GLY:O	1:B:156:GLU:HG2	2.17	0.44
1:A:238:ARG:NH2	1:A:261:GLU:OE2	2.50	0.44
1:B:246:PHE:CE1	1:B:255:ALA:HA	2.52	0.44
1:C:79:LEU:CG	1:C:154:MET:HE1	2.47	0.44
1:C:213:LYS:HZ2	1:C:269:HIS:HE1	1.65	0.44
1:B:120:GLN:HB2	3:B:995:HOH:O	2.17	0.44
1:C:83:GLU:HG3	1:C:84:ASP:N	2.32	0.44
1:C:342:MET:HA	1:C:342:MET:CE	2.48	0.43
1:C:342:MET:HA	1:C:342:MET:HE3	1.99	0.43
1:C:268:HIS:O	1:C:271:PRO:HD2	2.19	0.43
1:A:220:TYR:CZ	1:A:246:PHE:HB2	2.52	0.43
1:C:92:LYS:O	1:C:95:PRO:HD2	2.18	0.43
1:C:181:ILE:O	1:C:185:ARG:HG3	2.18	0.43
1:A:314:VAL:HG23	3:A:1062:HOH:O	2.19	0.43
1:A:210:PHE:CZ	1:A:297:ILE:HG12	2.53	0.43
1:B:213:LYS:NZ	1:B:269:HIS:CE1	2.81	0.43
1:A:210:PHE:CE2	1:A:297:ILE:HG12	2.54	0.43
1:A:240:VAL:HG22	3:A:1040:HOH:O	2.18	0.43
1:B:105:TYR:O	1:B:107:PRO:HD3	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:MET:CE	1:A:187:PHE:HA	2.45	0.42
1:C:249:PRO:O	1:C:252:ILE:HG13	2.19	0.42
1:A:291:ILE:HB	1:A:292:PRO:HD3	2.01	0.42
1:B:168:TRP:CE3	1:B:213:LYS:HE2	2.54	0.42
1:C:79:LEU:CD2	1:C:154:MET:HE1	2.49	0.42
1:C:190:SER:O	1:C:191:GLU:HB2	2.19	0.42
1:C:220:TYR:CE1	1:C:243:LEU:HD22	2.54	0.42
1:A:212:GLN:OE1	2:A:991:IN0:H251	2.20	0.42
1:A:356:SER:O	1:A:360:ARG:HG3	2.19	0.42
1:C:132:PHE:HE1	1:C:143:ILE:HB	1.85	0.42
1:A:213:LYS:HZ2	1:A:265:ASN:ND2	2.18	0.42
1:B:270:ILE:N	1:B:271:PRO:CD	2.83	0.42
2:A:991:IN0:H33	2:A:991:IN0:H7	1.88	0.42
1:A:101:HIS:HE1	3:A:1029:HOH:O	2.02	0.42
1:B:85:ASP:HB3	1:B:88:ILE:HD12	2.02	0.42
1:B:342:MET:HA	1:B:342:MET:CE	2.50	0.42
1:A:190:SER:O	1:A:191:GLU:HB2	2.19	0.42
1:B:195:PRO:HD3	3:B:1144:HOH:O	2.19	0.41
1:A:329:THR:HG21	3:A:1025:HOH:O	2.19	0.41
1:B:34:ASN:N	3:B:1074:HOH:O	2.52	0.41
1:B:125:PHE:N	1:B:126:PRO:CD	2.84	0.41
1:C:79:LEU:HG	1:C:154:MET:HE1	2.02	0.41
1:C:54:PHE:CE2	1:C:288:PHE:CE1	3.08	0.41
1:B:121:VAL:HG22	1:B:128:ILE:HD11	2.01	0.41
1:B:213:LYS:HZ3	1:B:269:HIS:HE1	1.68	0.41
1:B:246:PHE:CD1	1:B:255:ALA:HA	2.55	0.41
1:B:297:ILE:HD13	1:B:338:ILE:HG23	2.02	0.41
1:C:151:GLY:HA2	1:C:154:MET:CE	2.51	0.41
1:B:90:VAL:O	1:B:94:VAL:HG23	2.20	0.41
1:C:369:GLN:O	1:C:370:ASN:CG	2.59	0.41
2:C:995:IN0:H33	2:C:995:IN0:H7	1.82	0.41
1:A:218:ARG:HD2	1:A:219:ASP:OD1	2.20	0.41
1:C:125:PHE:N	1:C:126:PRO:CD	2.84	0.41
1:A:111:PHE:HB3	1:A:122:LEU:HB3	2.01	0.41
1:A:367:ARG:O	1:C:66:ARG:NH2	2.54	0.41
1:B:307:GLN:CD	1:B:307:GLN:H	2.23	0.41
1:C:65:MET:CE	1:C:187:PHE:HA	2.49	0.41
1:C:146:ILE:HD13	1:C:146:ILE:HA	1.90	0.41
1:C:196:LEU:O	1:C:196:LEU:HD23	2.21	0.41
1:C:265:ASN:C	1:C:265:ASN:ND2	2.74	0.41
1:A:116:GLU:HG3	1:A:117:LYS:H	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:VAL:HG11	1:B:288:PHE:HA	2.01	0.41
1:C:228:ARG:HB3	1:C:230:PHE:CE2	2.56	0.41
1:B:203:ARG:HH11	1:B:275:THR:HG21	1.85	0.40
1:C:210:PHE:HD2	1:C:293:GLN:OE1	2.04	0.40
1:C:248:LYS:HA	1:C:249:PRO:HD3	1.93	0.40
1:A:75:VAL:HG13	1:A:100:PHE:CE2	2.56	0.40
1:C:81:THR:HG23	1:C:116:GLU:HB3	2.02	0.40
1:B:357:SER:HB3	3:B:1131: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	319/340 (94%)	306 (96%)	13 (4%)	0	100	100
1	B	320/340 (94%)	308 (96%)	9 (3%)	3 (1%)	17	11
1	C	316/340 (93%)	304 (96%)	10 (3%)	2 (1%)	25	18
All	All	955/1020 (94%)	918 (96%)	32 (3%)	5 (0%)	29	22

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	369	GLN
1	C	369	GLN
1	B	85	ASP
1	B	356	SER
1	C	162	VAL

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	288/303 (95%)	275 (96%)	13 (4%)	27	24
1	B	288/303 (95%)	274 (95%)	14 (5%)	25	21
1	C	284/303 (94%)	265 (93%)	19 (7%)	16	11
All	All	860/909 (95%)	814 (95%)	46 (5%)	22	19

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ARG
1	A	121	VAL
1	A	154	MET
1	A	166	GLN
1	A	194	ASP
1	A	203	ARG
1	A	221	LEU
1	A	240	VAL
1	A	243	LEU
1	A	262	LEU
1	A	265	ASN
1	A	344	GLU
1	A	351	ASP
1	B	77	ARG
1	B	104	LEU
1	B	120	GLN
1	B	121	VAL
1	B	158	LEU
1	B	166	GLN
1	B	203	ARG
1	B	209	LEU
1	B	214	THR
1	B	221	LEU
1	B	262	LEU
1	B	265	ASN
1	B	307	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	342	MET
1	C	39	SER
1	C	83	GLU
1	C	104	LEU
1	C	120	GLN
1	C	121	VAL
1	C	122	LEU
1	C	194	ASP
1	C	203	ARG
1	C	209	LEU
1	C	214	THR
1	C	242	LYS
1	C	243	LEU
1	C	252	ILE
1	C	262	LEU
1	C	265	ASN
1	C	342	MET
1	C	358	LYS
1	C	361	GLN
1	C	368	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	225	GLN
1	A	265	ASN
1	A	269	HIS
1	A	308	GLN
1	B	38	ASN
1	B	59	GLN
1	B	101	HIS
1	B	161	HIS
1	B	265	ASN
1	B	269	HIS
1	B	340	GLN
1	C	59	GLN
1	C	98	HIS
1	C	120	GLN
1	C	224	GLN
1	C	225	GLN
1	C	265	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	269	HIS
1	C	307	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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
2	IN0	C	995	-	34,43,43	1.29	3 (8%)	43,63,63	1.01	4 (9%)
2	IN0	B	992	-	34,43,43	1.44	4 (11%)	43,63,63	1.04	2 (4%)
2	IN0	A	991	-	34,43,43	1.19	3 (8%)	43,63,63	0.98	4 (9%)

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
2	IN0	C	995	-	-	2/18/45/45	0/3/4/4
2	IN0	B	992	-	-	2/18/45/45	0/3/4/4
2	IN0	A	991	-	-	1/18/45/45	0/3/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	992	IN0	C1-C7	4.23	1.56	1.52
2	C	995	IN0	C1-C7	3.48	1.55	1.52
2	B	992	IN0	C2-C1	2.79	1.43	1.40
2	A	991	IN0	C28-C17	2.47	1.41	1.37
2	B	992	IN0	C43-C10	2.41	1.58	1.54
2	C	995	IN0	C28-C17	2.40	1.41	1.37
2	C	995	IN0	C43-C10	2.31	1.58	1.54
2	A	991	IN0	C27-C26	2.17	1.41	1.36
2	A	991	IN0	C1-C7	2.14	1.54	1.52
2	B	992	IN0	C28-C17	2.02	1.41	1.37

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	991	IN0	C5-C4-N3	2.82	118.80	115.78
2	C	995	IN0	C38-N23-C11	-2.41	119.48	123.33
2	B	992	IN0	C2-N3-C4	-2.41	119.01	122.99
2	C	995	IN0	C33-C15-C17	-2.40	120.61	123.40
2	C	995	IN0	C2-N3-C4	-2.17	119.40	122.99
2	C	995	IN0	C5-C4-N3	2.16	118.09	115.78
2	A	991	IN0	C33-C15-C17	-2.15	120.90	123.40
2	B	992	IN0	C43-N3-C2	2.12	121.05	118.35
2	A	991	IN0	C38-N23-C11	-2.05	120.06	123.33
2	A	991	IN0	C61-C38-N23	2.04	112.71	109.01

There are no chirality outliers.

All (5) torsion outliers are listed below:

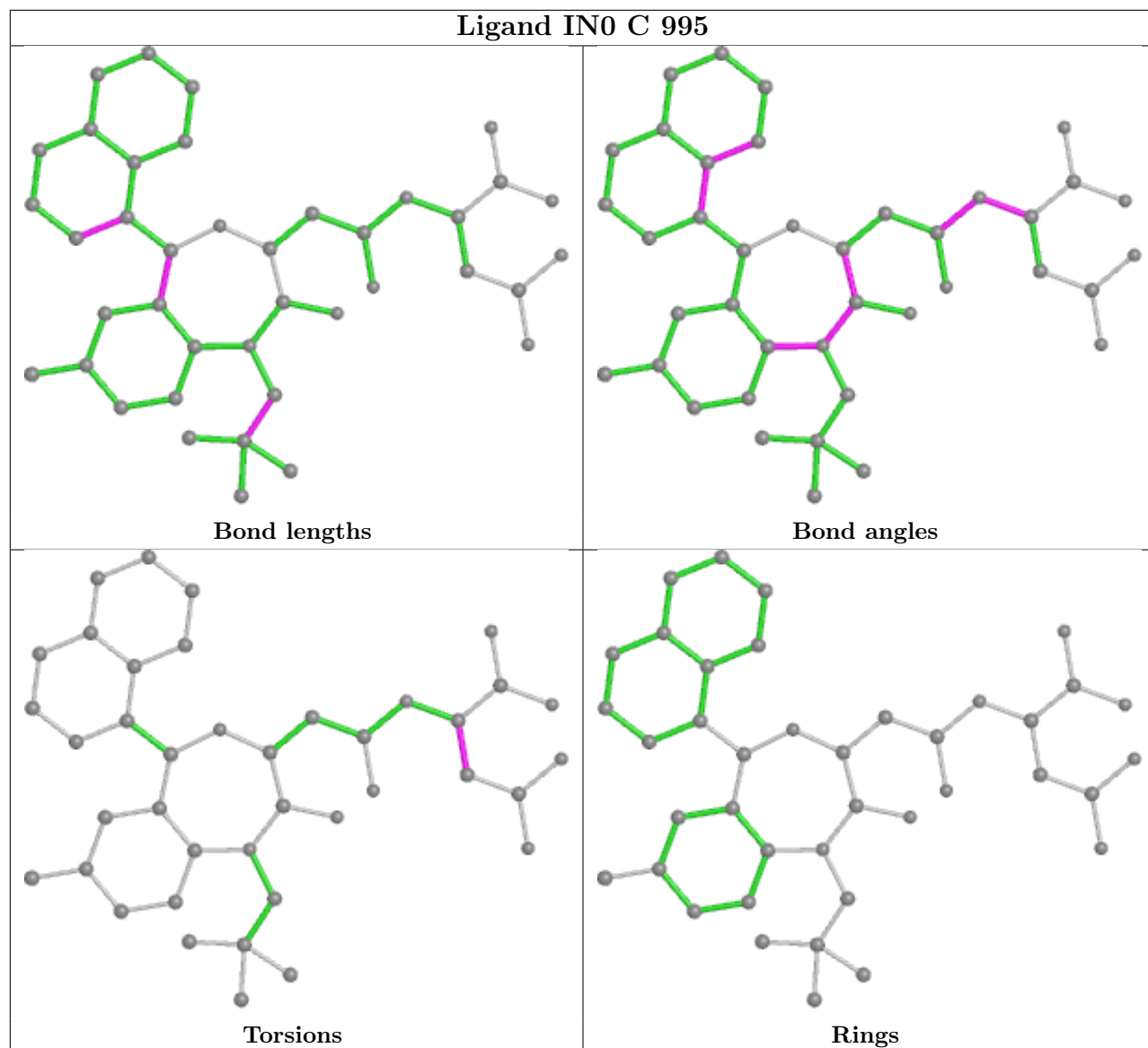
Mol	Chain	Res	Type	Atoms
2	A	991	IN0	C60-C38-C61-C62
2	B	992	IN0	N23-C38-C61-C62
2	B	992	IN0	C60-C38-C61-C62
2	C	995	IN0	N23-C38-C61-C62
2	C	995	IN0	C60-C38-C61-C62

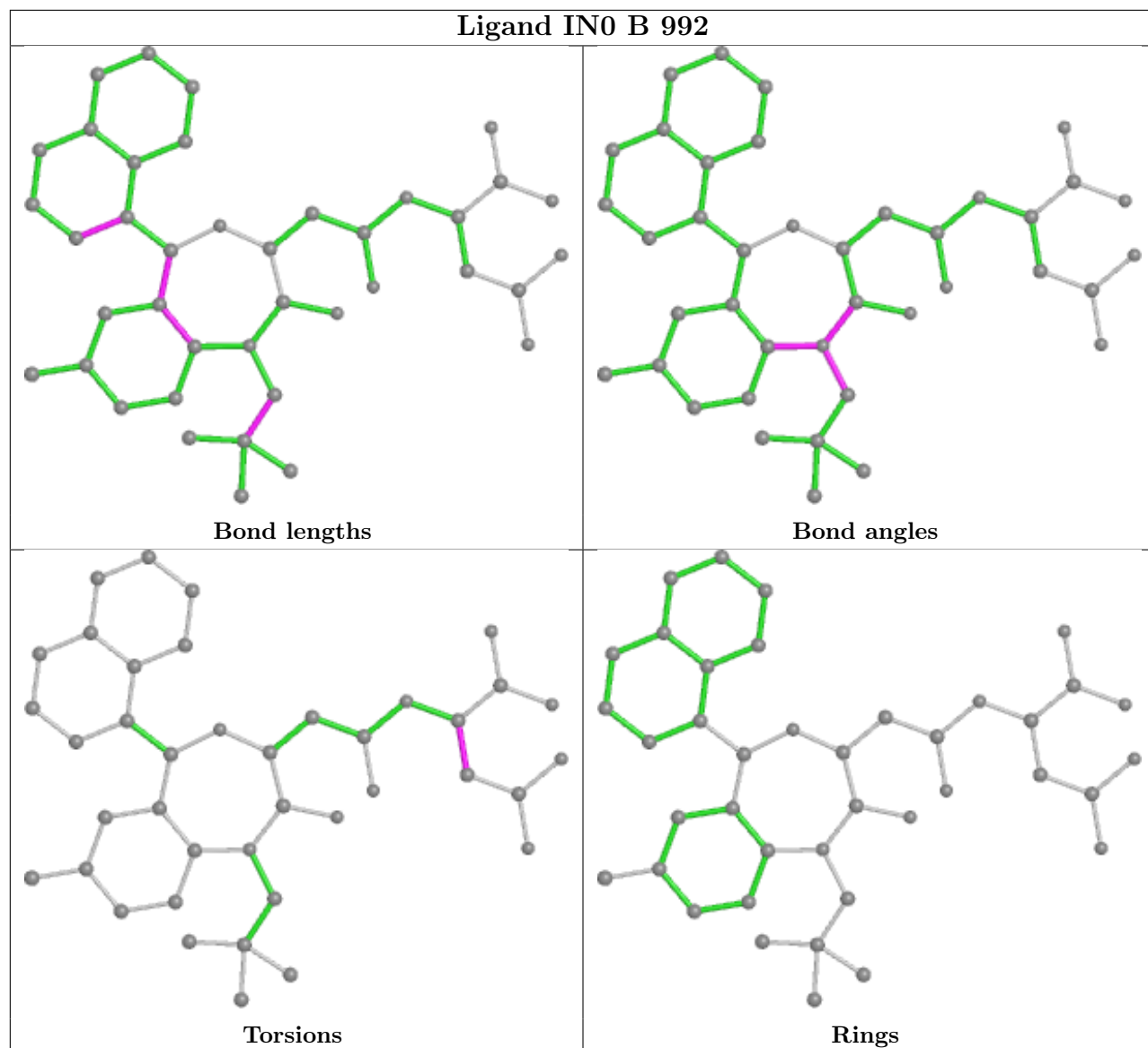
There are no ring outliers.

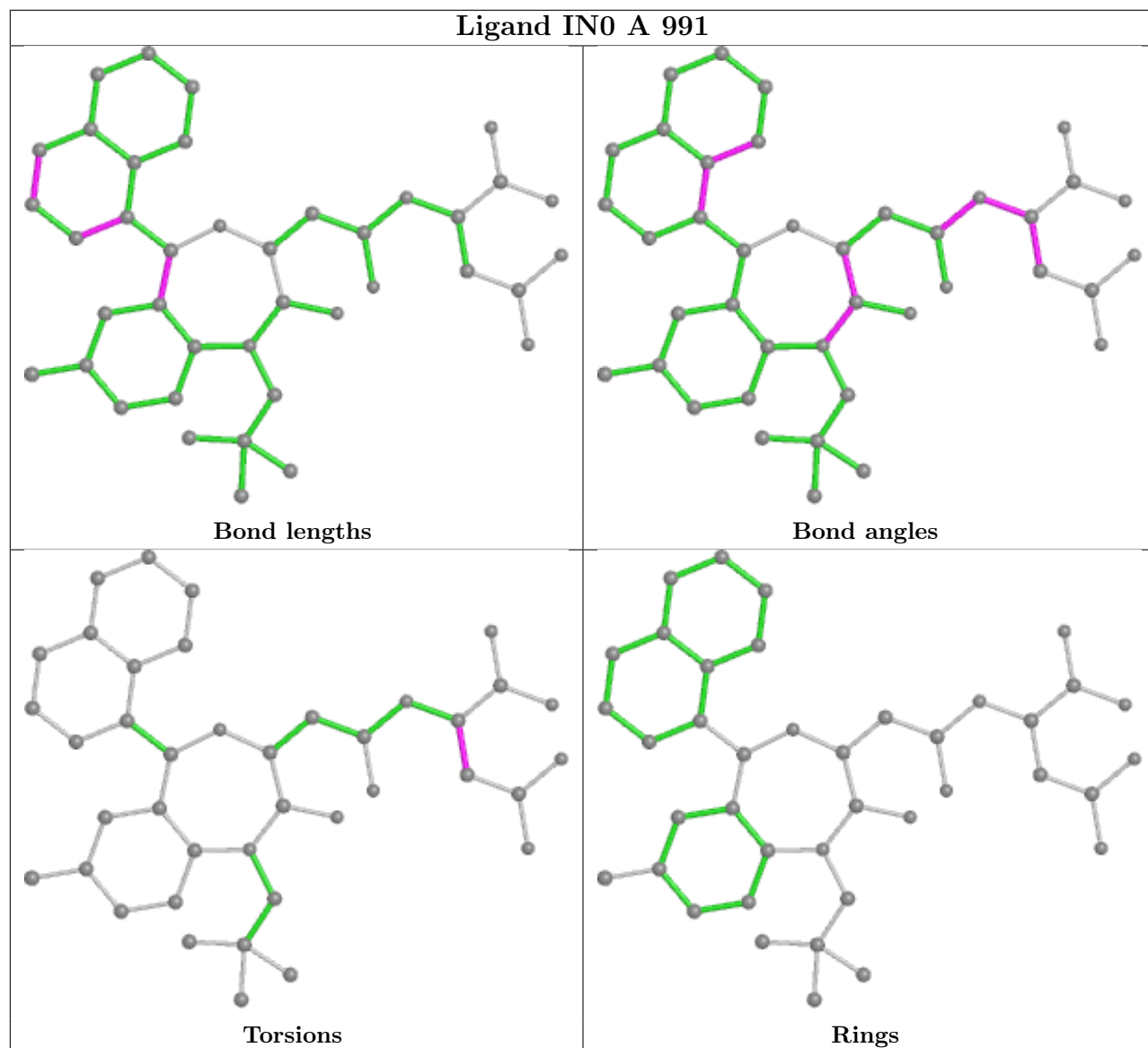
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	995	IN0	1	0
2	B	992	IN0	1	0
2	A	991	IN0	3	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](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	323/340 (95%)	0.11	9 (2%) 53 62	13, 26, 48, 74	0
1	B	324/340 (95%)	0.03	9 (2%) 53 62	9, 23, 50, 67	0
1	C	320/340 (94%)	0.02	12 (3%) 40 49	9, 24, 53, 68	0
All	All	967/1020 (94%)	0.05	30 (3%) 49 58	9, 25, 51, 74	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	370	ASN	8.5
1	B	370	ASN	5.1
1	C	370	ASN	5.0
1	C	115	LYS	4.3
1	A	52	ARG	4.0
1	B	369	GLN	3.8
1	A	315	LYS	3.4
1	C	89	SER	3.2
1	A	316	ILE	3.0
1	B	243	LEU	2.8
1	B	252	ILE	2.7
1	A	351	ASP	2.7
1	A	94	VAL	2.7
1	C	92	LYS	2.6
1	C	52	ARG	2.6
1	B	254	LEU	2.6
1	C	88	ILE	2.5
1	C	113	GLU	2.5
1	C	314	VAL	2.5
1	B	314	VAL	2.4
1	C	311	LYS	2.4
1	B	313	ALA	2.3
1	A	194	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	90	VAL	2.2
1	A	368	THR	2.2
1	C	119	ARG	2.2
1	B	251	ASN	2.2
1	C	161	HIS	2.1
1	B	247	ALA	2.1
1	A	120	GLN	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

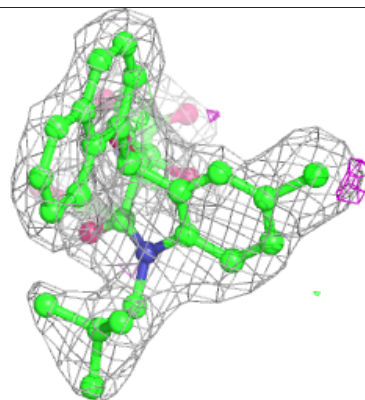
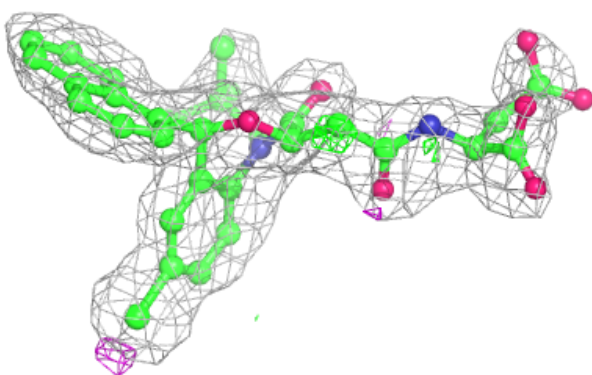
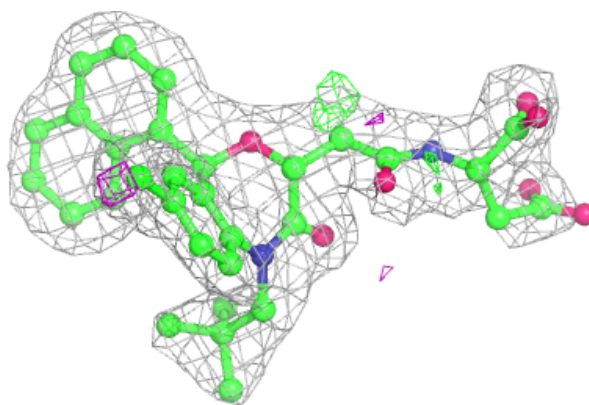
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	IN0	C	995	40/40	0.91	0.17	11,27,55,60	0
2	IN0	A	991	40/40	0.92	0.14	18,25,67,70	0
2	IN0	B	992	40/40	0.94	0.14	7,17,55,62	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

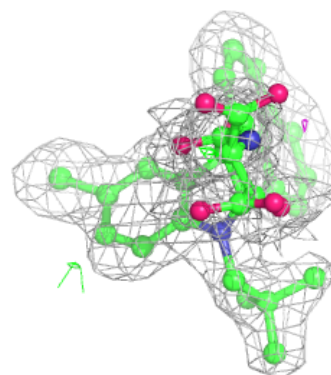
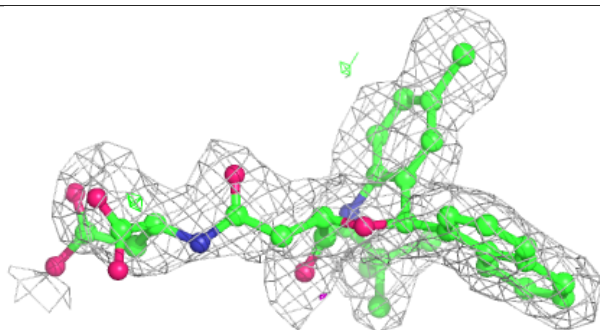
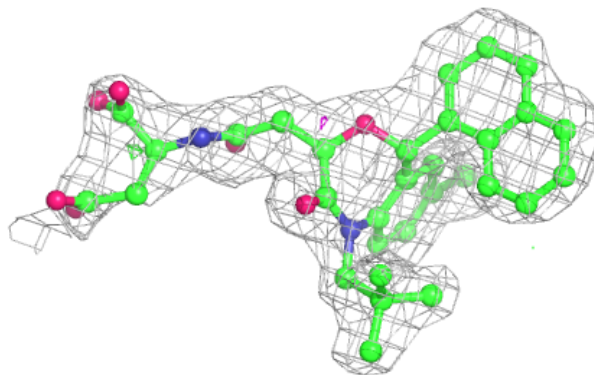
Electron density around IN0 C 995:

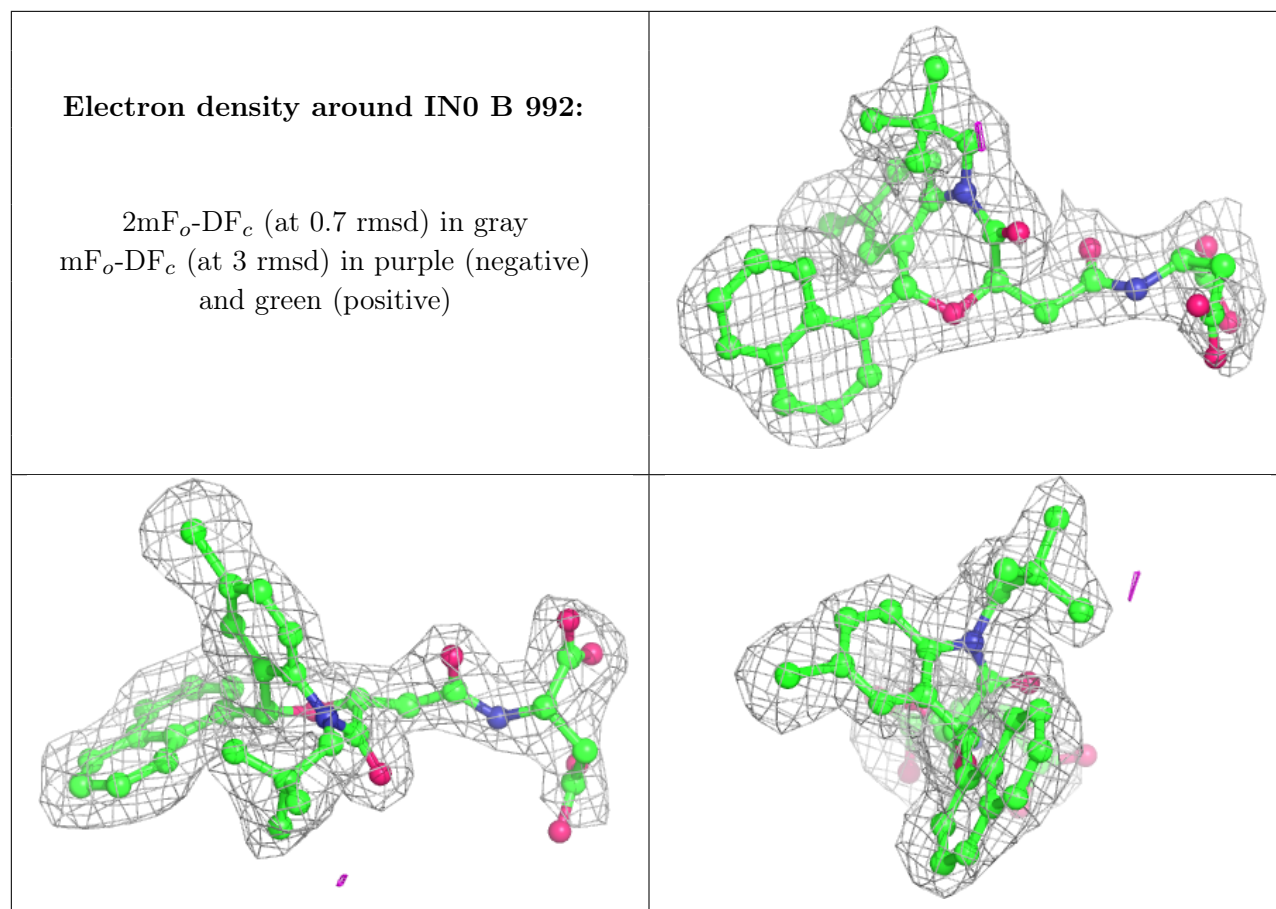
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around INO A 991:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.