



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2023 – 09:57 AM EDT

PDB ID : 3ADX
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

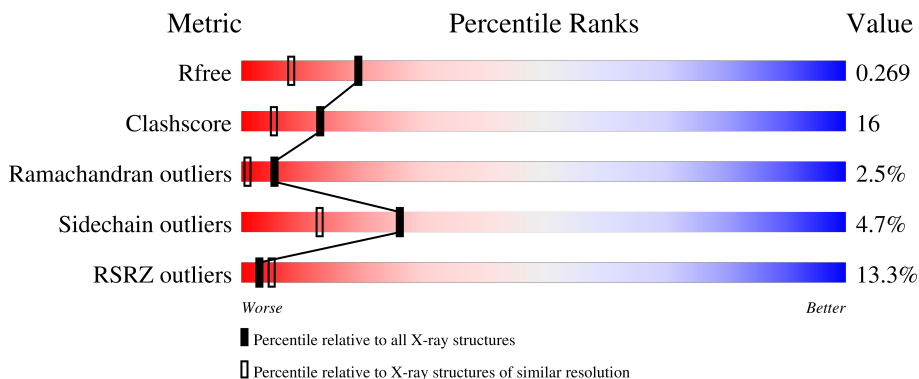
1 Overall quality at a glance

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}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (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	
1	B	287	

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.

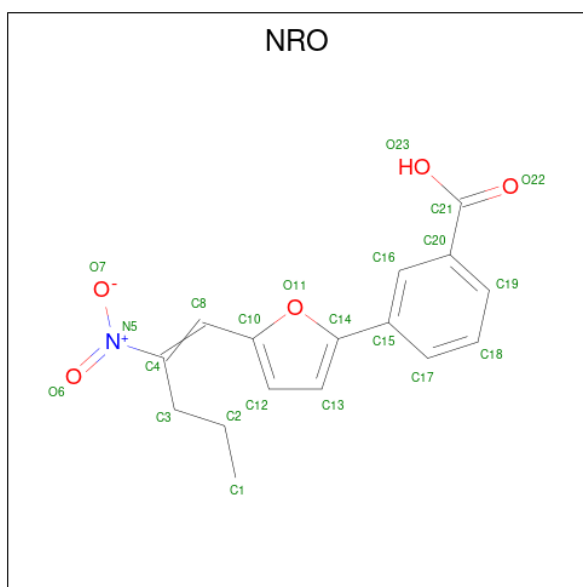
- Molecule 1 is a protein called Peroxisome proliferator-activated receptor gamma.

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

There are 8 discrepancies between the modelled and reference sequences:

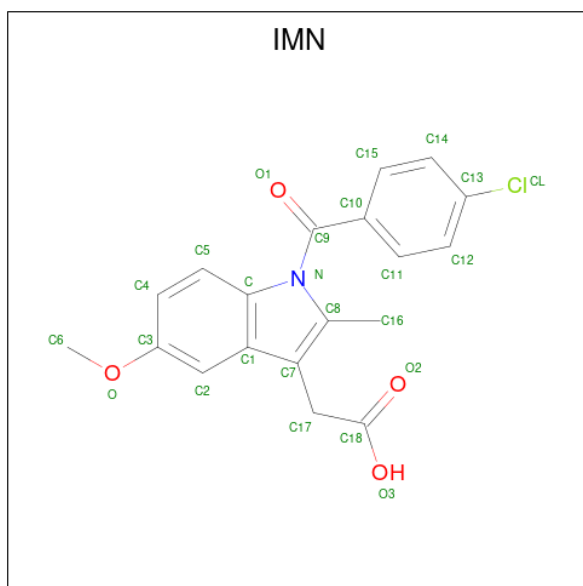
Chain	Residue	Modelled	Actual	Comment	Reference
A	191	GLY	-	expression tag	UNP P37231
A	192	SER	-	expression tag	UNP P37231
A	193	HIS	-	expression tag	UNP P37231
A	194	MET	-	expression tag	UNP P37231
B	191	GLY	-	expression tag	UNP P37231
B	192	SER	-	expression tag	UNP P37231
B	193	HIS	-	expression tag	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 (three-letter code: NRO) (formula: C₁₆H₁₅NO₅).



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

- Molecule 3 is INDOMETHACIN (three-letter code: IMN) (formula: $C_{19}H_{16}ClNO_4$).



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

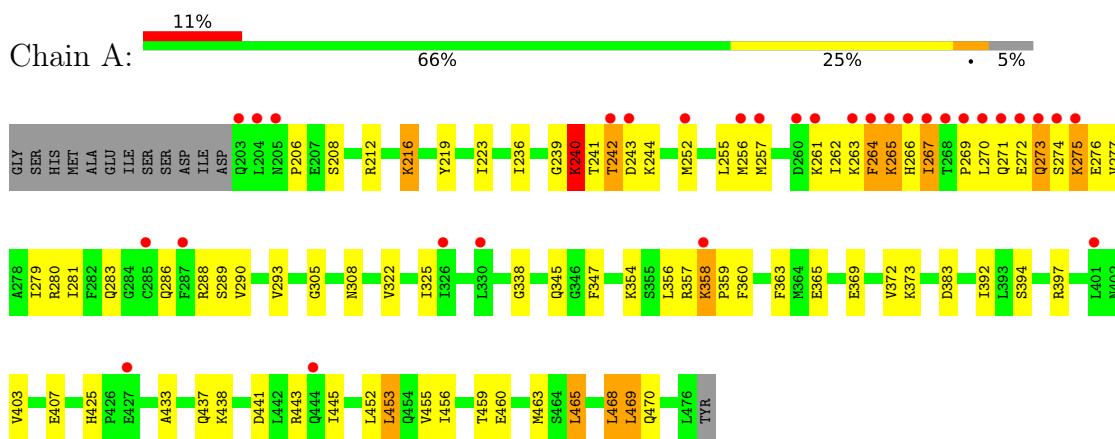
- Molecule 4 is water.

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

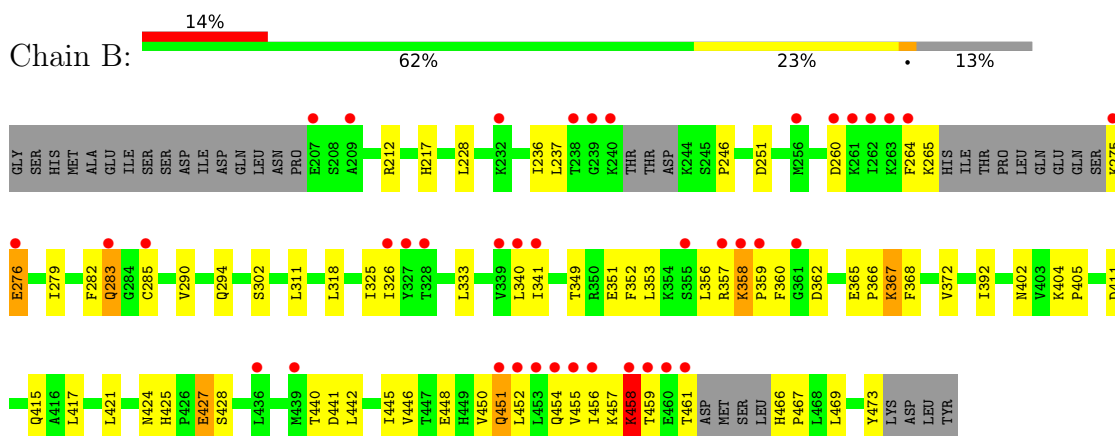
3 Residue-property plots [i](#)

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)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.246 , 0.275 0.238 , 0.269	Depositor DCC
R_{free} test set	2325 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	36.4	Xtrriage
Anisotropy	0.552	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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	0.36	0/2222	0.58	1/2995 (0.0%)
1	B	0.34	0/2047	0.53	0/2751
All	All	0.35	0/4269	0.56	1/5746 (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	206	PRO	N-CA-CB	5.87	110.35	103.30

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	76	0
1	B	2015	0	2084	67	0
2	A	22	0	13	5	0
3	A	25	0	15	3	0
3	B	25	0	15	4	0
4	A	40	0	0	3	0
4	B	31	0	0	0	0
All	All	4343	0	4365	142	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 16.

All (142) 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:B:358:LYS:HZ3	1:B:359:PRO:HD2	1.38	0.88
1:A:242:THR:O	1:A:244:LYS:N	2.12	0.81
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:A:242:THR:C	1:A:244:LYS:H	1.90	0.75
1:B:358:LYS:HZ3	1:B:359:PRO:CD	2.00	0.73
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:B:358:LYS:HZ3	1:B:358:LYS:HB3	1.55	0.70
1:A:239:GLY:O	1:A:240:LYS:HG2	1.90	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:263:LYS:C	1:A:265:LYS:H	1.99	0.65
1:A:465:LEU:HD12	1:A:469:LEU:HB3	1.79	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
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:358:LYS:HB3	1:B:358:LYS:NZ	2.13	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:CB	1:B:359:PRO:HD2	2.31	0.61
1:B:466:HIS:HB3	1:B:467:PRO:HD3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:242:THR:C	1:A:244:LYS:N	2.57	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:A:281:ILE:HG23	2:A:1:NRO:H16	1.86	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: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:353:LEU:O	1:B:356:LEU:HG	2.08	0.53
1:B:357:ARG:HD2	1:B:358:LYS:HB2	1.91	0.53
1:A:264:PHE:O	1:A:265:LYS:C	2.47	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: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:A:272:GLU:C	1:A:274:SER:H	2.11	0.52
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:B:457:LYS:C	1:B:459:THR:H	2.13	0.52
1:B:212:ARG:HH11	1:B:212:ARG:HG2	1.75	0.52
1:A:460:GLU:HG3	1:A:463:MET:HE2	1.91	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: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:402:ASN:OD1	1:B:405:PRO:HD3	2.12	0.49
1:A:363:PHE:CZ	1:A:452:LEU:HB3	2.48	0.49
1:A:255:LEU:C	1:A:255:LEU:HD13	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:357:ARG:HH22	1:A:460:GLU:CD	2.18	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
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:452:LEU:C	1:B:452:LEU:HD23	2.36	0.45
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:360:PHE:C	1:B:362:ASP:H	2.21	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:341:ILE:HG22	3:B:3:IMN:H161	2.00	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:373:LYS:HG3	1:A:438:LYS:NZ	2.34	0.43
1:B:251:ASP:OD1	1:B:251:ASP:C	2.57	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:A:263:LYS:C	1:A:265:LYS:N	2.65	0.41
1:A:239:GLY:O	1:A:240:LYS:CG	2.66	0.41
1:B:411:ASP:O	1:B:415:GLN:HG3	2.21	0.41
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%)	3 0
1	B	243/287 (85%)	225 (93%)	15 (6%)	3 (1%)	13 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	515/574 (90%)	480 (93%)	22 (4%)	13 (2%)	5 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
1	B	458	LYS
1	A	267	ILE

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	243/258 (94%)	232 (96%)	11 (4%)	27 15
1	B	224/258 (87%)	213 (95%)	11 (5%)	25 12
All	All	467/516 (90%)	445 (95%)	22 (5%)	26 13

All (22) 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	252	MET
1	A	256	MET

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Mol	Chain	Res	Type
1	A	372	VAL
1	A	453	LEU
1	A	465	LEU
1	A	468	LEU
1	A	469	LEU
1	A	470	GLN
1	B	260	ASP
1	B	276	GLU
1	B	283	GLN
1	B	294	GLN
1	B	311	LEU
1	B	318	LEU
1	B	367	LYS
1	B	424	ASN
1	B	427	GLU
1	B	451	GLN
1	B	458	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) 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	314	GLN
1	A	410	GLN
1	A	425	HIS
1	A	430	GLN
1	B	217	HIS
1	B	283	GLN
1	B	424	ASN
1	B	430	GLN
1	B	437	GLN
1	B	449	HIS
1	B	466	HIS
1	B	470	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	NRO	A	1	1	16,23,23	6.15	7 (43%)	15,31,31	0.85	0
3	IMN	A	2	-	24,27,27	1.65	5 (20%)	29,39,39	1.56	5 (17%)
3	IMN	B	3	-	24,27,27	1.71	9 (37%)	29,39,39	1.51	5 (17%)

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	-	3/9/19/19	0/2/2/2
3	IMN	A	2	-	-	6/10/14/14	0/3/3/3
3	IMN	B	3	-	-	6/10/14/14	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	NRO	C8-C4	20.37	1.57	1.33
2	A	1	NRO	O6-N5	11.23	1.42	1.22
2	A	1	NRO	C16-C20	4.31	1.44	1.37
2	A	1	NRO	C19-C20	3.49	1.45	1.39
3	A	2	IMN	C2-C3	3.27	1.42	1.37
3	B	3	IMN	C8-N	3.09	1.41	1.36
3	B	3	IMN	C15-C10	3.03	1.44	1.39
3	A	2	IMN	C8-N	2.93	1.41	1.36
2	A	1	NRO	C20-C21	2.91	1.55	1.49
3	A	2	IMN	C15-C10	2.79	1.44	1.39
2	A	1	NRO	C18-C17	2.78	1.43	1.36
3	B	3	IMN	C11-C10	2.61	1.43	1.39
3	A	2	IMN	C11-C10	2.57	1.43	1.39
3	A	2	IMN	C10-C9	2.56	1.54	1.50
3	B	3	IMN	C5-C4	2.53	1.41	1.36
3	B	3	IMN	C4-C3	2.42	1.43	1.38
3	B	3	IMN	C2-C3	2.24	1.41	1.37
2	A	1	NRO	C18-C19	2.18	1.43	1.38
3	B	3	IMN	C12-C13	2.17	1.42	1.38
3	B	3	IMN	C10-C9	2.05	1.53	1.50
3	B	3	IMN	C8-C7	-2.04	1.34	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2	IMN	C10-C9-N	5.40	124.26	117.95
3	B	3	IMN	C10-C9-N	4.14	122.78	117.95
3	B	3	IMN	C6-O-C3	-3.38	110.17	117.51
3	B	3	IMN	C16-C8-N	2.73	125.81	122.37
3	A	2	IMN	C6-O-C3	-2.71	111.64	117.51
3	A	2	IMN	C16-C8-N	2.49	125.51	122.37
3	B	3	IMN	C16-C8-C7	-2.46	123.92	129.24
3	B	3	IMN	C7-C17-C18	-2.26	111.47	114.18
3	A	2	IMN	C16-C8-C7	-2.13	124.64	129.24
3	A	2	IMN	C17-C7-C8	2.01	128.18	126.41

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	NRO	C2-C3-C4-C8
2	A	1	NRO	C8-C4-N5-O6

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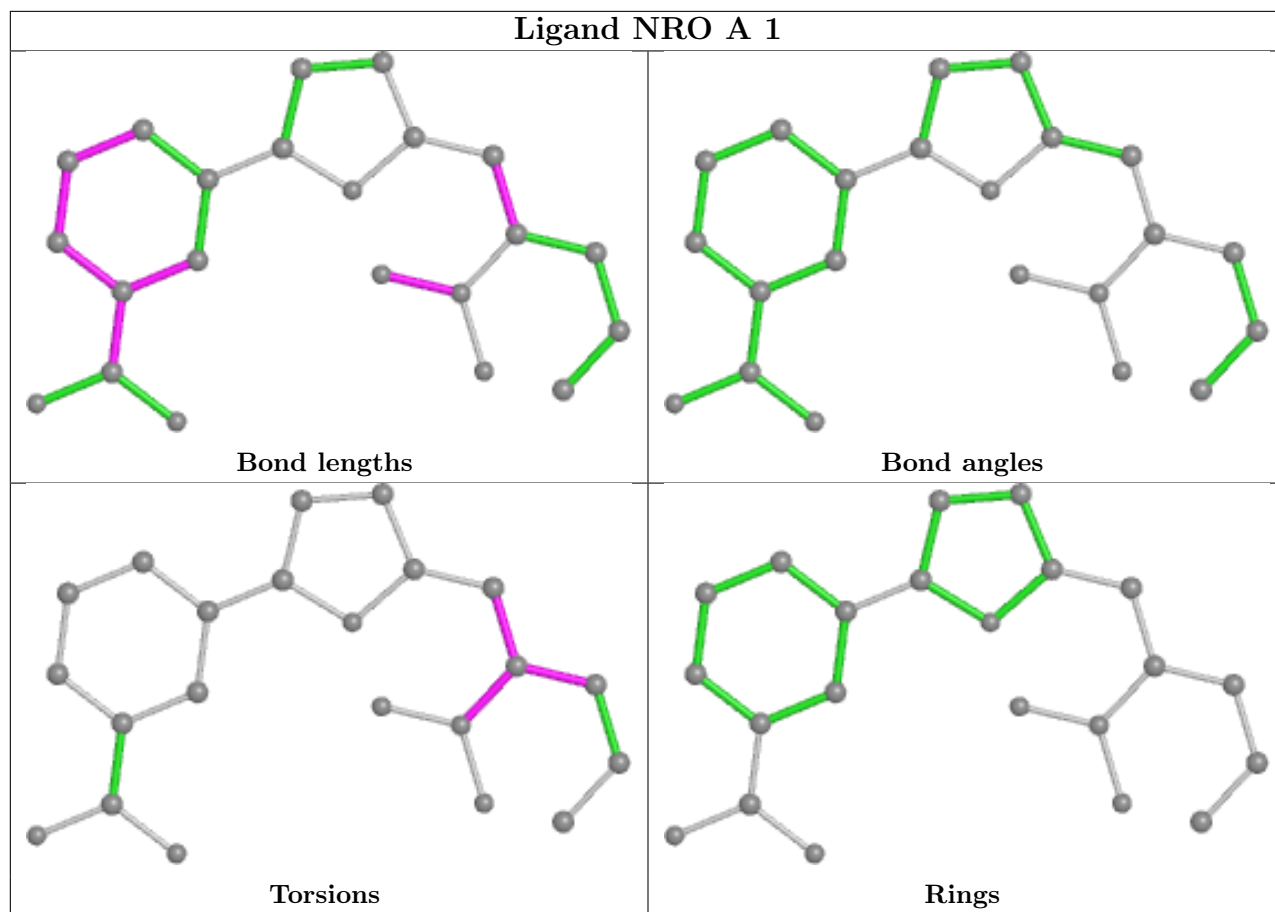
Mol	Chain	Res	Type	Atoms
3	A	2	IMN	C11-C10-C9-N
3	A	2	IMN	C15-C10-C9-N
3	B	3	IMN	C11-C10-C9-N
3	B	3	IMN	C15-C10-C9-N
3	B	3	IMN	C2-C3-O-C6
3	B	3	IMN	C4-C3-O-C6
3	A	2	IMN	C15-C10-C9-O1
3	B	3	IMN	C15-C10-C9-O1
3	B	3	IMN	C11-C10-C9-O1
3	A	2	IMN	C11-C10-C9-O1
3	A	2	IMN	C4-C3-O-C6
3	A	2	IMN	C2-C3-O-C6
2	A	1	NRO	N5-C4-C8-C10

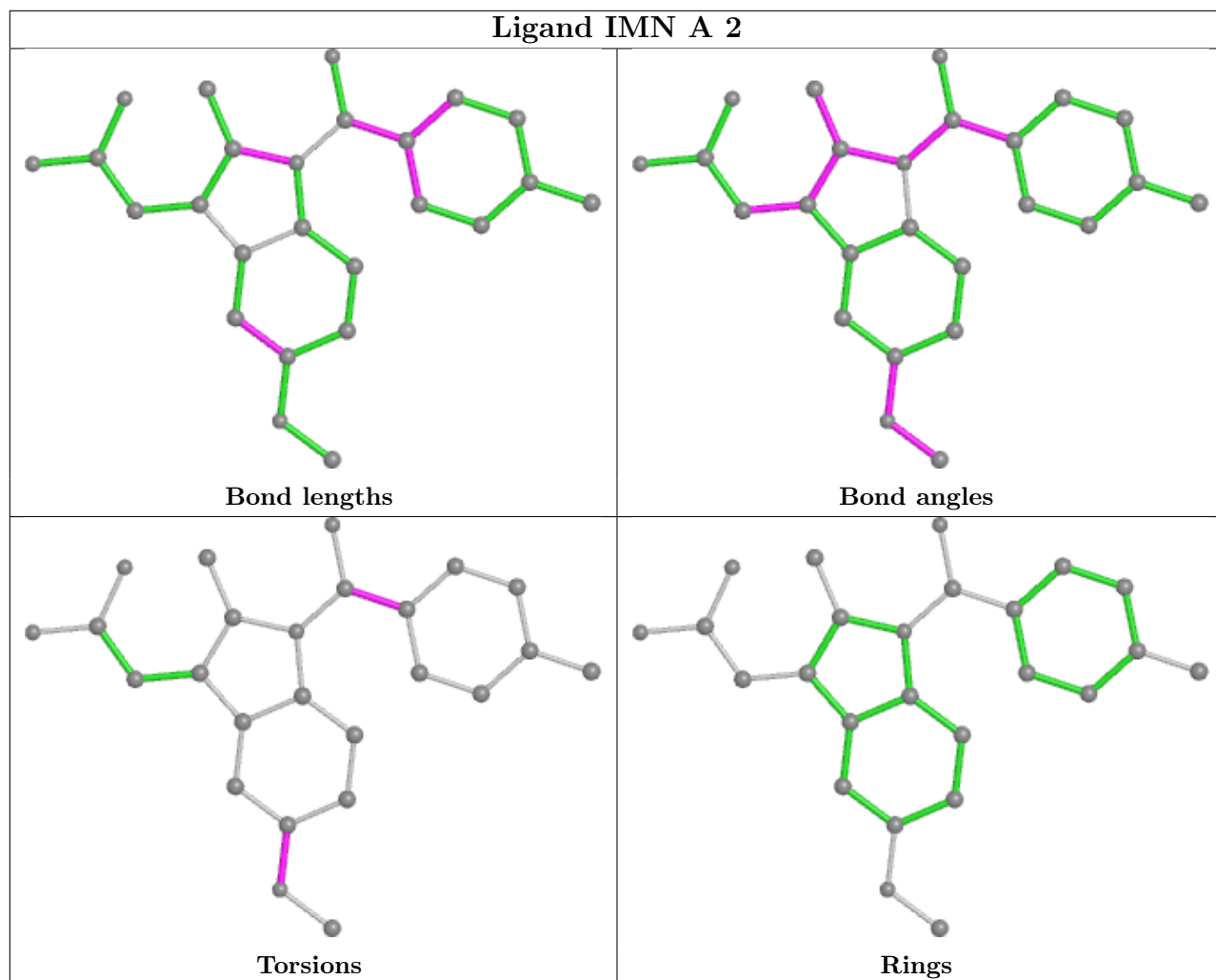
There are no ring outliers.

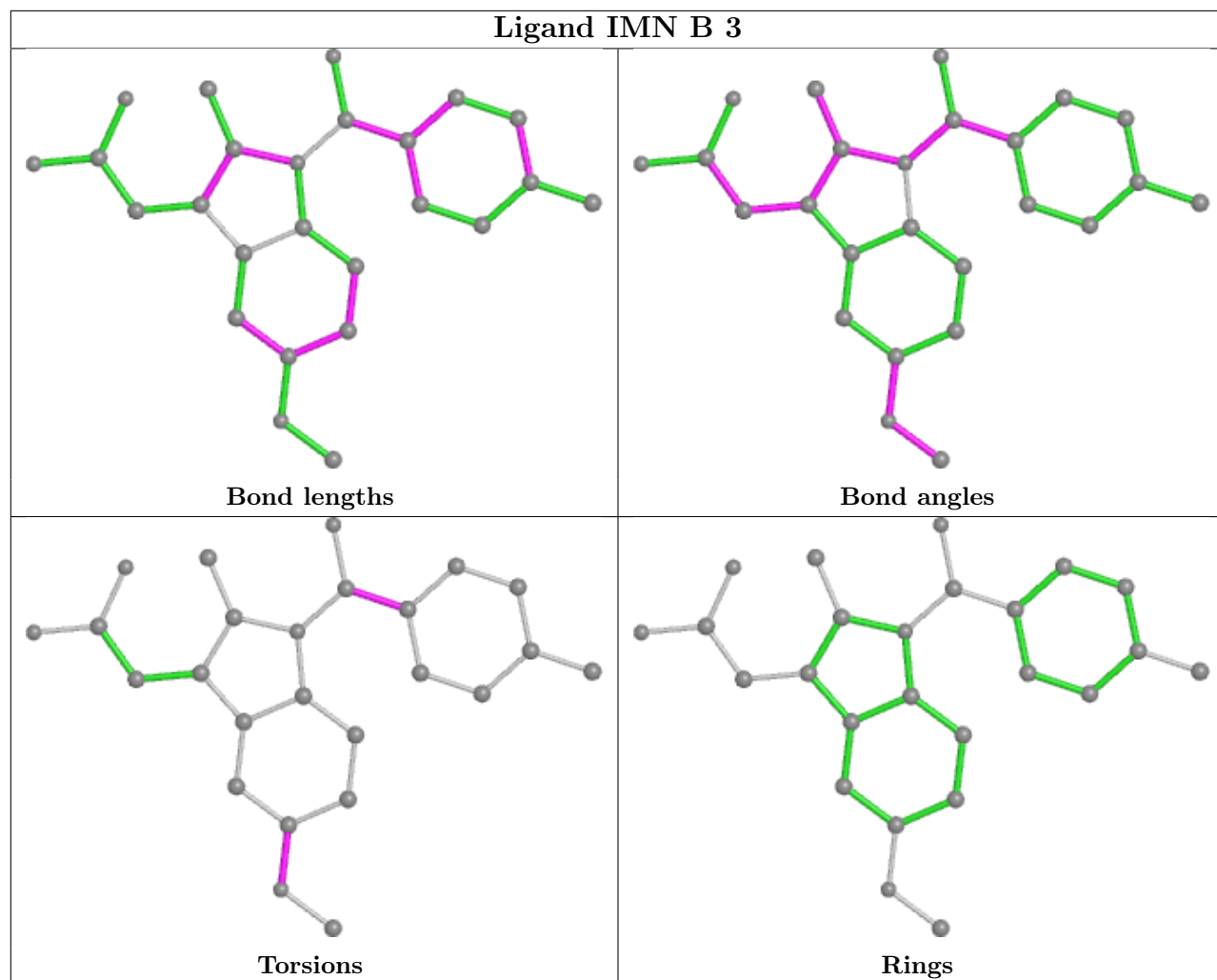
3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	NRO	5	0
3	A	2	IMN	3	0
3	B	3	IMN	4	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%)	0.81	31 (11%) 5 8	28, 43, 79, 96	0
1	B	251/287 (87%)	0.84	39 (15%) 2 3	28, 45, 79, 84	0
All	All	525/574 (91%)	0.83	70 (13%) 3 5	28, 44, 79, 96	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	270	LEU	10.4
1	A	269	PRO	9.3
1	A	266	HIS	8.3
1	A	265	LYS	8.0
1	A	275	LYS	7.5
1	A	268	THR	6.6
1	B	456	ILE	5.8
1	A	242	THR	5.7
1	B	461	THR	5.5
1	A	273	GLN	5.4
1	B	275	LYS	5.0
1	B	460	GLU	4.8
1	A	243	ASP	4.8
1	B	264	PHE	4.6
1	B	209	ALA	4.5
1	A	264	PHE	4.5
1	B	240	LYS	4.5
1	A	358	LYS	4.5
1	A	263	LYS	4.3
1	B	261	LYS	4.2
1	B	260	ASP	4.2
1	B	451	GLN	4.1
1	B	263	LYS	4.1
1	A	204	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	205	ASN	3.9
1	A	267	ILE	3.7
1	A	272	GLU	3.7
1	B	459	THR	3.7
1	B	458	LYS	3.6
1	B	207	GLU	3.5
1	B	436	LEU	3.5
1	B	455	VAL	3.5
1	A	203	GLN	3.5
1	B	359	PRO	3.4
1	B	262	ILE	3.2
1	B	454	GLN	3.1
1	B	232	LYS	3.0
1	B	357	ARG	2.9
1	B	339	VAL	2.9
1	B	238	THR	2.9
1	B	256	MET	2.9
1	A	271	GLN	2.8
1	A	274	SER	2.8
1	B	239	GLY	2.8
1	B	283	GLN	2.8
1	A	257	MET	2.8
1	B	355	SER	2.7
1	B	327	TYR	2.7
1	B	361	GLY	2.7
1	A	401	LEU	2.7
1	B	358	LYS	2.6
1	A	256	MET	2.6
1	A	444	GLN	2.6
1	A	287	PHE	2.5
1	A	427	GLU	2.5
1	A	260	ASP	2.5
1	A	261	LYS	2.5
1	A	252	MET	2.4
1	A	285	CYS	2.4
1	B	452	LEU	2.3
1	B	326	ILE	2.3
1	B	341	ILE	2.3
1	B	439	MET	2.3
1	B	285	CYS	2.3
1	B	328	THR	2.2
1	B	276	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	326	ILE	2.1
1	B	453	LEU	2.1
1	A	330	LEU	2.1
1	B	340	LEU	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](#)

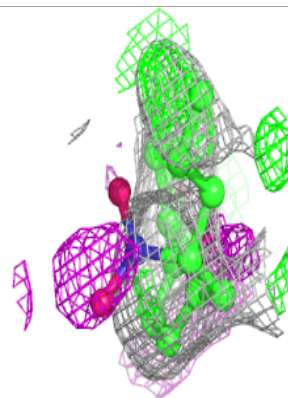
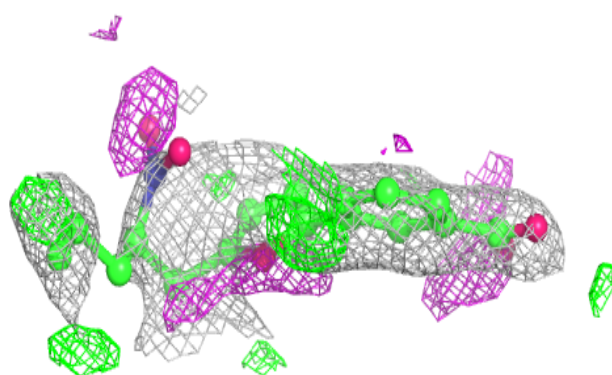
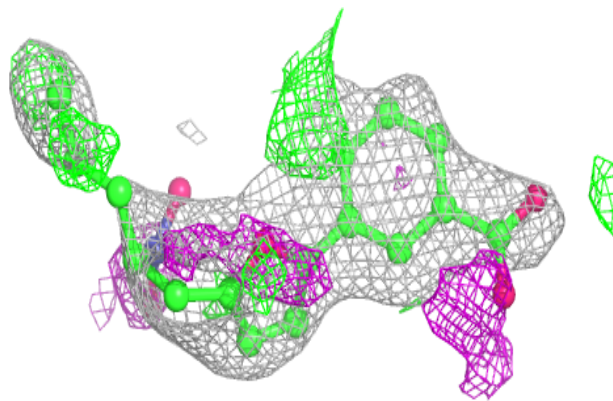
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists 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	NRO	A	1	22/22	0.58	0.36	77,80,83,84	0
3	IMN	B	3	25/25	0.66	0.28	76,79,81,82	0
3	IMN	A	2	25/25	0.73	0.23	53,59,64,64	0

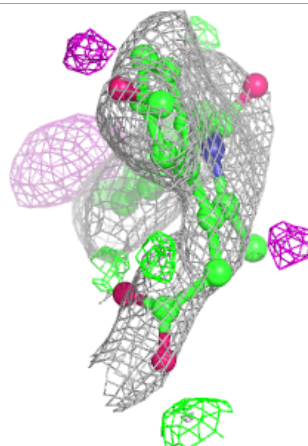
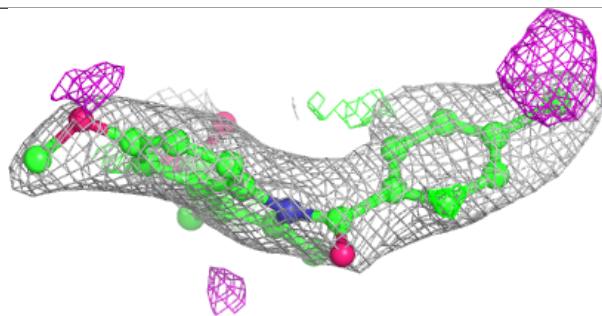
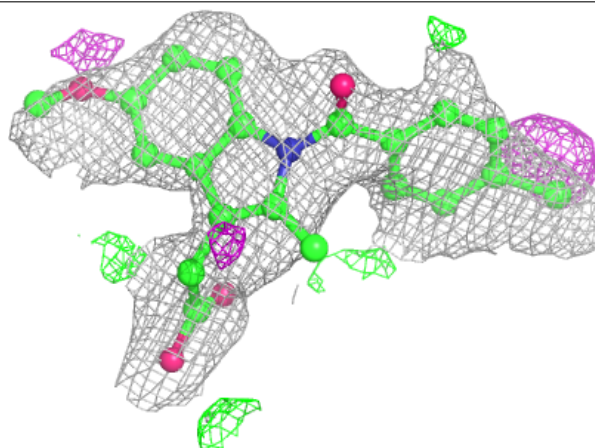
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

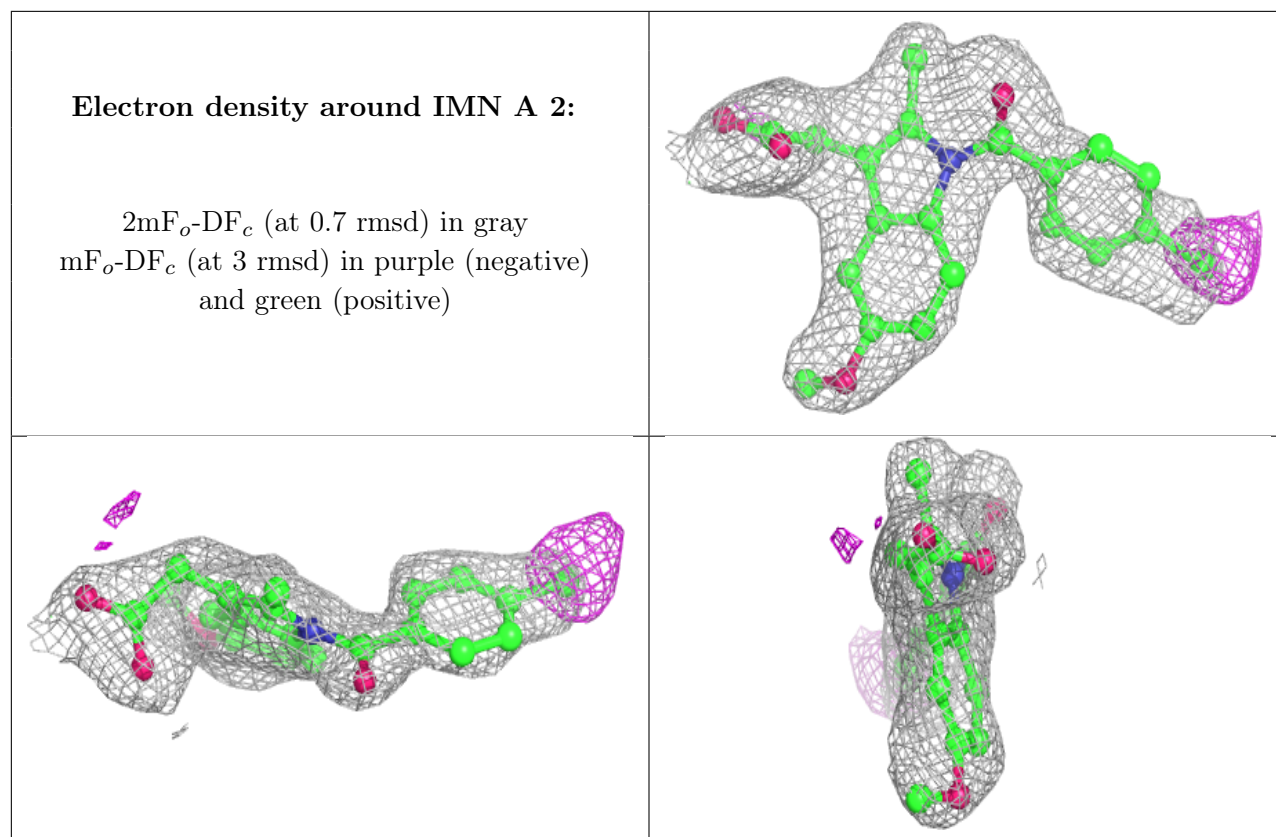
Electron density around NRO A 1:

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

**Electron density around IMN 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.