WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Oct 18, 2023 – 02:07 AM EDT

PDB ID	:	1LNY
Title	:	Crystal structure of the recombinant mouse-muscle adenylosuccinate synthetase complexed with 6-phosphoryl-IMP, GDP and Mg
Authors	:	Iancu, C.V.; Borza, T.; Fromm, H.J.; Honzatko, R.B.
Deposited on	:	2002-05-04
Resolution	:	2.20 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

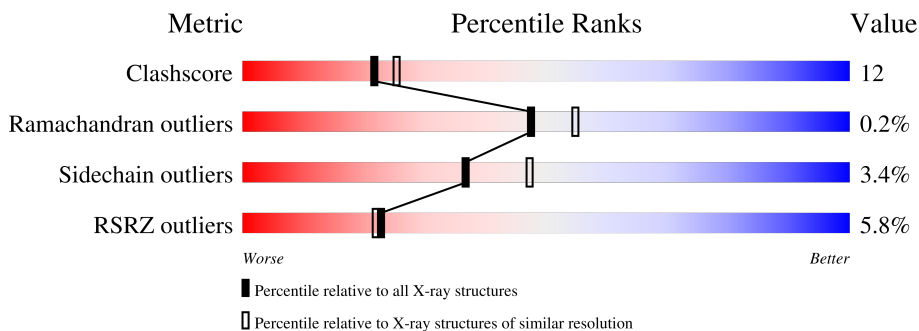|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.20 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		12
Ramachandran outliers		0.2%
Sidechain outliers		3.4%
RSRZ outliers		5.8%

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	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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% 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	457	7% 70% 22% · 6%
1	B	457	4% 70% 22% · 6%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 7130 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 Adenylosuccinate Synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	430	Total 3348	C 2130	N 588	O 618	S 12	0	0	0
1	B	431	Total 3353	C 2133	N 589	O 619	S 12	0	0	0

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Mg 1	0	0
2	B	1	Total 1	Mg 1	0	0

- Molecule 3 is 6-O-PHOSPHORYL INOSINE MONOPHOSPHATE (three-letter code: IMO) (formula: $C_{10}H_{14}N_4O_{11}P_2$).
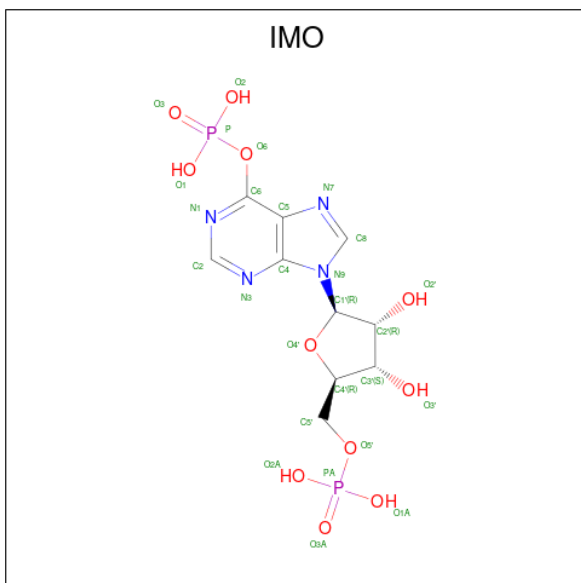
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	4	11	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	4	11	2		

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).
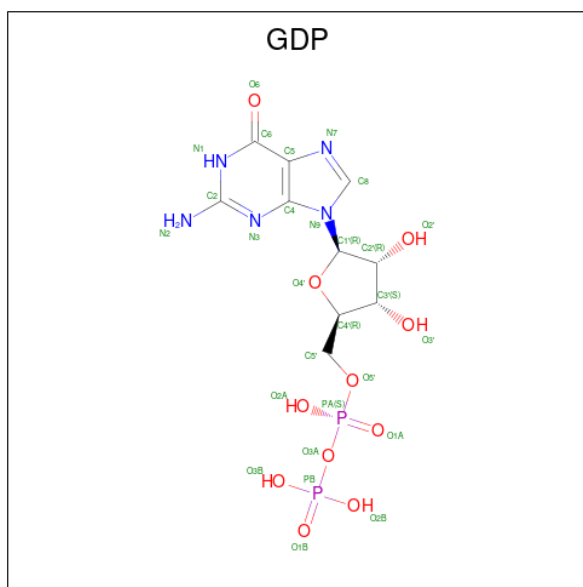
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
4	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	161	Total	O	0	0
			161	161		
5	B	156	Total	O	0	0
			156	156		

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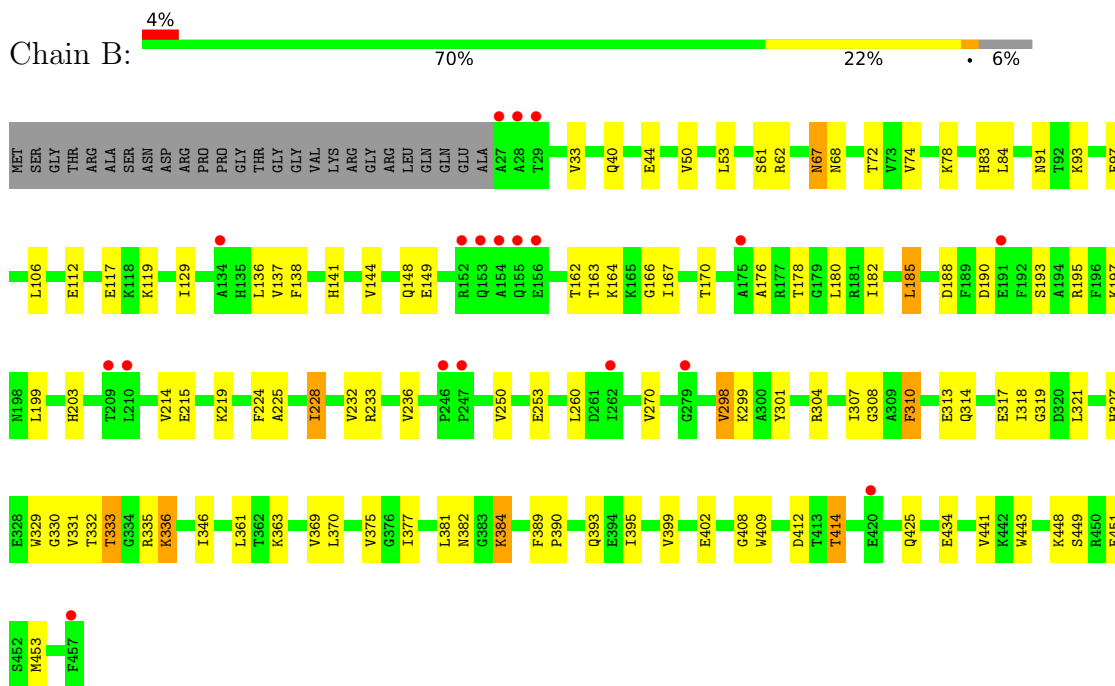 graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above 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: Adenylosuccinate Synthetase
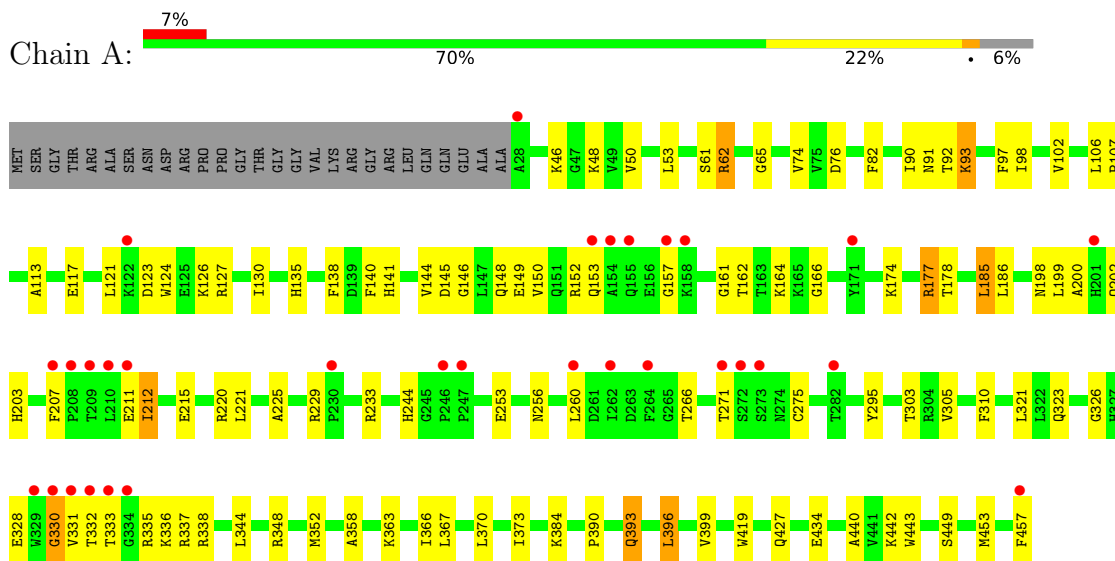
- Molecule 1: Adenylosuccinate Synthetase

4   Data and refinement statistics   ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	128.50Å 70.12Å 105.13Å 90.00° 90.46° 90.00°	Depositor
Resolution (Å)	5.00 – 2.20 40.52 – 2.15	Depositor EDS
% Data completeness (in resolution range)	(Not available) (5.00-2.20) 96.1 (40.52-2.15)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 2.16Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.207 , 0.259 0.202 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	36.0	Xtriage
Anisotropy	0.531	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 44.2	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.000 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.000 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.006 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.007 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7130	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.49% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, IMO, GDP

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	0.32	0/3418	0.60	0/4621
1	B	0.34	0/3423	0.60	0/4628
All	All	0.33	0/6841	0.60	0/9249

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	3348	0	3354	81	0
1	B	3353	0	3359	81	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	10	0	0
3	B	27	0	10	1	0
4	A	28	0	12	1	0
4	B	28	0	12	3	0
5	A	161	0	0	4	0
5	B	156	0	0	1	0
All	All	7130	0	6757	161	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 12.

All (161) 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:62:ARG:HB3	1:A:62:ARG:HH11	1.11	1.16
1:B:162:THR:HG22	1:B:164:LYS:H	1.13	1.12
1:A:162:THR:HG22	1:A:164:LYS:H	1.07	1.10
1:A:62:ARG:HB3	1:A:62:ARG:NH1	1.88	0.88
1:A:162:THR:HG22	1:A:164:LYS:N	1.89	0.87
1:B:330:GLY:HA3	1:B:333:THR:HG23	1.60	0.84
1:A:178:THR:HG22	1:A:199:LEU:HD13	1.60	0.81
1:A:178:THR:CG2	1:A:199:LEU:HD13	2.12	0.80
1:B:162:THR:HG22	1:B:164:LYS:N	1.98	0.75
1:A:148:GLN:O	1:A:152:ARG:HG3	1.86	0.75
1:A:62:ARG:HH11	1:A:62:ARG:CB	1.97	0.74
1:A:233:ARG:HG3	1:A:233:ARG:HH11	1.54	0.72
1:A:352:MET:HE1	1:B:236:VAL:HG12	1.69	0.72
1:B:144:VAL:O	1:B:148:GLN:HG3	1.90	0.72
1:B:412:ASP:OD2	1:B:414:THR:HB	1.89	0.72
1:B:409:TRP:HB3	1:B:425:GLN:HB2	1.73	0.71
1:A:113:ALA:O	1:A:117:GLU:HG3	1.93	0.69
1:B:40:GLN:HE22	1:B:299:LYS:H	1.41	0.69
1:B:304:ARG:HG2	1:B:304:ARG:HH11	1.59	0.67
1:A:140:PHE:O	1:A:144:VAL:HG23	1.94	0.67
1:B:62:ARG:HH21	1:B:62:ARG:HG3	1.59	0.66
1:A:153:GLN:O	1:A:157:GLY:HA2	1.96	0.65
1:B:434:GLU:HG3	1:B:441:VAL:HG23	1.79	0.65
1:B:176:ALA:HB3	1:B:178:THR:HG22	1.79	0.64
1:A:390:PRO:HG2	1:A:396:LEU:HD22	1.82	0.62
1:B:91:ASN:HD21	1:B:93:LYS:NZ	1.97	0.62
1:A:93:LYS:HD2	1:A:93:LYS:O	2.00	0.61
1:B:91:ASN:OD1	1:B:93:LYS:HG3	2.00	0.60
1:B:232:VAL:O	1:B:233:ARG:HG3	2.01	0.60
1:B:50:VAL:HG21	1:B:253:GLU:HG3	1.83	0.60
1:B:384:LYS:O	1:B:384:LYS:HD3	2.03	0.58
1:A:328:GLU:OE1	1:A:337:ARG:HD2	2.05	0.57
1:B:53:LEU:HD21	1:B:443:TRP:CZ2	2.40	0.56
1:B:67:ASN:HB3	1:B:84:LEU:HG	1.87	0.56
1:A:144:VAL:O	1:A:148:GLN:HG3	2.05	0.56
1:A:434:GLU:HG3	1:A:440:ALA:HA	1.88	0.55
1:A:106:LEU:HB2	1:A:107:PRO:HD3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:LEU:O	1:B:203:HIS:HD2	1.88	0.55
1:A:333:THR:HG23	1:A:335:ARG:H	1.70	0.55
1:B:215:GLU:O	1:B:219:LYS:HG3	2.07	0.55
1:B:233:ARG:HG3	1:B:233:ARG:HH11	1.71	0.55
1:B:331:VAL:HG13	1:B:332:THR:HG23	1.87	0.55
1:A:145:ASP:OD1	1:A:162:THR:HG21	2.06	0.55
1:A:198:ASN:O	1:A:202:GLN:HG3	2.07	0.55
1:B:185:LEU:HD22	1:B:225:ALA:HB2	1.88	0.54
1:B:336:LYS:O	1:B:336:LYS:HE2	2.08	0.54
1:A:135:HIS:CE1	1:A:174:LYS:HG3	2.43	0.54
1:A:74:VAL:HB	1:A:449:SER:HA	1.90	0.54
1:A:177:ARG:NH2	3:B:1455:IMO:O2A	2.40	0.53
1:B:381:LEU:O	1:B:382:ASN:HB2	2.08	0.53
1:B:106:LEU:HD22	1:B:228:ILE:HD12	1.90	0.53
1:B:448:LYS:HD2	4:B:1454:GDP:O2'	2.09	0.53
1:B:260:LEU:O	1:B:270:VAL:HB	2.08	0.53
1:B:166:GLY:O	1:B:170:THR:HG22	2.09	0.52
1:A:148:GLN:HG2	1:A:207:PHE:CZ	2.45	0.52
1:A:185:LEU:HD22	1:A:225:ALA:HB2	1.92	0.52
1:B:61:SER:HB3	1:B:97:PHE:HB3	1.92	0.52
1:A:98:ILE:HD12	1:A:130:ILE:CD1	2.39	0.52
1:A:146:GLY:O	1:A:150:VAL:HG23	2.09	0.52
1:B:377:ILE:HD11	1:B:402:GLU:OE1	2.09	0.52
1:A:419:TRP:CZ2	1:A:427:GLN:HB3	2.44	0.52
1:A:61:SER:HB3	1:A:97:PHE:HB3	1.91	0.52
1:B:106:LEU:HD13	1:B:224:PHE:HB3	1.92	0.52
1:A:82:PHE:HZ	1:A:90:ILE:HD11	1.75	0.51
1:A:186:LEU:HD21	1:A:229:ARG:HA	1.93	0.51
1:B:451:GLU:H	1:B:451:GLU:CD	2.12	0.51
1:B:93:LYS:O	1:B:93:LYS:HD2	2.11	0.51
1:A:233:ARG:HG3	1:A:233:ARG:NH1	2.19	0.51
1:B:162:THR:HG22	1:B:163:THR:N	2.26	0.51
1:A:149:GLU:HG2	5:A:610:HOH:O	2.10	0.50
1:A:50:VAL:HG21	1:A:253:GLU:HG3	1.91	0.50
1:B:193:SER:O	1:B:197:LYS:HG3	2.12	0.50
1:A:65:GLY:O	1:A:102:VAL:HG13	2.12	0.50
1:B:91:ASN:HD21	1:B:93:LYS:HZ2	1.59	0.50
1:A:140:PHE:HB3	1:A:212:ILE:HG12	1.94	0.49
1:B:62:ARG:HG3	1:B:62:ARG:NH2	2.26	0.49
1:B:167:ILE:O	1:B:170:THR:HG22	2.11	0.49
1:A:453:MET:HG3	5:A:744:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:GLU:O	1:A:212:ILE:HB	2.13	0.49
1:A:331:VAL:HG13	1:A:332:THR:N	2.27	0.49
1:A:390:PRO:HG2	1:A:396:LEU:CD2	2.42	0.49
1:B:40:GLN:HG2	1:B:346:ILE:HD11	1.94	0.49
1:A:323:GLN:NE2	1:A:336:LYS:HB3	2.28	0.49
1:A:344:LEU:O	1:A:348:ARG:HG3	2.13	0.49
1:B:78:LYS:HE2	1:B:119:LYS:O	2.12	0.49
1:B:138:PHE:O	1:B:141:HIS:HB2	2.14	0.48
1:B:180:LEU:HD21	1:B:195:ARG:HB3	1.94	0.48
1:B:233:ARG:HG3	1:B:233:ARG:NH1	2.28	0.48
1:B:317:GLU:HG3	1:B:318:ILE:N	2.28	0.48
1:B:72:THR:HB	4:B:1454:GDP:H3'	1.96	0.48
1:A:106:LEU:HD12	1:A:221:LEU:HD23	1.95	0.47
1:B:83:HIS:HB2	1:B:112:GLU:OE1	2.14	0.47
1:B:310:PHE:CG	1:B:313:GLU:HB2	2.49	0.47
1:B:408:GLY:O	1:B:425:GLN:HG2	2.14	0.47
1:B:149:GLU:HA	1:B:149:GLU:OE2	2.14	0.47
1:A:442:LYS:HE3	1:A:457:PHE:OXT	2.14	0.47
1:B:74:VAL:HB	1:B:449:SER:HA	1.96	0.46
1:A:48:LYS:NZ	1:A:453:MET:HG2	2.29	0.46
1:B:449:SER:HB2	1:B:451:GLU:OE2	2.16	0.46
1:A:53:LEU:HD21	1:A:443:TRP:CH2	2.50	0.46
1:B:333:THR:OG1	1:B:335:ARG:HG2	2.16	0.46
1:B:381:LEU:O	1:B:384:LYS:HG3	2.16	0.46
1:A:149:GLU:OE1	1:A:161:GLY:N	2.40	0.46
1:A:148:GLN:HG2	1:A:207:PHE:CE2	2.51	0.46
1:A:145:ASP:HB2	1:A:166:GLY:HA2	1.97	0.46
1:B:137:VAL:HG22	1:B:170:THR:HG21	1.96	0.46
1:B:321:LEU:HD23	1:B:370:LEU:HD21	1.98	0.46
1:A:91:ASN:OD1	1:A:93:LYS:HG3	2.16	0.45
1:A:295:TYR:CD1	1:A:358:ALA:HB3	2.51	0.45
1:B:214:VAL:HG23	1:B:215:GLU:N	2.31	0.45
1:A:203:HIS:HE1	5:A:765:HOH:O	1.98	0.45
1:A:266:THR:HB	1:A:393:GLN:HG3	1.97	0.45
1:A:393:GLN:HE21	1:A:393:GLN:HB3	1.61	0.45
1:B:136:LEU:HD21	1:B:182:ILE:HD13	1.99	0.45
1:B:314:GLN:O	1:B:319:GLY:HA3	2.17	0.45
1:A:46:LYS:O	1:A:50:VAL:HG23	2.16	0.45
1:A:200:ALA:HB1	1:A:212:ILE:HD13	1.99	0.45
1:A:185:LEU:CD2	1:A:225:ALA:HB2	2.47	0.45
1:B:304:ARG:HH11	1:B:304:ARG:CG	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:ILE:O	1:B:399:VAL:HG13	2.16	0.45
1:B:68:ASN:HB3	1:B:167:ILE:HG13	1.98	0.44
1:B:327:HIS:HA	1:B:329:TRP:CZ3	2.51	0.44
1:B:33:VAL:HG12	1:B:250:VAL:HB	1.99	0.44
1:A:363:LYS:HG2	4:A:1452:GDP:C5	2.53	0.44
1:B:117:GLU:C	1:B:119:LYS:H	2.20	0.44
1:B:185:LEU:CD2	1:B:225:ALA:HB2	2.47	0.43
1:B:162:THR:CG2	1:B:163:THR:N	2.80	0.43
1:B:363:LYS:HG2	4:B:1454:GDP:C5	2.54	0.43
1:A:91:ASN:HD21	1:A:93:LYS:HE3	1.83	0.43
1:A:145:ASP:OD2	1:A:162:THR:HG21	2.19	0.43
1:A:367:LEU:HD13	1:A:373:ILE:HD13	2.01	0.43
1:B:304:ARG:NH1	5:B:534:HOH:O	2.50	0.43
1:A:124:TRP:HA	1:A:127:ARG:NH1	2.33	0.43
1:A:138:PHE:O	1:A:141:HIS:HB2	2.19	0.43
1:A:321:LEU:HD23	1:A:370:LEU:HD21	2.01	0.42
1:A:326:GLY:HA2	1:A:366:ILE:CD1	2.49	0.42
1:A:140:PHE:CZ	1:A:199:LEU:HG	2.55	0.42
1:A:326:GLY:HA2	1:A:366:ILE:HD11	2.01	0.42
1:A:396:LEU:O	1:A:399:VAL:HG22	2.19	0.42
1:B:304:ARG:CG	1:B:304:ARG:NH1	2.82	0.42
1:A:303:THR:HA	1:A:338:ARG:O	2.20	0.42
1:B:389:PHE:HA	1:B:390:PRO:HD3	1.73	0.42
1:A:330:GLY:N	1:A:335:ARG:O	2.52	0.42
1:A:92:THR:HA	1:A:127:ARG:NE	2.35	0.42
1:A:305:VAL:HG22	1:A:337:ARG:HG2	2.02	0.41
1:A:256:ASN:HB2	1:A:275:CYS:SG	2.60	0.41
1:B:299:LYS:HB3	1:B:301:TYR:O	2.21	0.41
1:B:307:ILE:HG22	1:B:308:GLY:N	2.35	0.41
1:B:67:ASN:C	1:B:67:ASN:HD22	2.24	0.41
1:A:123:ASP:HB3	1:A:126:LYS:HD3	2.02	0.41
1:A:244:HIS:HE1	5:A:812:HOH:O	2.02	0.41
1:B:369:VAL:O	1:B:369:VAL:CG1	2.68	0.41
1:A:53:LEU:HD21	1:A:443:TRP:CZ2	2.56	0.41
1:A:260:LEU:O	1:A:271:THR:HG22	2.20	0.41
1:B:129:ILE:HD12	1:B:233:ARG:HD2	2.03	0.41
1:A:145:ASP:CG	1:A:162:THR:HG21	2.40	0.41
1:A:198:ASN:N	1:A:198:ASN:HD22	2.19	0.41
1:B:188:ASP:OD1	1:B:190:ASP:HB2	2.21	0.41
1:B:298:VAL:HG22	1:B:361:LEU:CD1	2.51	0.41
1:B:40:GLN:HE21	1:B:44:GLU:HG2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:LEU:O	1:B:382:ASN:CB	2.70	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	428/457 (94%)	405 (95%)	21 (5%)	2 (0%)	29	31
1	B	429/457 (94%)	407 (95%)	22 (5%)	0	100	100
All	All	857/914 (94%)	812 (95%)	43 (5%)	2 (0%)	47	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	ILE
1	A	330	GLY

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	354/373 (95%)	342 (97%)	12 (3%)	37	47
1	B	354/373 (95%)	342 (97%)	12 (3%)	37	47
All	All	708/746 (95%)	684 (97%)	24 (3%)	37	47

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	ARG
1	A	76	ASP
1	A	93	LYS
1	A	121	LEU
1	A	177	ARG
1	A	185	LEU
1	A	215	GLU
1	A	220	ARG
1	A	310	PHE
1	A	384	LYS
1	A	393	GLN
1	A	396	LEU
1	B	67	ASN
1	B	185	LEU
1	B	228	ILE
1	B	298	VAL
1	B	310	PHE
1	B	333	THR
1	B	336	LYS
1	B	375	VAL
1	B	384	LYS
1	B	393	GLN
1	B	414	THR
1	B	453	MET

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	153	GLN
1	A	198	ASN
1	A	203	HIS
1	A	217	GLN
1	A	323	GLN
1	A	382	ASN
1	B	40	GLN
1	B	64	GLN
1	B	67	ASN
1	B	155	GLN
1	B	198	ASN
1	B	203	HIS
1	B	217	GLN

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Mol	Chain	Res	Type
1	B	323	GLN
1	B	382	ASN
1	B	397	GLN
1	B	427	GLN
1	B	436	HIS
1	B	455	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 monosaccharides in this entry.

5.6   Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
4	GDP	B	1454	2	24,30,30	1.01	2 (8%)	30,47,47	0.80	2 (6%)
3	IMO	A	1451	2	24,29,29	2.70	2 (8%)	30,45,45	1.02	1 (3%)
4	GDP	A	1452	2	24,30,30	1.04	2 (8%)	30,47,47	0.81	2 (6%)
3	IMO	B	1455	2	24,29,29	2.70	2 (8%)	30,45,45	1.15	1 (3%)

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
4	GDP	B	1454	2	-	3/12/32/32	0/3/3/3
3	IMO	A	1451	2	-	0/9/31/31	0/3/3/3
4	GDP	A	1452	2	-	2/12/32/32	0/3/3/3
3	IMO	B	1455	2	-	0/9/31/31	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1455	IMO	O6-C6	-12.69	1.24	1.40
3	A	1451	IMO	O6-C6	-12.55	1.24	1.40
4	A	1452	GDP	C5-C6	-2.96	1.41	1.47
4	B	1454	GDP	C5-C6	-2.81	1.41	1.47
3	A	1451	IMO	P-O6	2.78	1.63	1.59
4	B	1454	GDP	C8-N7	-2.50	1.30	1.35
4	A	1452	GDP	C8-N7	-2.46	1.30	1.35
3	B	1455	IMO	C8-N7	-2.04	1.31	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1455	IMO	O6-C6-N1	4.73	125.67	116.56
3	A	1451	IMO	O6-C6-N1	3.98	124.21	116.56
4	A	1452	GDP	O6-C6-C5	2.07	128.42	124.37
4	A	1452	GDP	PA-O3A-PB	-2.06	125.77	132.83
4	B	1454	GDP	O6-C6-C5	2.02	128.31	124.37
4	B	1454	GDP	PA-O3A-PB	-2.01	125.92	132.83

There are no chirality outliers.

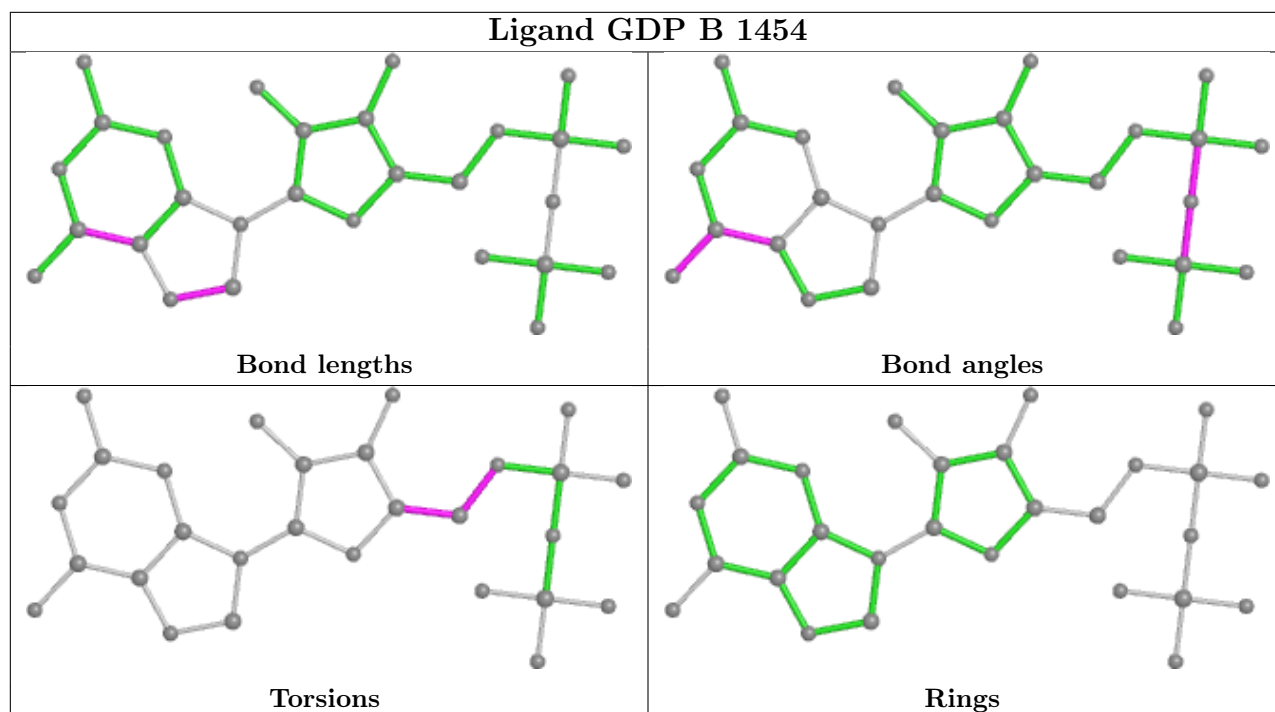All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1454	GDP	O4'-C4'-C5'-O5'
4	B	1454	GDP	C4'-C5'-O5'-PA
4	B	1454	GDP	C3'-C4'-C5'-O5'
4	A	1452	GDP	C5'-O5'-PA-O1A
4	A	1452	GDP	O4'-C4'-C5'-O5'

There are no ring outliers.
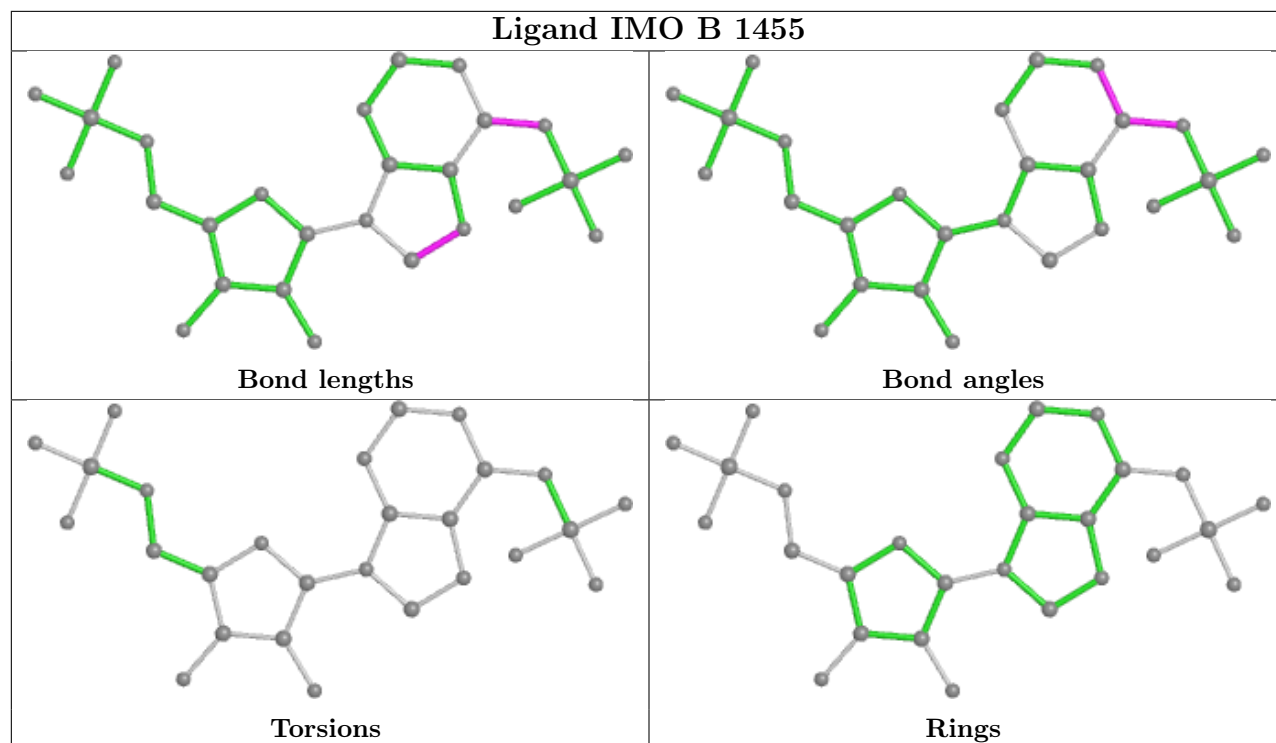
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1454	GDP	3	0
4	A	1452	GDP	1	0
3	B	1455	IMO	1	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 GDP B 1454

Ligand IMO A 1451

Bond lengths

Bond angles

Torsions

Rings

Ligand GDP A 1452

Bond lengths

Bond angles

Torsions

Rings

Ligand IMO B 1455

Bond lengths

Bond angles

Torsions

Rings
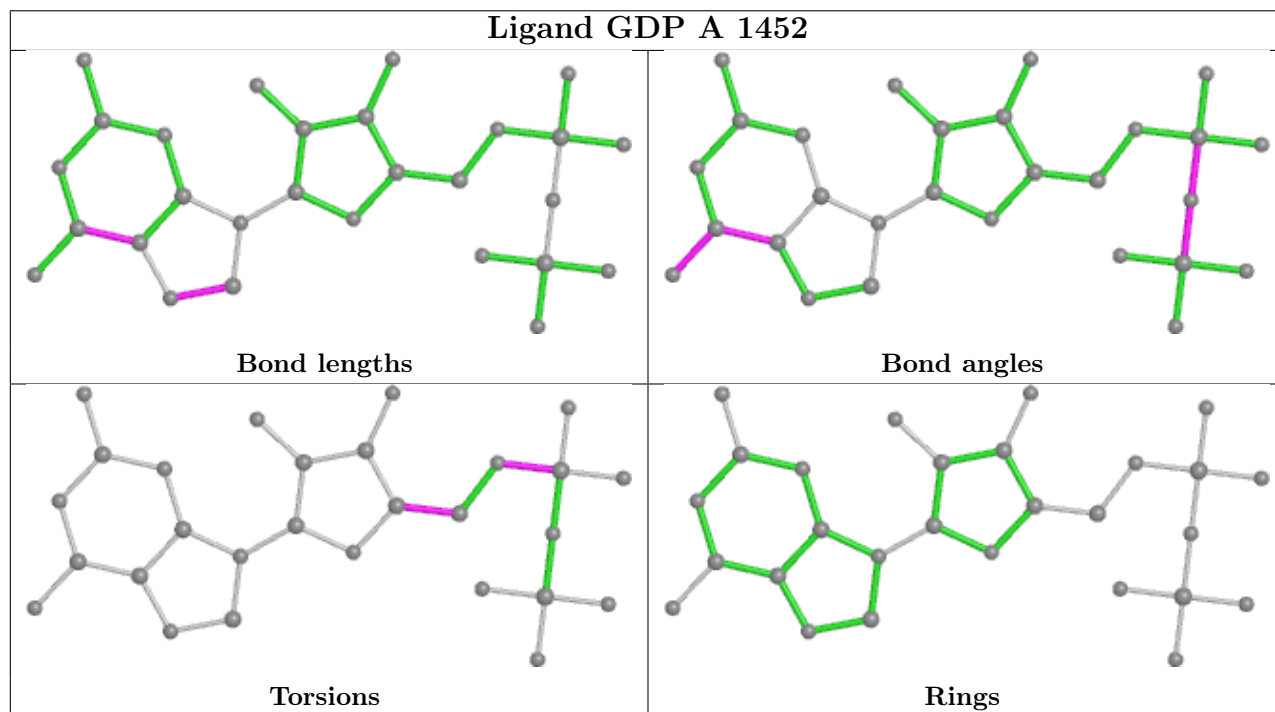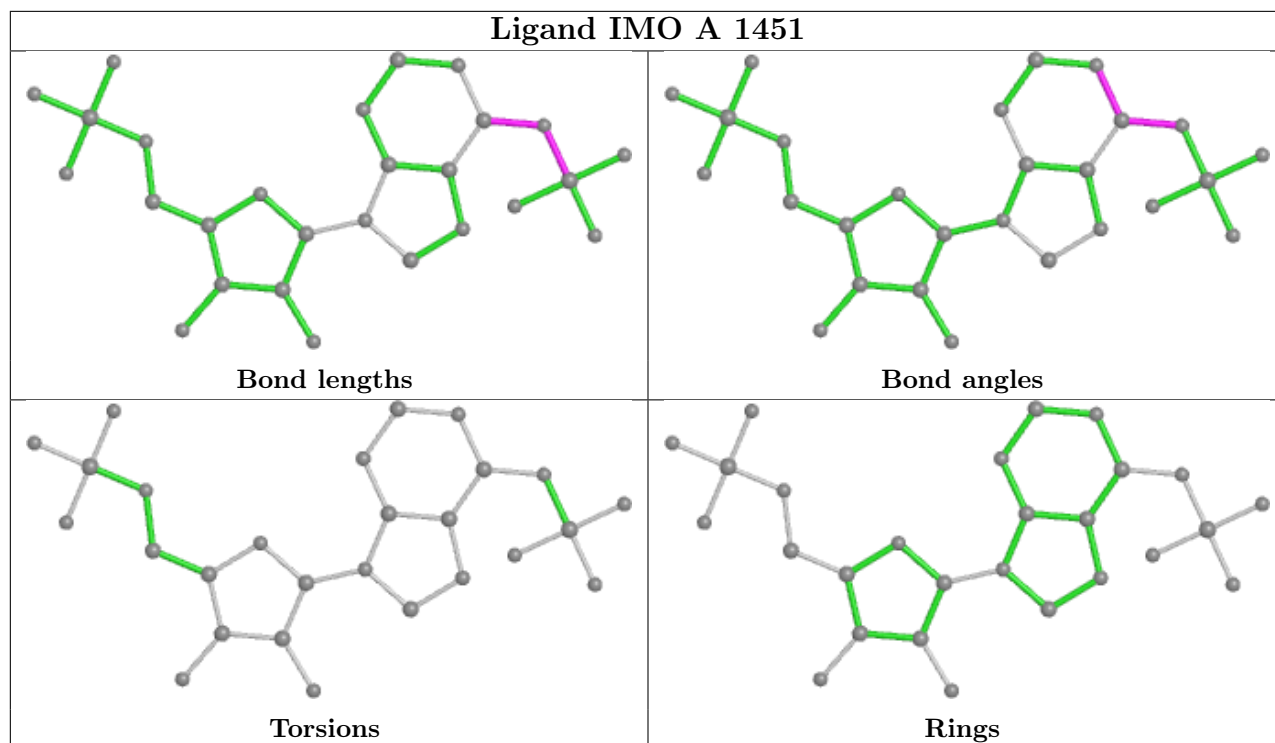
5.7 Other polymers ⓘ

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 ⓘ

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	430/457 (94%)	0.32	31 (7%)	15	14	25, 38, 61, 78	0
1	B	431/457 (94%)	0.16	19 (4%)	34	32	24, 36, 56, 74	0
All	All	861/914 (94%)	0.24	50 (5%)	23	22	24, 37, 60, 78	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	330	GLY	6.8
1	A	207	PHE	6.4
1	A	210	LEU	6.2
1	A	334	GLY	5.1
1	B	27	ALA	4.9
1	A	209	THR	4.9
1	B	28	ALA	4.9
1	A	28	ALA	4.9
1	B	154	ALA	4.6
1	B	156	GLU	4.3
1	A	155	GLN	4.2
1	A	332	THR	4.2
1	B	155	GLN	4.0
1	A	331	VAL	4.0
1	A	211	GLU	3.8
1	A	122	LYS	3.7
1	A	208	PRO	3.6
1	A	154	ALA	3.5
1	B	29	THR	3.3
1	A	201	HIS	3.3
1	A	260	LEU	3.1
1	A	457	PHE	3.1
1	A	246	PRO	3.0
1	A	262	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	157	GLY	2.9
1	A	329	TRP	2.8
1	B	247	PRO	2.8
1	A	171	TYR	2.7
1	A	273	SER	2.6
1	B	420	GLU	2.6
1	A	272	SER	2.5
1	A	333	THR	2.5
1	B	210	LEU	2.5
1	A	271	THR	2.4
1	B	175	ALA	2.3
1	B	209	THR	2.3
1	A	153	GLN	2.3
1	B	191	GLU	2.2
1	A	230	PRO	2.2
1	A	247	PRO	2.2
1	A	158	LYS	2.2
1	B	134	ALA	2.2
1	B	246	PRO	2.2
1	B	457	PHE	2.2
1	A	264	PHE	2.1
1	B	153	GLN	2.1
1	B	152	ARG	2.1
1	B	262	ILE	2.0
1	B	279	GLY	2.0
1	A	282	THR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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(Å²)	Q<0.9
2	MG	B	1456	1/1	0.91	0.06	34,34,34,34	0
3	IMO	B	1455	27/27	0.92	0.13	35,37,44,46	0
4	GDP	A	1452	28/28	0.94	0.11	30,34,37,40	0
3	IMO	A	1451	27/27	0.95	0.14	31,40,46,50	0
2	MG	A	1453	1/1	0.96	0.09	35,35,35,35	0
4	GDP	B	1454	28/28	0.96	0.11	27,33,36,37	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.
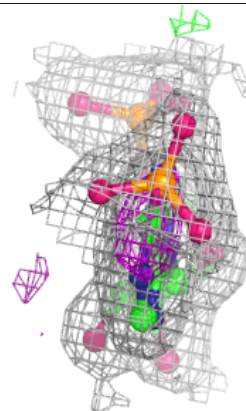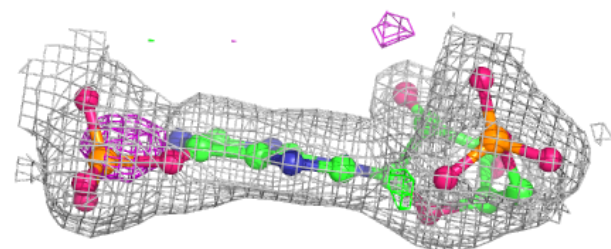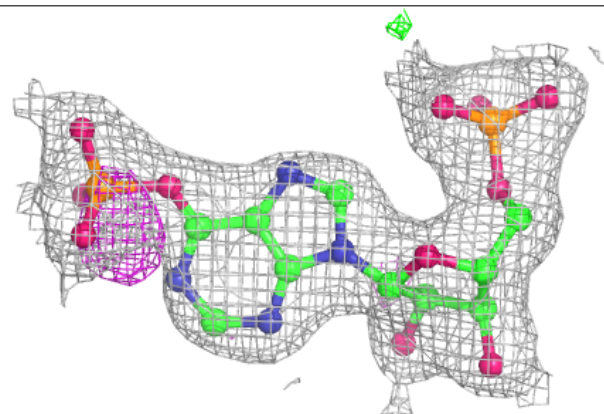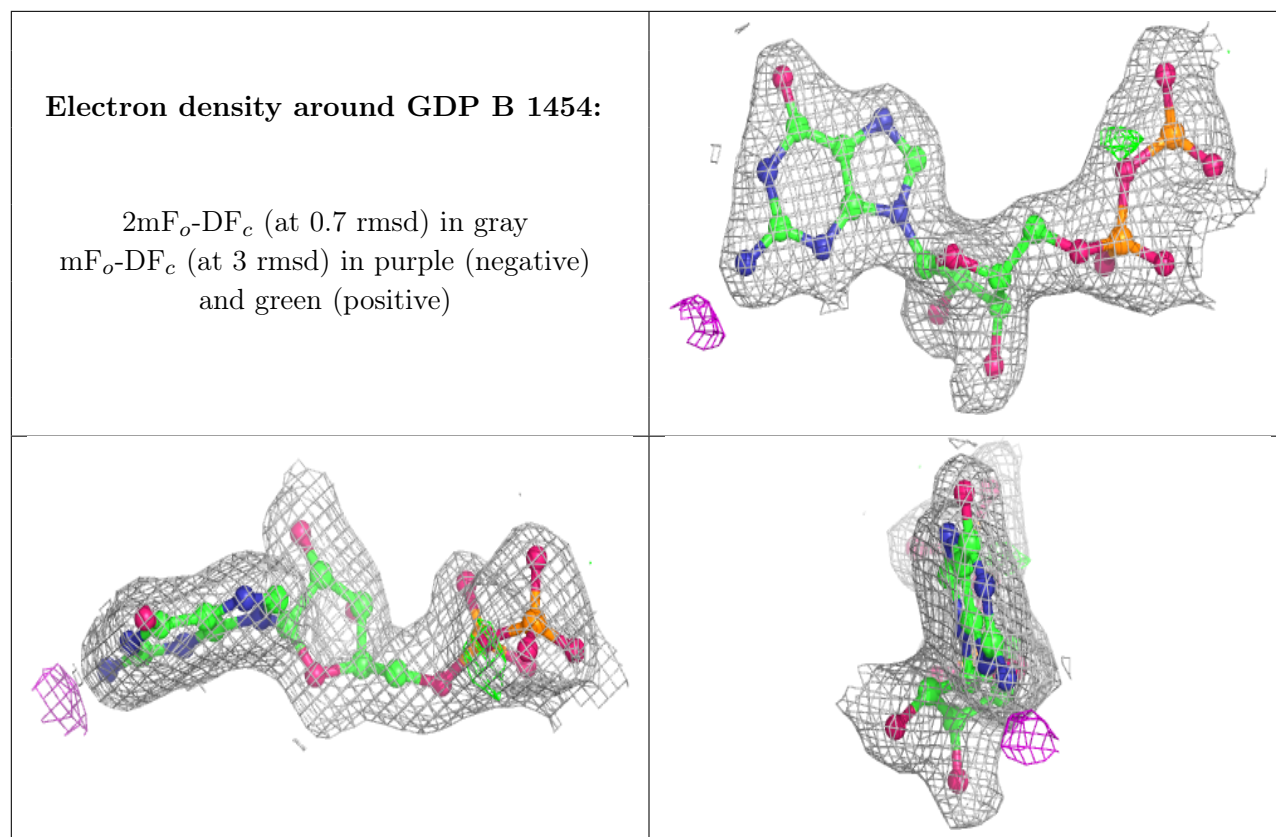
Electron density around IMO B 1455:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
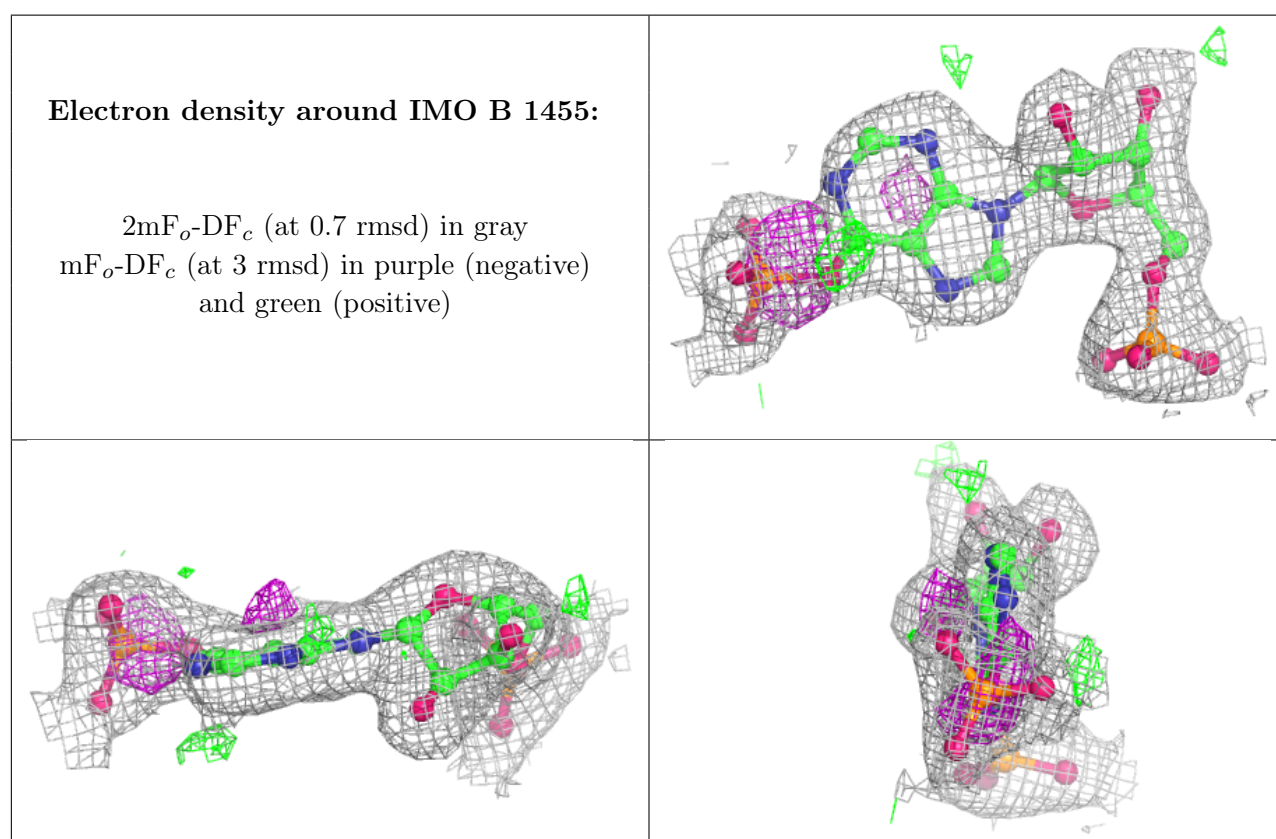
Electron density around GDP A 1452:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
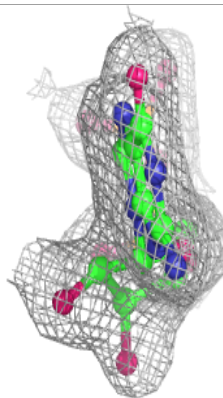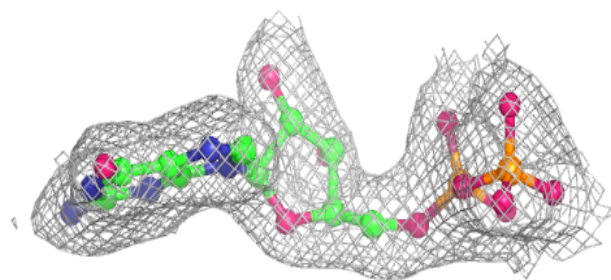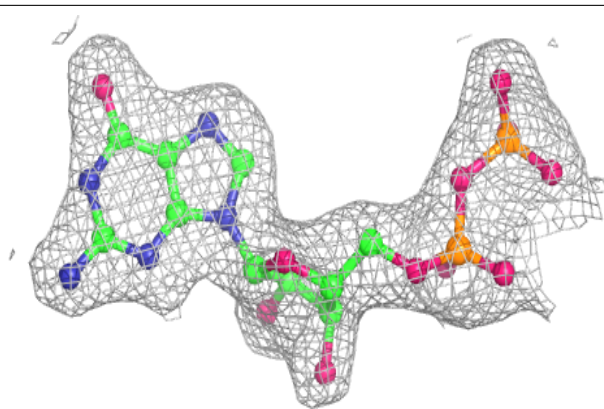
Electron density around IMO A 1451:

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 GDP B 1454:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.