



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:14 AM UTC

PDB ID : 3ADX / pdb_00003adx
Title : Human PPARgamma ligand-binding domain in complex with indomethacin and nitro-233
Authors : Waku, T.; Shiraki, T.; Oyama, T.; Morikawa, K.
Deposited on : 2010-01-29
Resolution : 1.95 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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

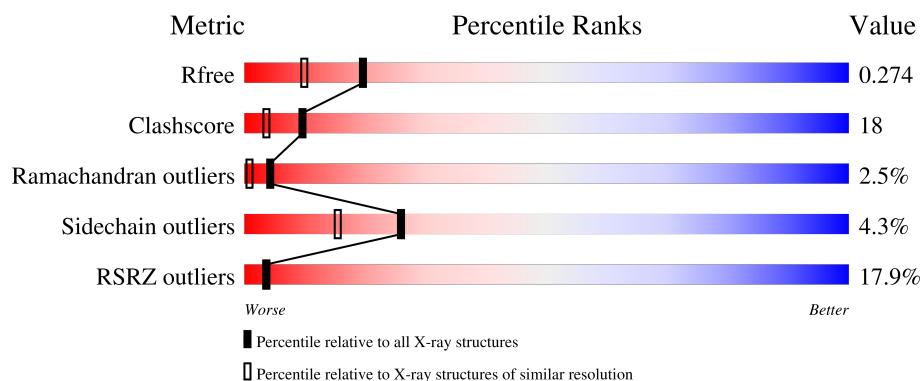
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	287	17% 64% 25% 6% 5%
1	B	287	16% 60% 25% • 13%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4343 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.

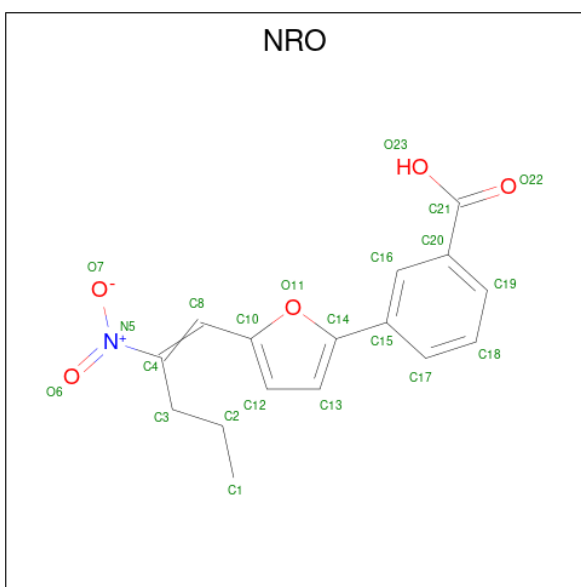
- Molecule 1 is a protein called Peroxisome proliferator-activated receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2185	1409	358	408	10			
1	B	251	Total	C	N	O	S	0	0	0
			2015	1306	330	370	9			

There are 8 discrepancies between the modelled and reference sequences:

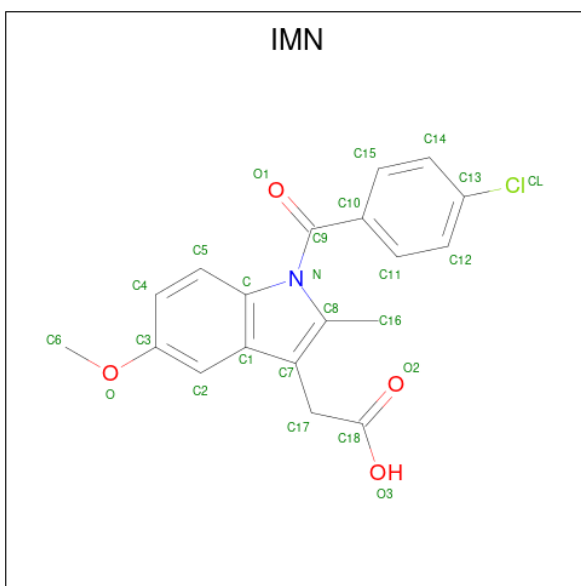
Chain	Residue	Modelled	Actual	Comment	Reference
A	191	GLY	-	expression tag	UNP P37231
A	192	SER	-	expression tag	UNP P37231
A	193	HIS	-	expression tag	UNP P37231
A	194	MET	-	expression tag	UNP P37231
B	191	GLY	-	expression tag	UNP P37231
B	192	SER	-	expression tag	UNP P37231
B	193	HIS	-	expression tag	UNP P37231
B	194	MET	-	expression tag	UNP P37231

- Molecule 2 is 3-[5-(2-nitropent-1-en-1-yl)furan-2-yl]benzoic acid (CCD ID: NRO) (formula: C₁₆H₁₅NO₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			22	16	1	5		

- Molecule 3 is INDOMETHACIN (CCD ID: IMN) (formula: $C_{19}H_{16}ClNO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0
			25	19	1	1	4	
3	B	1	Total	C	Cl	N	O	0
			25	19	1	1	4	

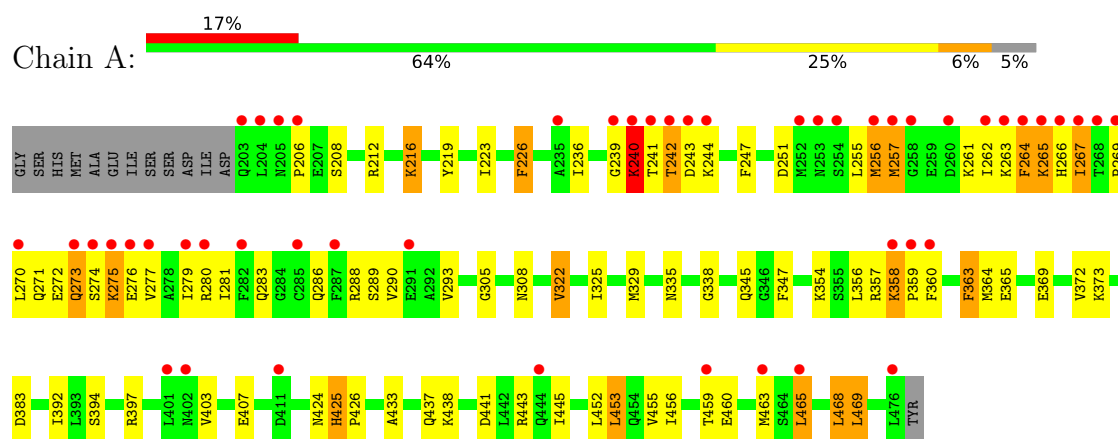
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	40	Total 40	O 40	0	0
4	B	31	Total 31	O 31	0	0

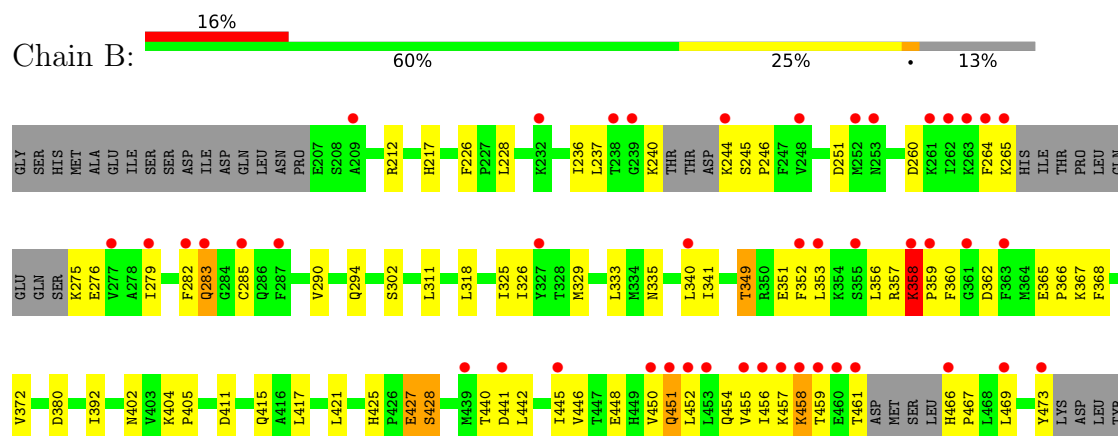
3 Residue-property plots [i](#)

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



- Molecule 1: Peroxisome proliferator-activated receptor gamma



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	93.05Å 61.74Å 118.48Å 90.00° 102.85° 90.00°	Depositor
Resolution (Å)	27.70 – 1.95 27.70 – 1.95	Depositor EDS
% Data completeness (in resolution range)	93.2 (27.70-1.95) 93.3 (27.70-1.95)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 1.95Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.246 , 0.275 0.245 , 0.274	Depositor DCC
R_{free} test set	2325 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	36.4	Xtriage
Anisotropy	0.552	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 39.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4343	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.05% 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: NRO, IMN

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	0.43	0/2222	0.89	10/2995 (0.3%)
1	B	0.39	0/2047	0.83	2/2751 (0.1%)
All	All	0.41	0/4269	0.86	12/5746 (0.2%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	335	ASN	N-CA-C	-6.38	99.63	109.14
1	A	206	PRO	N-CA-CB	6.38	110.35	103.33
1	A	364	MET	N-CA-C	5.92	119.69	112.23
1	A	322	VAL	N-CA-C	5.87	116.05	110.42
1	B	335	ASN	N-CA-C	-5.84	100.44	109.14
1	A	363	PHE	N-CA-C	5.71	117.31	111.14
1	A	226	PHE	CA-C-N	5.35	125.42	119.32
1	A	226	PHE	C-N-CA	5.35	125.42	119.32
1	A	425	HIS	CA-C-N	5.30	124.76	119.24
1	A	425	HIS	C-N-CA	5.30	124.76	119.24
1	A	247	PHE	N-CA-C	-5.19	102.00	110.20
1	B	428	SER	N-CA-C	5.06	116.73	108.63

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	2185	0	2238	81	0
1	B	2015	0	2084	74	0
2	A	22	0	13	5	0
3	A	25	0	15	3	0
3	B	25	0	15	5	0
4	A	40	0	0	3	0
4	B	31	0	0	0	0
All	All	4343	0	4365	154	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 18.

All (154) 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:358:LYS:HB2	1:A:359:PRO:HD3	1.41	1.01
1:B:349:THR:HG22	1:B:352:PHE:H	1.33	0.91
1:A:242:THR:O	1:A:244:LYS:N	2.12	0.81
1:B:358:LYS:HZ3	1:B:358:LYS:HB3	1.44	0.81
1:B:358:LYS:HZ3	1:B:359:PRO:HD2	1.45	0.80
1:A:242:THR:C	1:A:244:LYS:H	1.90	0.80
1:B:264:PHE:O	1:B:265:LYS:HB2	1.83	0.79
1:B:358:LYS:HE3	1:B:459:THR:OG1	1.83	0.78
1:B:358:LYS:HB3	1:B:359:PRO:HD2	1.66	0.78
1:A:288:ARG:HG3	2:A:1:NRO:H1A	1.63	0.77
1:B:441:ASP:O	1:B:445:ILE:HD13	1.88	0.72
1:A:354:LYS:O	1:A:354:LYS:HD3	1.88	0.72
1:B:358:LYS:NZ	1:B:359:PRO:HD2	2.06	0.71
1:A:239:GLY:O	1:A:240:LYS:HG2	1.90	0.70
1:A:263:LYS:C	1:A:265:LYS:H	1.99	0.70
1:B:217:HIS:HE1	1:B:302:SER:O	1.74	0.69
1:B:283:GLN:HE21	1:B:283:GLN:N	1.91	0.67
1:A:271:GLN:HE21	1:A:271:GLN:HA	1.59	0.66
1:A:465:LEU:HD12	1:A:469:LEU:HB3	1.79	0.65
1:B:358:LYS:HZ3	1:B:359:PRO:CD	2.09	0.65
1:A:358:LYS:HB2	1:A:359:PRO:CD	2.25	0.65
1:A:270:LEU:HD23	1:A:270:LEU:O	1.97	0.64
1:A:274:SER:O	1:A:276:GLU:N	2.30	0.64
1:A:286:GLN:NE2	1:A:465:LEU:HA	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:PHE:O	1:B:372:VAL:HG23	1.98	0.64
1:A:453:LEU:HD21	4:A:1003:HOH:O	1.97	0.64
1:A:293:VAL:HG22	1:A:322:VAL:HG21	1.80	0.64
1:A:465:LEU:HD12	1:A:469:LEU:CB	2.29	0.63
1:A:455:VAL:O	1:A:459:THR:HG22	1.98	0.63
1:A:459:THR:HG23	1:A:460:GLU:HG2	1.80	0.63
1:B:358:LYS:HB3	1:B:359:PRO:CD	2.28	0.63
1:B:264:PHE:O	1:B:265:LYS:CB	2.48	0.62
1:B:325:ILE:HD11	1:B:392:ILE:HG13	1.80	0.62
1:A:271:GLN:HA	1:A:271:GLN:NE2	2.15	0.62
1:B:358:LYS:HB3	1:B:358:LYS:NZ	2.13	0.62
1:A:242:THR:C	1:A:244:LYS:N	2.57	0.62
1:B:358:LYS:CB	1:B:359:PRO:HD2	2.31	0.61
1:B:466:HIS:HB3	1:B:467:PRO:HD3	1.83	0.60
1:B:283:GLN:HE21	1:B:283:GLN:CA	2.12	0.60
1:B:358:LYS:CE	1:B:359:PRO:HD2	2.32	0.60
1:A:465:LEU:HD11	4:A:1003:HOH:O	2.02	0.59
1:B:341:ILE:HG22	3:B:3:IMN:C16	2.32	0.59
1:A:236:ILE:HG23	1:A:244:LYS:O	2.02	0.59
1:B:228:LEU:HD23	1:B:333:LEU:HD21	1.83	0.59
1:A:264:PHE:O	1:A:265:LYS:C	2.47	0.58
1:B:458:LYS:HD2	1:B:458:LYS:N	2.19	0.58
1:A:305:GLY:HA2	1:A:308:ASN:HD22	1.67	0.57
1:A:272:GLU:C	1:A:274:SER:H	2.11	0.57
1:A:441:ASP:O	1:A:445:ILE:HG12	2.04	0.57
1:B:402:ASN:O	1:B:405:PRO:HD2	2.05	0.56
1:B:457:LYS:C	1:B:459:THR:H	2.13	0.56
1:A:281:ILE:HG23	2:A:1:NRO:H16	1.86	0.56
1:B:226:PHE:CG	1:B:329:MET:HE1	2.40	0.56
1:B:448:GLU:O	1:B:451:GLN:HG3	2.06	0.56
1:A:289:SER:OG	3:A:2:IMN:H171	2.06	0.56
1:B:357:ARG:NH1	1:B:358:LYS:HG3	2.22	0.55
1:B:365:GLU:HB3	1:B:366:PRO:HD3	1.88	0.55
1:A:433:ALA:O	1:A:437:GLN:HG3	2.06	0.55
1:A:263:LYS:C	1:A:265:LYS:N	2.65	0.55
1:A:383:ASP:OD2	1:A:425:HIS:HE1	1.90	0.55
1:B:452:LEU:O	1:B:456:ILE:HG13	2.06	0.54
1:B:466:HIS:O	1:B:469:LEU:HB2	2.07	0.54
1:B:466:HIS:HA	1:B:469:LEU:HD12	1.89	0.54
1:B:341:ILE:HG22	3:B:3:IMN:H162	1.89	0.53
1:B:353:LEU:O	1:B:356:LEU:HG	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:ARG:HD2	1:B:358:LYS:HB2	1.91	0.53
1:A:255:LEU:C	1:A:255:LEU:HD13	2.34	0.53
1:B:349:THR:HG22	1:B:352:PHE:N	2.15	0.53
1:B:326:ILE:HG23	3:B:3:IMN:H62	1.90	0.53
1:A:256:MET:HE1	1:A:280:ARG:HH22	1.74	0.53
1:A:264:PHE:O	1:A:266:HIS:N	2.42	0.53
1:A:279:ILE:O	1:A:283:GLN:HG2	2.08	0.53
1:B:340:LEU:O	3:B:3:IMN:H163	2.09	0.53
1:A:242:THR:CG2	1:A:244:LYS:HD2	2.40	0.52
1:A:286:GLN:NE2	1:A:465:LEU:HD13	2.25	0.52
1:A:460:GLU:HG3	1:A:463:MET:HE2	1.90	0.52
1:B:212:ARG:HH11	1:B:212:ARG:HG2	1.75	0.52
1:A:219:TYR:CE1	1:A:223:ILE:HD11	2.45	0.52
1:B:357:ARG:HH11	1:B:358:LYS:HG3	1.75	0.51
1:A:357:ARG:HH22	1:A:460:GLU:CD	2.18	0.51
1:B:226:PHE:CD1	1:B:329:MET:HE1	2.45	0.51
1:A:325:ILE:HD11	1:A:392:ILE:CG1	2.41	0.51
1:B:237:LEU:HD21	1:B:340:LEU:HG	1.93	0.51
1:B:452:LEU:C	1:B:452:LEU:HD23	2.36	0.50
1:B:402:ASN:OD1	1:B:405:PRO:HD3	2.12	0.49
1:A:226:PHE:CG	1:A:329:MET:HE1	2.48	0.49
1:B:360:PHE:C	1:B:362:ASP:H	2.21	0.49
1:A:363:PHE:CZ	1:A:452:LEU:HB3	2.48	0.49
1:B:290:VAL:HG21	1:B:473:TYR:HD1	1.78	0.48
1:A:272:GLU:HA	1:A:280:ARG:HD2	1.95	0.48
1:B:279:ILE:HD11	1:B:461:THR:HG23	1.95	0.48
1:B:455:VAL:O	1:B:458:LYS:HD3	2.13	0.48
1:A:281:ILE:HG12	2:A:1:NRO:O22	2.14	0.48
1:A:403:VAL:O	1:A:407:GLU:HG3	2.14	0.48
1:B:290:VAL:HG21	1:B:473:TYR:CD1	2.49	0.47
1:B:404:LYS:HB3	1:B:405:PRO:HD3	1.96	0.47
1:A:360:PHE:HB3	3:A:2:IMN:H12	1.96	0.47
1:B:251:ASP:OD1	1:B:251:ASP:C	2.57	0.47
1:A:263:LYS:O	1:A:265:LYS:N	2.47	0.47
1:A:267:ILE:HG21	2:A:1:NRO:H18	1.96	0.47
1:A:273:GLN:O	1:A:275:LYS:N	2.48	0.47
1:A:257:MET:O	1:A:261:LYS:HG2	2.14	0.47
1:A:277:VAL:HG12	1:A:280:ARG:NH2	2.31	0.46
1:A:286:GLN:HE21	1:A:465:LEU:HD13	1.80	0.46
1:A:443:ARG:HG3	1:B:440:THR:CG2	2.45	0.46
1:A:255:LEU:HD11	1:A:280:ARG:HH21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:LYS:HD2	1:B:367:LYS:N	2.30	0.46
1:A:286:GLN:HE22	1:A:465:LEU:HA	1.81	0.46
1:B:454:GLN:O	1:B:457:LYS:HG2	2.15	0.45
1:A:216:LYS:HG3	4:A:1060:HOH:O	2.17	0.45
1:A:242:THR:HG23	1:A:244:LYS:CG	2.46	0.45
1:B:325:ILE:HD11	1:B:392:ILE:CG1	2.44	0.45
1:B:442:LEU:O	1:B:446:VAL:HG23	2.17	0.45
1:A:365:GLU:O	1:A:369:GLU:HG3	2.17	0.45
1:B:282:PHE:O	1:B:285:CYS:HB3	2.17	0.45
1:A:208:SER:O	1:A:212:ARG:HG2	2.17	0.44
1:A:456:ILE:HA	1:A:459:THR:HG22	1.99	0.44
1:B:279:ILE:CD1	1:B:461:THR:HG23	2.47	0.44
1:A:290:VAL:HG13	1:A:468:LEU:HD12	1.98	0.44
1:B:326:ILE:HG23	3:B:3:IMN:C6	2.46	0.44
1:B:358:LYS:HE2	1:B:359:PRO:HD2	2.00	0.44
1:B:446:VAL:O	1:B:450:VAL:HG23	2.18	0.44
1:A:242:THR:HG23	1:A:244:LYS:HG3	1.99	0.44
1:A:267:ILE:HG21	2:A:1:NRO:C18	2.48	0.43
1:A:272:GLU:C	1:A:274:SER:N	2.76	0.43
1:A:356:LEU:HD12	3:A:2:IMN:CL	2.55	0.43
1:A:465:LEU:CD1	1:A:469:LEU:HD23	2.48	0.43
1:A:277:VAL:HG12	1:A:280:ARG:HH22	1.83	0.43
1:A:338:GLY:HA3	1:A:347:PHE:CZ	2.54	0.43
1:B:236:ILE:CG2	1:B:246:PRO:HG2	2.48	0.43
1:B:244:LYS:O	1:B:245:SER:C	2.61	0.43
1:A:373:LYS:HG3	1:A:438:LYS:NZ	2.34	0.43
1:B:380:ASP:OD1	1:B:380:ASP:C	2.62	0.43
1:A:262:ILE:HG21	1:A:264:PHE:CE2	2.53	0.42
1:A:263:LYS:CB	1:A:345:GLN:HE22	2.32	0.42
1:B:358:LYS:CB	1:B:359:PRO:CD	2.92	0.42
1:A:456:ILE:HA	1:A:459:THR:CG2	2.50	0.42
1:B:417:LEU:O	1:B:421:LEU:HG	2.20	0.42
1:A:358:LYS:CB	1:A:359:PRO:HD3	2.28	0.42
1:B:275:LYS:HE3	1:B:275:LYS:HB2	1.90	0.42
1:B:349:THR:HG22	1:B:351:GLU:N	2.35	0.42
1:A:212:ARG:HA	1:A:212:ARG:HD2	1.86	0.42
1:A:263:LYS:HB3	1:A:345:GLN:HE22	1.85	0.42
1:A:394:SER:O	1:A:397:ARG:HG2	2.20	0.42
1:B:425:HIS:HB3	1:B:428:SER:OG	2.21	0.41
1:B:457:LYS:C	1:B:459:THR:N	2.79	0.41
1:A:239:GLY:O	1:A:240:LYS:CG	2.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:ASN:C	1:A:426:PRO:HD3	2.45	0.41
1:B:411:ASP:O	1:B:415:GLN:HG3	2.21	0.41
1:B:454:GLN:O	1:B:455:VAL:C	2.64	0.41
1:A:251:ASP:OD1	1:A:251:ASP:C	2.63	0.40
1:B:367:LYS:N	1:B:367:LYS:CD	2.85	0.40
1:B:427:GLU:HG3	1:B:428:SER:H	1.86	0.40
1:A:460:GLU:HG3	1:A:463:MET:CE	2.51	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	272/287 (95%)	255 (94%)	7 (3%)	10 (4%)	2	0
1	B	243/287 (85%)	225 (93%)	15 (6%)	3 (1%)	10	4
All	All	515/574 (90%)	480 (93%)	22 (4%)	13 (2%)	4	1

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	243	ASP
1	A	269	PRO
1	A	275	LYS
1	A	358	LYS
1	A	265	LYS
1	B	358	LYS
1	A	273	GLN
1	B	276	GLU
1	A	240	LYS
1	A	242	THR
1	A	264	PHE

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Mol	Chain	Res	Type
1	B	458	LYS
1	A	267	ILE

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	243/258 (94%)	233 (96%)	10 (4%)	27	17
1	B	224/258 (87%)	214 (96%)	10 (4%)	24	14
All	All	467/516 (90%)	447 (96%)	20 (4%)	26	15

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	216	LYS
1	A	240	LYS
1	A	241	THR
1	A	256	MET
1	A	257	MET
1	A	372	VAL
1	A	453	LEU
1	A	465	LEU
1	A	468	LEU
1	A	469	LEU
1	B	240	LYS
1	B	260	ASP
1	B	283	GLN
1	B	294	GLN
1	B	311	LEU
1	B	318	LEU
1	B	349	THR
1	B	358	LYS
1	B	427	GLU
1	B	451	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	253	ASN
1	A	271	GLN
1	A	283	GLN
1	A	286	GLN
1	A	294	GLN
1	A	308	ASN
1	A	312	ASN
1	A	314	GLN
1	A	345	GLN
1	A	410	GLN
1	A	425	HIS
1	B	217	HIS
1	B	253	ASN
1	B	283	GLN
1	B	323	HIS
1	B	424	ASN
1	B	449	HIS
1	B	466	HIS
1	B	470	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 ⓘ

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	NRO	A	1	1	22,23,23	4.14	11 (50%)	23,31,31	1.46	3 (13%)
3	IMN	B	3	-	27,27,27	1.61	7 (25%)	39,39,39	1.26	5 (12%)
3	IMN	A	2	-	27,27,27	1.53	7 (25%)	39,39,39	1.26	5 (12%)

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	NRO	A	1	1	-	11/17/19/19	0/2/2/2
3	IMN	B	3	-	-	10/14/14/14	0/3/3/3
3	IMN	A	2	-	-	8/14/14/14	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	NRO	C8-C4	11.49	1.57	1.35
2	A	1	NRO	O6-N5	11.07	1.42	1.22
2	A	1	NRO	C8-C10	5.75	1.55	1.43
2	A	1	NRO	C19-C20	3.87	1.45	1.39
2	A	1	NRO	C16-C20	3.61	1.44	1.39
2	A	1	NRO	C16-C15	3.46	1.44	1.39
3	B	3	IMN	C15-C10	3.35	1.44	1.39
3	A	2	IMN	C15-C10	3.08	1.44	1.39
2	A	1	NRO	C20-C21	2.90	1.55	1.49
2	A	1	NRO	C15-C14	-2.88	1.41	1.48
3	B	3	IMN	C11-C10	2.88	1.43	1.39
3	A	2	IMN	C11-C10	2.82	1.43	1.39
2	A	1	NRO	C18-C19	2.70	1.43	1.38
2	A	1	NRO	C17-C15	2.63	1.43	1.39
3	A	2	IMN	C5-C	2.62	1.43	1.39
3	B	3	IMN	C4-C3	2.53	1.43	1.38
3	A	2	IMN	C10-C9	2.51	1.54	1.50
2	A	1	NRO	C18-C17	2.41	1.43	1.38
3	A	2	IMN	C2-C3	2.37	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	3	IMN	C5-C	2.28	1.43	1.39
3	B	3	IMN	C12-C13	2.21	1.42	1.38
3	B	3	IMN	C1-C	2.15	1.43	1.41
3	A	2	IMN	C12-C13	2.02	1.41	1.38
3	B	3	IMN	C10-C9	2.01	1.53	1.50
3	A	2	IMN	C16-C8	2.00	1.52	1.49

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	NRO	O11-C14-C15	4.25	121.76	116.73
3	B	3	IMN	C6-O-C3	-3.42	110.17	117.50
3	A	2	IMN	C10-C9-N	3.30	124.26	117.92
3	A	2	IMN	C5-C-C1	-3.22	118.35	121.95
2	A	1	NRO	C12-C13-C14	2.99	108.97	107.04
3	B	3	IMN	C5-C-C1	-2.83	118.79	121.95
3	A	2	IMN	C6-O-C3	-2.73	111.64	117.50
3	B	3	IMN	C16-C8-C7	-2.65	123.92	128.07
3	B	3	IMN	C10-C9-N	2.53	122.78	117.92
3	B	3	IMN	C16-C8-N	2.50	125.81	122.07
3	A	2	IMN	C16-C8-N	2.29	125.51	122.07
2	A	1	NRO	C12-C10-C8	-2.24	124.77	132.73
3	A	2	IMN	C16-C8-C7	-2.19	124.64	128.07

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	NRO	C2-C3-C4-C8
2	A	1	NRO	C3-C4-C8-C10
2	A	1	NRO	N5-C4-C8-C10
2	A	1	NRO	C3-C4-N5-O6
2	A	1	NRO	C8-C4-N5-O6
2	A	1	NRO	O11-C10-C8-C4
2	A	1	NRO	C12-C10-C8-C4
3	B	3	IMN	C10-C9-N-C8
3	B	3	IMN	O1-C9-N-C8
2	A	1	NRO	O11-C14-C15-C16
3	B	3	IMN	C2-C3-O-C6
3	B	3	IMN	C4-C3-O-C6
2	A	1	NRO	O11-C14-C15-C17
2	A	1	NRO	C13-C14-C15-C16

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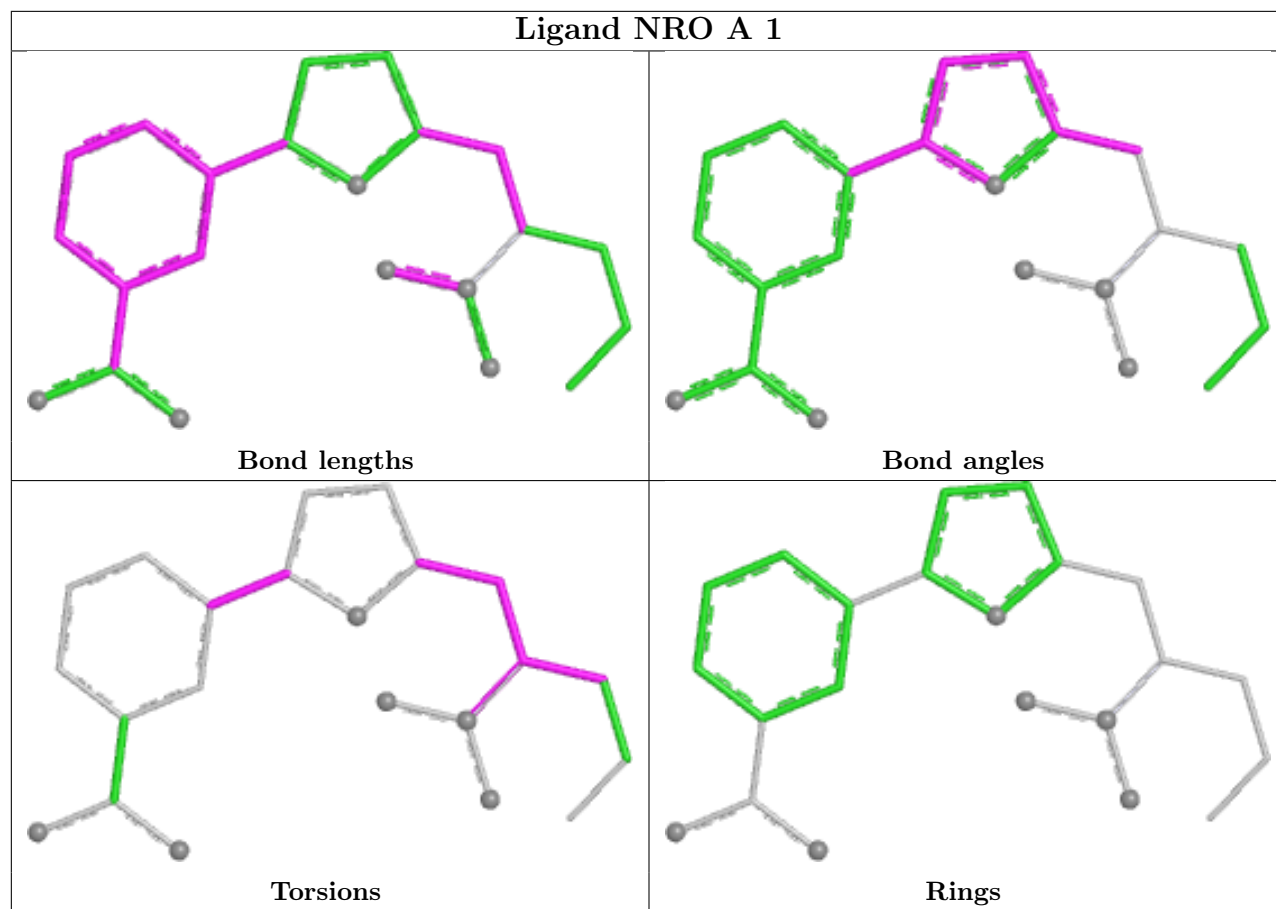
Mol	Chain	Res	Type	Atoms
2	A	1	NRO	C13-C14-C15-C17
3	B	3	IMN	O1-C9-N-C
3	A	2	IMN	C15-C10-C9-O1
3	B	3	IMN	C15-C10-C9-O1
3	B	3	IMN	C11-C10-C9-O1
3	B	3	IMN	C15-C10-C9-N
3	A	2	IMN	C11-C10-C9-O1
3	A	2	IMN	C15-C10-C9-N
3	B	3	IMN	C11-C10-C9-N
3	A	2	IMN	O1-C9-N-C8
3	A	2	IMN	C11-C10-C9-N
3	B	3	IMN	C10-C9-N-C
3	A	2	IMN	C4-C3-O-C6
3	A	2	IMN	C2-C3-O-C6
3	A	2	IMN	C10-C9-N-C8

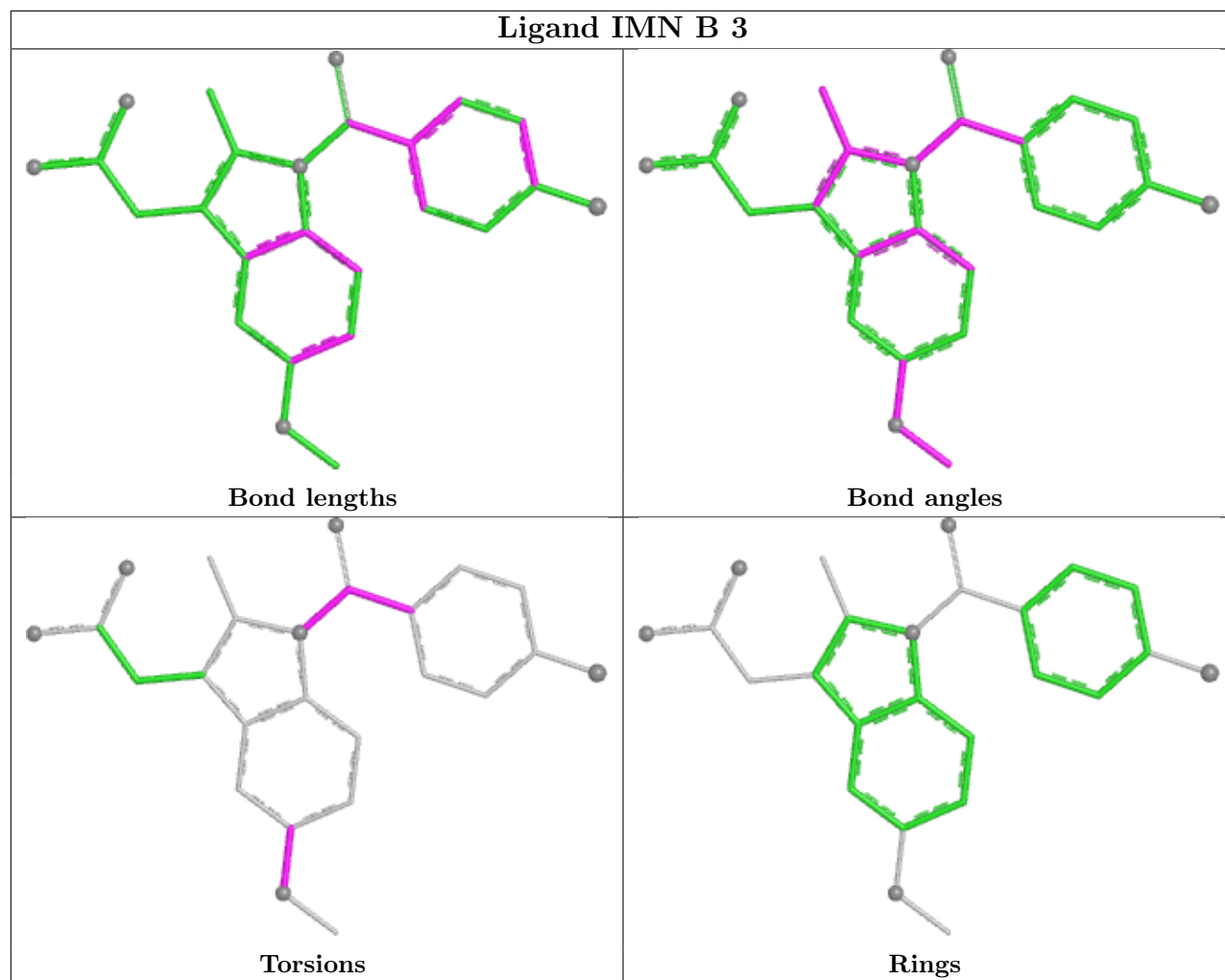
There are no ring outliers.

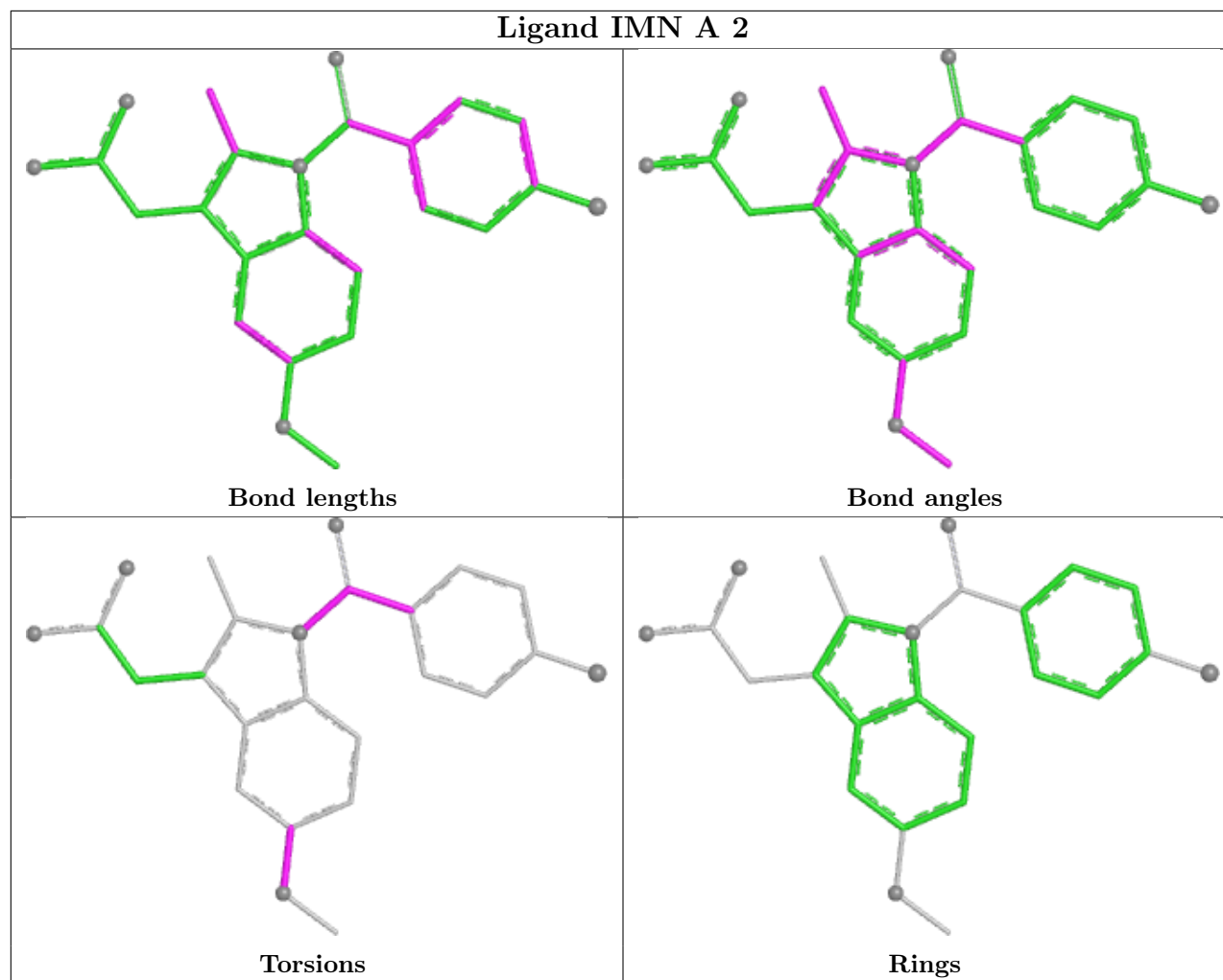
3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	NRO	5	0
3	B	3	IMN	5	0
3	A	2	IMN	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	274/287 (95%)	1.05	49 (17%) 3 3	28, 43, 79, 96	0
1	B	251/287 (87%)	1.09	45 (17%) 3 3	28, 45, 79, 84	0
All	All	525/574 (91%)	1.07	94 (17%) 3 3	28, 44, 79, 96	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	205	ASN	7.9
1	A	242	THR	7.4
1	A	268	THR	5.2
1	A	264	PHE	4.5
1	B	459	THR	4.5
1	A	267	ILE	4.4
1	A	266	HIS	4.3
1	A	269	PRO	4.3
1	A	204	LEU	4.2
1	B	453	LEU	4.2
1	A	359	PRO	4.0
1	B	455	VAL	4.0
1	A	262	ILE	4.0
1	A	275	LYS	3.9
1	B	264	PHE	3.9
1	B	283	GLN	3.9
1	B	456	ILE	3.8
1	A	203	GLN	3.8
1	B	457	LYS	3.7
1	B	239	GLY	3.7
1	B	363	PHE	3.7
1	B	279	ILE	3.6
1	A	277	VAL	3.6
1	A	401	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	358	LYS	3.5
1	B	458	LYS	3.5
1	B	209	ALA	3.5
1	A	258	GLY	3.5
1	B	460	GLU	3.4
1	B	461	THR	3.4
1	A	243	ASP	3.4
1	B	451	GLN	3.4
1	B	361	GLY	3.4
1	B	287	PHE	3.4
1	B	473	TYR	3.3
1	A	279	ILE	3.3
1	A	257	MET	3.2
1	A	244	LYS	3.2
1	A	444	GLN	3.2
1	B	262	ILE	3.2
1	A	270	LEU	3.2
1	A	273	GLN	3.1
1	B	282	PHE	3.1
1	B	265	LYS	3.1
1	B	359	PRO	3.1
1	A	476	LEU	3.1
1	B	263	LYS	3.1
1	A	240	LYS	3.0
1	A	241	THR	2.9
1	A	252	MET	2.9
1	A	287	PHE	2.9
1	B	445	ILE	2.8
1	A	274	SER	2.8
1	A	256	MET	2.8
1	B	327	TYR	2.8
1	B	261	LYS	2.7
1	A	239	GLY	2.7
1	A	411	ASP	2.7
1	A	260	ASP	2.7
1	A	254	SER	2.7
1	B	244	LYS	2.6
1	B	450	VAL	2.6
1	A	235	ALA	2.6
1	A	206	PRO	2.6
1	B	441	ASP	2.6
1	A	459	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	355	SER	2.5
1	B	252	MET	2.5
1	B	277	VAL	2.5
1	A	265	LYS	2.5
1	A	402	ASN	2.4
1	A	282	PHE	2.4
1	A	285	CYS	2.4
1	A	465	LEU	2.4
1	B	469	LEU	2.4
1	B	238	THR	2.4
1	B	466	HIS	2.4
1	A	463	MET	2.4
1	A	263	LYS	2.3
1	A	276	GLU	2.3
1	A	358	LYS	2.3
1	B	232	LYS	2.3
1	B	340	LEU	2.3
1	B	248	VAL	2.2
1	A	291	GLU	2.2
1	B	452	LEU	2.2
1	B	253	ASN	2.2
1	A	360	PHE	2.1
1	B	352	PHE	2.1
1	A	253	ASN	2.1
1	B	285	CYS	2.1
1	B	353	LEU	2.1
1	B	439	MET	2.0
1	A	280	ARG	2.0

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 oligosaccharides in this entry.

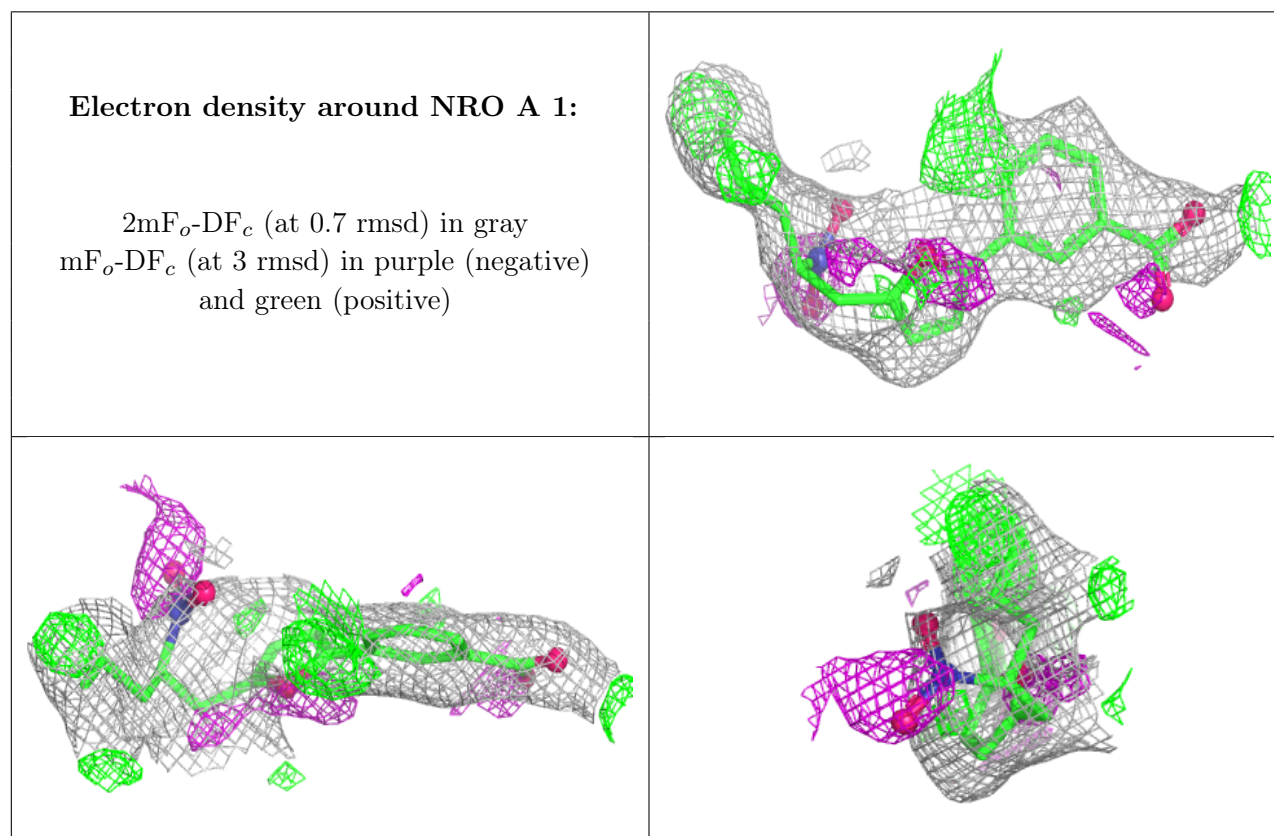
6.4 Ligands [i](#)

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.

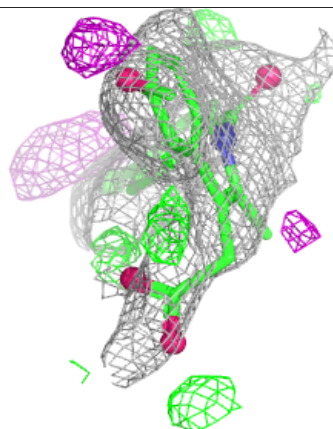
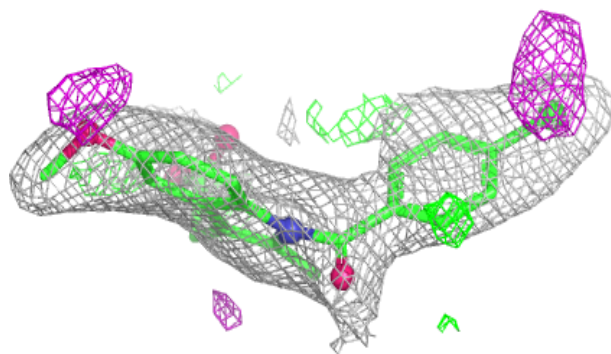
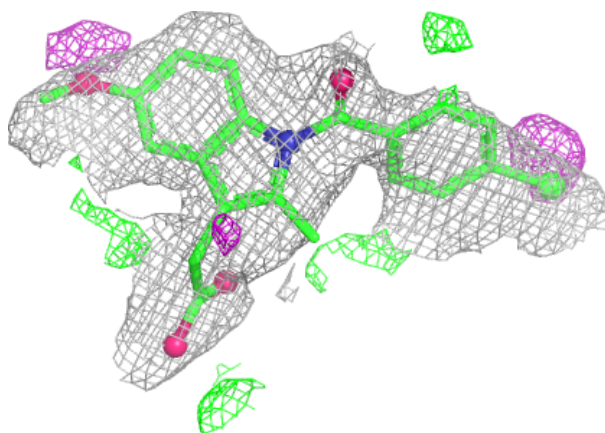
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NRO	A	1	22/22	0.62	0.23	77,80,83,84	0
3	IMN	B	3	25/25	0.73	0.21	76,79,81,82	0
3	IMN	A	2	25/25	0.80	0.15	53,59,64,64	0

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.

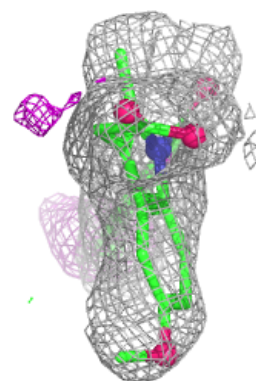
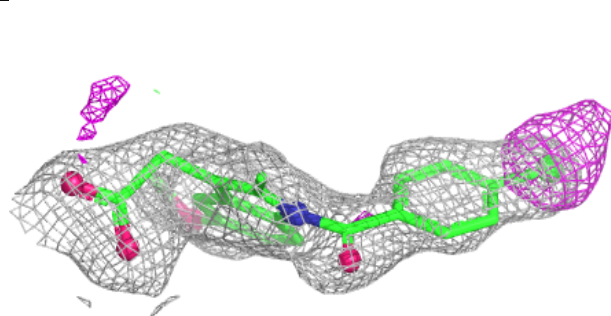
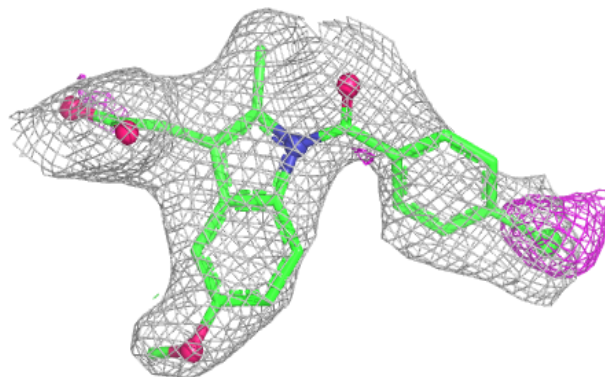


Electron density around IMN B 3:

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

**Electron density around IMN A 2:**

$2mF_o-DF_c$ (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.