WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Dec 10, 2023 – 10:36 pm GMT

PDB ID : 2J14
Title : 3,4,5-Trisubstituted Isoxazoles as Novel PPARdelta Agonists: Part2
Authors : Epple, R.; Azimioara, M.; Russo, R.; Xie, Y.; Wang, X.; Cow, C.; Wityak, J.; Karanewsky, D.; Bursulaya, B.; Kreusch, A.; Tuntland, T.; Gerken, A.; Iskandar, M.; Saez, E.; Seidel, H.M.; Tian, S.S.
Deposited on : 2006-08-08
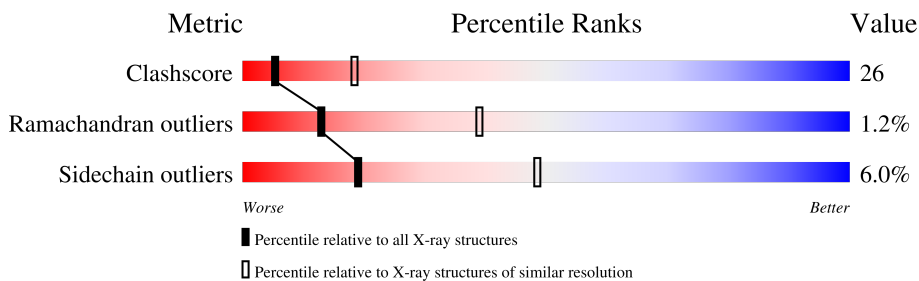Resolution : 2.80 Å(reported)

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 2.80 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	Percentile Ranks	Value
Clashscore		26
Ramachandran outliers		1.2%
Sidechain outliers		6.0%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	285	47% 40% • 11%
1	B	285	45% 39% • 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GNI	A	1440	-	-	X	-
2	GNI	B	1439	-	-	X	-

WORLD WIDE
PDB
PROTEIN DATA BANK

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4273 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 DELTA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	0	1
			2044	1321	343	371	9			
1	B	252	Total	C	N	O	S	0	0	1
			2030	1316	342	363	9			

- Molecule 2 is (3-{4-[2-(2,4-DICHLORO-PHENOXY)-ETHYLCARBAMOYL]-5-PHE NYL-ISOXAZOL-3-YL}-PHENYL)-ACETIC ACID (three-letter code: GNI) (formula: $C_{26}H_{20}Cl_2N_2O_5$).
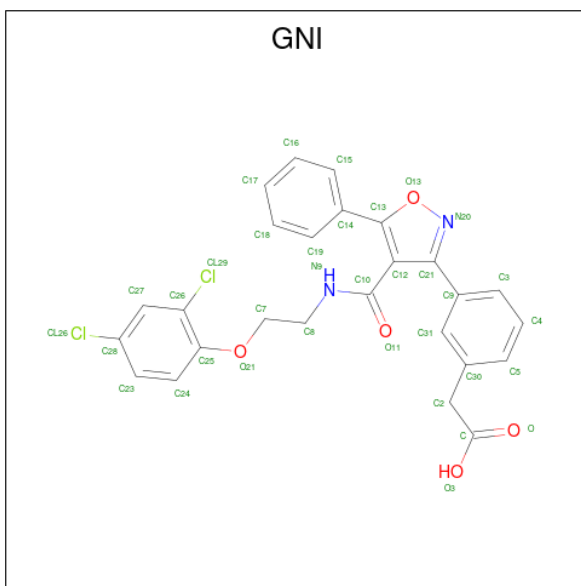
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			35	26	2	2	5		
2	B	1	Total	C	Cl	N	O	0	0
			35	26	2	2	5		

- Molecule 3 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	69	Total 69	O 69	0	0
3	B	60	Total 60	O 60	0	0

3 Residue-property plots ⓘ

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. 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. 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.

Note EDS was not executed.

• Molecule 1: PEROXISOME PROLIFERATOR-ACTIVATED RECEPTOR DELTA

Chain A:
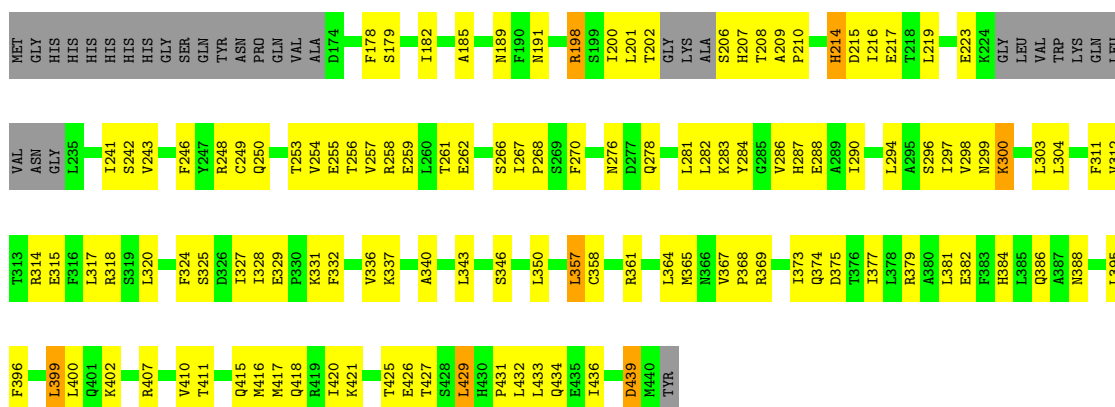
• Molecule 1: PEROXISOME PROLIFERATOR-ACTIVATED RECEPTOR DELTA

Chain B:
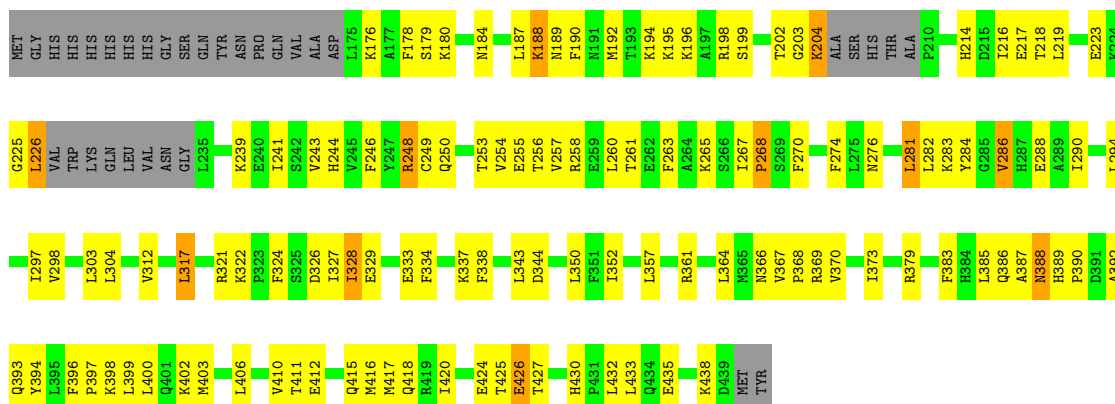
4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	39.38Å 93.39Å 92.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.70 – 2.80	Depositor
% Data completeness (in resolution range)	97.6 (46.70-2.80)	Depositor
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.224 , 0.284	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4273	wwPDB-VP
Average B, all atoms (Å^2)	35.0	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: GNI

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	0.33	0/2086	0.55	0/2816
1	B	0.34	0/2072	0.54	0/2793
All	All	0.34	0/4158	0.55	0/5609

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2044	0	2076	103	0
1	B	2030	0	2080	111	0
2	A	35	0	19	10	0
2	B	35	0	19	10	0
3	A	69	0	0	5	0
3	B	60	0	0	5	0
All	All	4273	0	4194	219	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 26.

All (219) 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:1439:GNI:H7C1	2:B:1439:GNI:CL29	1.95	1.03
1:A:216:ILE:HD12	1:A:216:ILE:H	1.40	0.85
1:B:281:LEU:HD13	1:B:364:LEU:HD21	1.60	0.83
1:B:255:GLU:HA	1:B:258:ARG:HD2	1.59	0.82
1:B:411:THR:O	1:B:415:GLN:HG3	1.79	0.82
1:A:253:THR:O	1:A:257:VAL:HG23	1.80	0.80
1:B:343:LEU:HD11	1:B:399:LEU:HD21	1.66	0.78
1:B:254:VAL:HG12	1:B:258:ARG:HE	1.48	0.78
1:B:364:LEU:HD13	1:B:370:VAL:HG21	1.66	0.77
1:A:411:THR:O	1:A:415:GLN:HG3	1.84	0.77
1:A:298:VAL:CG2	2:A:1440:GNI:H17	2.15	0.75
1:B:250:GLN:O	1:B:254:VAL:HG23	1.87	0.75
1:A:249:CYS:HA	2:A:1440:GNI:H7C1	1.68	0.75
1:B:297:ILE:HG12	1:B:304:LEU:HB2	1.67	0.74
1:B:298:VAL:HG21	2:B:1439:GNI:H17	1.67	0.74
1:B:198:ARG:O	1:B:202:THR:HG22	1.88	0.74
1:B:338:PHE:HD1	1:B:402:LYS:HD2	1.52	0.73
2:A:1440:GNI:H31	2:A:1440:GNI:O11	1.89	0.73
1:A:286:VAL:HG11	1:A:436:ILE:HD13	1.71	0.72
1:A:253:THR:HG21	2:A:1440:GNI:H2C1	1.72	0.71
1:B:254:VAL:HG22	1:B:433:LEU:HD11	1.72	0.70
1:A:327:ILE:HD11	1:A:417:MET:HE2	1.73	0.70
1:A:357:LEU:HD13	1:A:377:ILE:HD11	1.72	0.70
1:B:243:VAL:HG13	1:B:427:THR:HG22	1.74	0.69
1:B:398:LYS:HE2	3:B:2049:HOH:O	1.94	0.67
1:A:375:ASP:O	1:A:379:ARG:HG3	1.95	0.67
1:A:298:VAL:HG22	2:A:1440:GNI:H17	1.76	0.66
1:A:288:GLU:HG3	1:A:410:VAL:HG21	1.75	0.66
1:B:192:MET:HG2	1:B:297:ILE:HD12	1.79	0.65
1:A:298:VAL:HG12	1:A:299:ASN:N	2.13	0.64
1:B:322:LYS:HE2	1:B:326:ASP:OD1	1.99	0.63
1:B:203:GLY:O	1:B:204:LYS:HB2	1.99	0.63
1:A:415:GLN:O	1:A:418:GLN:HB3	1.98	0.62
1:B:281:LEU:CD1	1:B:364:LEU:HD21	2.28	0.62
2:B:1439:GNI:CL29	2:B:1439:GNI:C7	2.80	0.62
1:A:294:LEU:HB3	2:A:1440:GNI:H16	1.82	0.62
1:A:426:GLU:HB2	3:A:2065:HOH:O	1.99	0.62
1:B:202:THR:HG23	1:B:202:THR:O	1.99	0.62
1:B:282:LEU:O	1:B:286:VAL:HB	2.00	0.62
1:B:254:VAL:HG22	1:B:433:LEU:CD1	2.29	0.62
1:A:421:LYS:O	1:A:421:LYS:HD3	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:GLN:O	1:B:394:TYR:HB2	1.99	0.61
1:A:270:PHE:CE1	1:A:278:GLN:HG2	2.36	0.61
1:B:188:LYS:HD2	1:B:188:LYS:O	2.01	0.61
1:A:178:PHE:CE1	1:A:182:ILE:HD11	2.35	0.61
1:B:317:LEU:HD23	1:B:328:ILE:HD13	1.83	0.61
1:A:216:ILE:H	1:A:216:ILE:CD1	2.12	0.61
1:B:283:LYS:HE3	1:B:435:GLU:O	2.02	0.60
1:A:250:GLN:O	1:A:254:VAL:HG23	2.00	0.60
1:B:369:ARG:O	1:B:373:ILE:HG13	2.03	0.59
1:A:217:GLU:HG3	3:A:2013:HOH:O	2.03	0.59
1:B:219:LEU:O	1:B:223:GLU:HG2	2.03	0.59
1:A:255:GLU:O	1:A:259:GLU:HG3	2.03	0.58
1:B:288:GLU:HG3	1:B:410:VAL:HG21	1.85	0.58
1:A:216:ILE:HD12	1:A:216:ILE:N	2.16	0.58
1:A:276:ASN:HB2	1:A:365:MET:CE	2.34	0.58
1:B:286:VAL:O	1:B:290:ILE:HG13	2.04	0.57
1:B:253:THR:O	1:B:257:VAL:HG23	2.05	0.57
1:B:430:HIS:HB3	1:B:433:LEU:HD13	1.87	0.57
1:B:303:LEU:CD2	1:B:312:VAL:HB	2.35	0.57
1:B:366:ASN:O	1:B:370:VAL:HG23	2.05	0.57
1:B:430:HIS:HD2	1:B:432:LEU:H	1.53	0.56
1:A:253:THR:CG2	2:A:1440:GNI:H2C1	2.34	0.56
1:A:257:VAL:HG22	1:A:286:VAL:HG21	1.87	0.56
1:A:257:VAL:HG22	1:A:286:VAL:CG2	2.35	0.56
1:A:328:ILE:C	1:A:328:ILE:HD12	2.25	0.56
1:A:320:LEU:O	1:A:325:SER:HB3	2.06	0.56
1:B:195:LYS:HD3	3:B:2007:HOH:O	2.05	0.56
1:B:192:MET:HG2	1:B:297:ILE:CD1	2.36	0.56
1:B:267:ILE:HD12	1:B:268:PRO:N	2.20	0.56
1:A:243:VAL:HG13	1:A:427:THR:HG22	1.88	0.55
1:A:314:ARG:NE	1:A:318:ARG:HH21	2.04	0.55
1:A:185:ALA:O	1:A:189:ASN:ND2	2.36	0.55
1:A:324:PHE:O	1:A:327:ILE:HG22	2.07	0.55
1:A:395:LEU:O	1:A:399:LEU:HB2	2.06	0.54
1:B:239:LYS:HD2	1:B:426:GLU:OE2	2.07	0.54
1:B:196:LYS:O	1:B:199:SER:HB3	2.06	0.54
1:A:298:VAL:CG1	1:A:299:ASN:N	2.71	0.54
1:B:178:PHE:CE2	1:B:268:PRO:HG2	2.43	0.54
1:B:225:GLY:O	1:B:226:LEU:HB3	2.08	0.54
1:B:415:GLN:O	1:B:418:GLN:HB3	2.07	0.54
1:A:286:VAL:HG13	1:A:287:HIS:N	2.22	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:THR:CG2	1:B:290:ILE:HG12	2.38	0.53
1:A:254:VAL:HG13	1:A:432:LEU:HD23	1.89	0.53
1:B:267:ILE:HB	1:B:268:PRO:HD2	1.91	0.53
2:A:1440:GNI:O11	2:A:1440:GNI:C31	2.56	0.53
1:B:256:THR:HG21	1:B:290:ILE:HG12	1.89	0.53
1:B:190:PHE:HZ	1:B:260:LEU:HD23	1.74	0.53
1:B:298:VAL:HG22	1:B:303:LEU:CB	2.39	0.52
1:A:297:ILE:HG23	1:A:304:LEU:HB2	1.91	0.52
1:B:284:TYR:HB3	1:B:361:ARG:HD2	1.92	0.52
1:A:312:VAL:HG12	1:A:317:LEU:HD21	1.92	0.52
2:B:1439:GNI:O11	2:B:1439:GNI:H31	2.09	0.52
1:B:333:GLU:O	1:B:337:LYS:HE3	2.10	0.52
1:A:282:LEU:O	1:A:286:VAL:HB	2.09	0.52
1:B:198:ARG:HD2	1:B:198:ARG:N	2.26	0.51
1:B:298:VAL:HG22	1:B:303:LEU:HB2	1.91	0.51
1:A:201:LEU:HD21	1:A:304:LEU:HG	1.91	0.51
1:A:304:LEU:HD23	1:A:311:PHE:HD1	1.75	0.51
1:B:367:VAL:HB	1:B:368:PRO:HD3	1.93	0.51
1:A:327:ILE:CD1	1:A:417:MET:HE2	2.41	0.50
1:B:321:ARG:NH2	1:B:424:GLU:OE1	2.42	0.50
1:B:324:PHE:O	1:B:328:ILE:HG23	2.10	0.50
1:B:180:LYS:HG2	1:B:184:ASN:ND2	2.26	0.50
1:B:327:ILE:CD1	1:B:417:MET:HE2	2.40	0.50
1:A:421:LYS:HD3	1:A:421:LYS:C	2.33	0.50
1:B:254:VAL:HG13	1:B:432:LEU:HD23	1.93	0.50
2:B:1439:GNI:C14	2:B:1439:GNI:H9	2.24	0.50
1:A:198:ARG:NH1	1:A:296:SER:O	2.45	0.49
1:B:294:LEU:O	1:B:297:ILE:HG22	2.11	0.49
1:A:294:LEU:O	1:A:298:VAL:HG23	2.12	0.49
1:B:385:LEU:HD12	1:B:396:PHE:HD1	1.77	0.49
2:B:1439:GNI:O11	2:B:1439:GNI:C31	2.60	0.49
1:A:281:LEU:CD1	1:A:364:LEU:HD21	2.43	0.49
1:B:194:LYS:O	1:B:198:ARG:HG2	2.13	0.49
1:B:297:ILE:HG23	1:B:297:ILE:O	2.13	0.49
1:B:267:ILE:HD11	1:B:270:PHE:H	1.78	0.48
1:A:357:LEU:O	1:A:374:GLN:HB2	2.13	0.48
1:A:254:VAL:O	1:A:258:ARG:HG3	2.13	0.48
1:B:290:ILE:O	1:B:294:LEU:HG	2.14	0.48
1:B:263:PHE:CE2	1:B:352:ILE:HD11	2.48	0.48
1:A:328:ILE:HA	2:A:1440:GNI:O13	2.14	0.48
1:A:215:ASP:OD1	1:A:217:GLU:HB3	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:LEU:O	1:A:223:GLU:HG3	2.12	0.48
1:A:284:TYR:HB3	1:A:361:ARG:HD2	1.96	0.48
1:A:298:VAL:HG21	2:A:1440:GNI:H17	1.95	0.47
1:B:180:LYS:HG2	1:B:184:ASN:HD21	1.80	0.47
1:B:189:ASN:ND2	1:B:263:PHE:HA	2.29	0.47
1:B:303:LEU:HD23	1:B:312:VAL:HB	1.96	0.47
1:A:254:VAL:HG22	1:A:433:LEU:CD1	2.45	0.47
1:A:314:ARG:NE	1:A:318:ARG:NH2	2.63	0.47
1:A:258:ARG:HG2	1:A:258:ARG:HH11	1.80	0.47
1:A:241:ILE:HG23	1:A:242:SER:N	2.30	0.47
1:B:328:ILE:HG13	1:B:329:GLU:N	2.29	0.47
1:A:343:LEU:HD21	1:A:395:LEU:HD11	1.96	0.46
1:A:200:ILE:C	1:A:202:THR:H	2.19	0.46
1:A:276:ASN:HB2	1:A:365:MET:HE2	1.96	0.46
1:A:303:LEU:H	1:A:303:LEU:HD23	1.79	0.46
1:B:387:ALA:O	1:B:390:PRO:HD3	2.15	0.46
1:B:267:ILE:HD12	1:B:267:ILE:C	2.35	0.46
1:A:346:SER:HB2	1:A:384:HIS:HE1	1.81	0.46
1:A:416:MET:O	1:A:420:ILE:HG13	2.15	0.46
1:B:249:CYS:HA	2:B:1439:GNI:H7C2	1.98	0.46
1:A:179:SER:HA	1:A:350:LEU:HD21	1.98	0.46
1:B:412:GLU:O	1:B:416:MET:HG3	2.16	0.46
1:B:420:ILE:O	1:B:424:GLU:HB2	2.15	0.46
1:A:185:ALA:HB1	1:A:266:SER:CB	2.46	0.46
1:B:241:ILE:O	1:B:244:HIS:HB3	2.15	0.46
1:B:254:VAL:HG12	1:B:258:ARG:NE	2.23	0.46
1:A:209:ALA:HA	1:A:210:PRO:HD3	1.74	0.45
1:A:331:LYS:HD2	1:A:331:LYS:N	2.32	0.45
1:A:243:VAL:O	1:A:246:PHE:HB3	2.15	0.45
1:A:314:ARG:CZ	1:A:318:ARG:HH21	2.29	0.45
1:A:286:VAL:HG13	1:A:287:HIS:H	1.81	0.45
1:B:276:ASN:HD22	1:B:276:ASN:N	2.13	0.45
1:A:300:LYS:HE2	3:A:2034:HOH:O	2.17	0.45
1:A:191:ASN:ND2	1:A:259:GLU:OE1	2.48	0.45
1:B:179:SER:HA	1:B:350:LEU:HD21	1.99	0.45
1:A:250:GLN:OE1	1:A:429:LEU:HA	2.17	0.45
1:A:254:VAL:HG22	1:A:433:LEU:HD13	1.99	0.45
1:A:346:SER:CB	1:A:384:HIS:HE1	2.30	0.45
1:B:303:LEU:HD21	1:B:312:VAL:HB	1.97	0.45
1:B:261:THR:O	1:B:265:LYS:HG3	2.17	0.44
1:B:246:PHE:CE2	1:B:250:GLN:NE2	2.86	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:ILE:C	1:B:328:ILE:HD12	2.37	0.44
1:A:198:ARG:HA	1:A:198:ARG:HD2	1.81	0.44
1:A:284:TYR:CB	1:A:361:ARG:HD2	2.47	0.44
1:A:214:HIS:N	1:A:214:HIS:CD2	2.84	0.43
1:B:394:TYR:O	1:B:397:PRO:HG2	2.18	0.43
1:B:176:LYS:HB3	1:B:383:PHE:HE2	1.83	0.43
1:B:214:HIS:CD2	1:B:218:THR:HG21	2.53	0.43
1:B:246:PHE:HE1	1:B:417:MET:HE1	1.82	0.43
1:B:430:HIS:CD2	1:B:432:LEU:H	2.33	0.43
1:B:357:LEU:HD22	1:B:373:ILE:CG2	2.48	0.43
1:B:389:HIS:HB3	1:B:392:ALA:HB3	2.00	0.43
1:B:438:LYS:NZ	1:B:438:LYS:HB3	2.34	0.43
1:A:189:ASN:OD1	1:A:262:GLU:HB3	2.19	0.43
1:A:337:LYS:O	1:A:340:ALA:HB3	2.19	0.43
1:A:396:PHE:CZ	1:A:400:LEU:HD11	2.54	0.43
1:A:432:LEU:HD11	1:B:274:PHE:CE2	2.54	0.43
1:B:343:LEU:HD11	1:B:399:LEU:CD2	2.44	0.43
1:A:369:ARG:O	1:A:373:ILE:HG13	2.18	0.43
1:B:334:PHE:CZ	1:B:406:LEU:HD21	2.54	0.43
1:B:327:ILE:HG13	1:B:416:MET:CE	2.49	0.42
1:A:208:THR:HG21	3:A:2010:HOH:O	2.19	0.42
1:A:367:VAL:HB	1:A:368:PRO:HD3	2.01	0.42
1:B:194:LYS:HG3	1:B:198:ARG:HD3	1.99	0.42
1:A:202:THR:O	1:A:206:SER:HA	2.20	0.42
1:A:185:ALA:HB1	1:A:266:SER:HB3	2.01	0.42
1:B:223:GLU:HA	1:B:223:GLU:OE1	2.19	0.42
1:A:312:VAL:HG12	1:A:317:LEU:CD2	2.49	0.42
1:A:261:THR:HG21	1:B:274:PHE:CE1	2.54	0.42
1:B:216:ILE:H	1:B:216:ILE:HG13	1.70	0.42
1:B:294:LEU:HB3	2:B:1439:GNI:H16	2.02	0.42
1:B:265:LYS:HE2	3:B:2020:HOH:O	2.20	0.42
1:B:379:ARG:NH1	3:B:2040:HOH:O	2.53	0.41
1:A:358:CYS:O	1:A:361:ARG:HG2	2.21	0.41
1:A:364:LEU:HB2	1:A:367:VAL:HG22	2.01	0.41
1:A:431:PRO:HA	1:A:434:GLN:HB2	2.02	0.41
1:B:400:LEU:O	1:B:403:MET:HB2	2.21	0.41
1:A:402:LYS:HA	1:A:402:LYS:HD3	1.77	0.41
1:A:202:THR:HG22	1:A:202:THR:OXT	2.21	0.41
1:A:283:LYS:HD2	3:A:2067:HOH:O	2.19	0.41
1:B:248:ARG:HB3	2:B:1439:GNI:C23	2.50	0.41
1:B:284:TYR:CB	1:B:361:ARG:HD2	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:PHE:O	1:A:336:VAL:HG23	2.21	0.41
1:B:267:ILE:HB	1:B:268:PRO:CD	2.51	0.41
1:B:344:ASP:HB2	3:B:2032:HOH:O	2.20	0.41
1:A:214:HIS:CD2	1:A:214:HIS:H	2.39	0.41
1:B:202:THR:O	1:B:204:LYS:HD3	2.20	0.41
1:B:263:PHE:O	1:B:267:ILE:HG23	2.21	0.41
1:A:328:ILE:HD12	1:A:329:GLU:N	2.35	0.40
1:B:294:LEU:CB	2:B:1439:GNI:H16	2.51	0.40
1:A:256:THR:CG2	1:A:290:ILE:HG12	2.52	0.40
1:A:367:VAL:N	1:A:368:PRO:CD	2.85	0.40
1:A:350:LEU:HD13	1:A:381:LEU:HA	2.03	0.40
1:B:225:GLY:O	1:B:226:LEU:HD23	2.21	0.40
1:B:267:ILE:HD11	1:B:270:PHE:HB2	2.02	0.40
1:B:388:ASN:O	1:B:388:ASN:ND2	2.55	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	248/285 (87%)	228 (92%)	15 (6%)	5 (2%)	7	24
1	B	246/285 (86%)	227 (92%)	18 (7%)	1 (0%)	34	66
All	All	494/570 (87%)	455 (92%)	33 (7%)	6 (1%)	13	39

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	207	HIS
1	A	300	LYS
1	A	439	ASP
1	B	268	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	425	THR
1	A	268	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	225/251 (90%)	212 (94%)	13 (6%)	20	50
1	B	223/251 (89%)	209 (94%)	14 (6%)	18	46
All	All	448/502 (89%)	421 (94%)	27 (6%)	19	48

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	198	ARG
1	A	214	HIS
1	A	248	ARG
1	A	267	ILE
1	A	315	GLU
1	A	357	LEU
1	A	382	GLU
1	A	386	GLN
1	A	388	ASN
1	A	399	LEU
1	A	407	ARG
1	A	429	LEU
1	A	439	ASP
1	B	187	LEU
1	B	188	LYS
1	B	204	LYS
1	B	217	GLU
1	B	226	LEU
1	B	248	ARG
1	B	281	LEU
1	B	286	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	317	LEU
1	B	328	ILE
1	B	386	GLN
1	B	388	ASN
1	B	425	THR
1	B	426	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	ASN
1	A	214	HIS
1	A	221	GLN
1	A	384	HIS
1	A	388	ASN
1	A	401	GLN
1	A	418	GLN
1	A	430	HIS
1	B	184	ASN
1	B	191	ASN
1	B	276	ASN
1	B	278	GLN
1	B	388	ASN
1	B	401	GLN
1	B	418	GLN
1	B	430	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	GNI	B	1439	-	31,38,38	0.82	0	36,52,52	1.54	5 (13%)
2	GNI	A	1440	-	31,38,38	0.82	0	36,52,52	0.91	1 (2%)

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	GNI	B	1439	-	-	4/11/23/23	0/4/4/4
2	GNI	A	1440	-	-	4/11/23/23	0/4/4/4

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1439	GNI	O21-C25-C26	5.85	123.62	116.40
2	B	1439	GNI	O21-C25-C24	-3.16	117.13	123.97
2	B	1439	GNI	C7-C8-N9	-2.66	105.54	111.83
2	B	1439	GNI	C25-C26-CL29	2.34	122.17	119.43
2	B	1439	GNI	O-C-C2	-2.22	116.70	123.04
2	A	1440	GNI	O-C-C2	-2.22	116.71	123.04

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1439	GNI	C26-C25-O21-C7
2	B	1439	GNI	C24-C25-O21-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	1440	GNI	C26-C25-O21-C7
2	A	1440	GNI	O3-C-C2-C30
2	B	1439	GNI	O3-C-C2-C30
2	A	1440	GNI	O-C-C2-C30
2	B	1439	GNI	O-C-C2-C30
2	A	1440	GNI	C24-C25-O21-C7

There are no ring outliers.

2 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1439	GNI	10	0
2	A	1440	GNI	10	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 then 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.

Ligand GNI B 1439

Bond lengths

Bond angles

Torsions

Rings

Ligand GNI A 1440

Bond lengths

Bond angles

Torsions

Rings
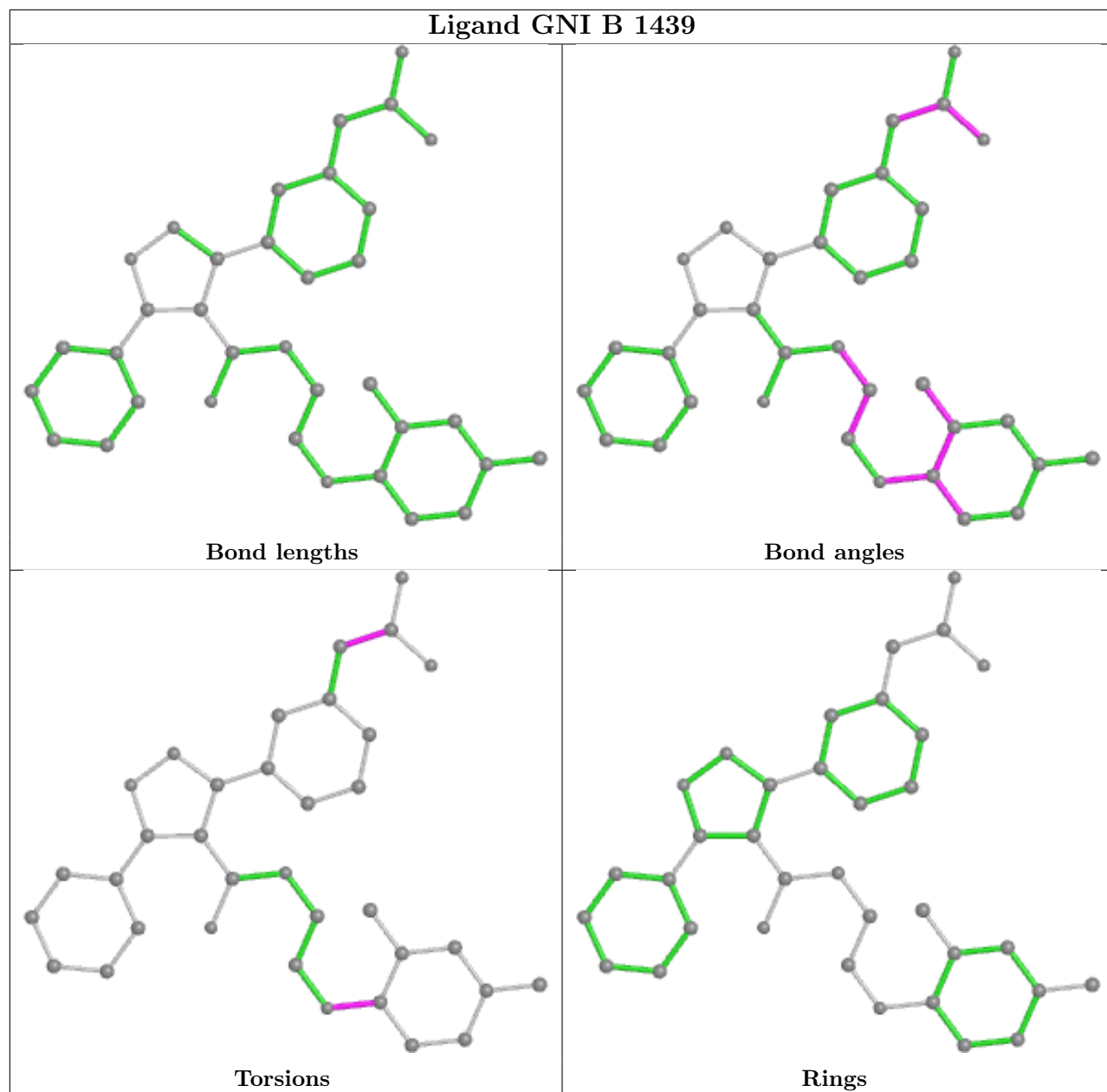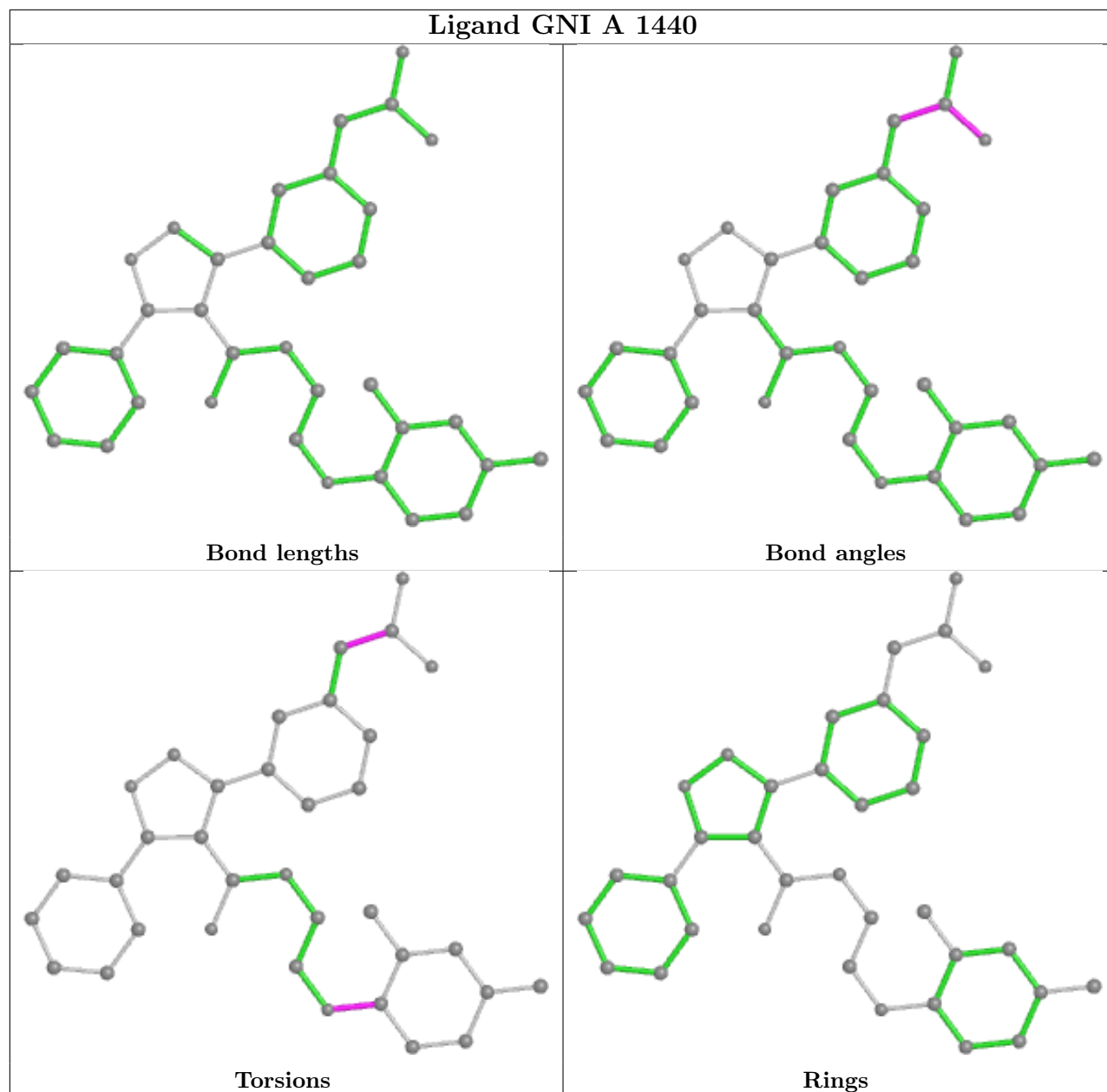
5.7 Other polymers ⓘ

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.