



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:30 AM UTC

PDB ID : 6IO0 / pdb_00006io0
Title : Human IDH1 R132C mutant complexed with compound A.
Authors : Suzuki, M.; Baba, D.; Hanzawa, H.
Deposited on : 2018-10-29
Resolution : 2.20 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

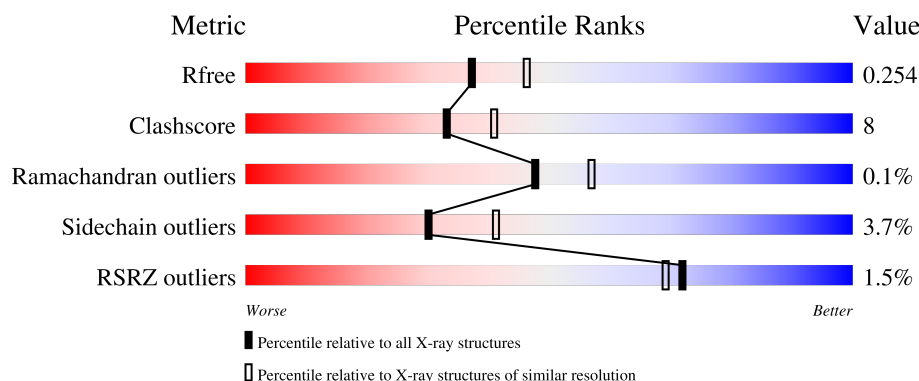
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 $\leq 5\%$. 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	414	 2% 84% 12% ..
1	B	414	 % 75% 20% ..

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
5	GOL	B	502	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6667 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.

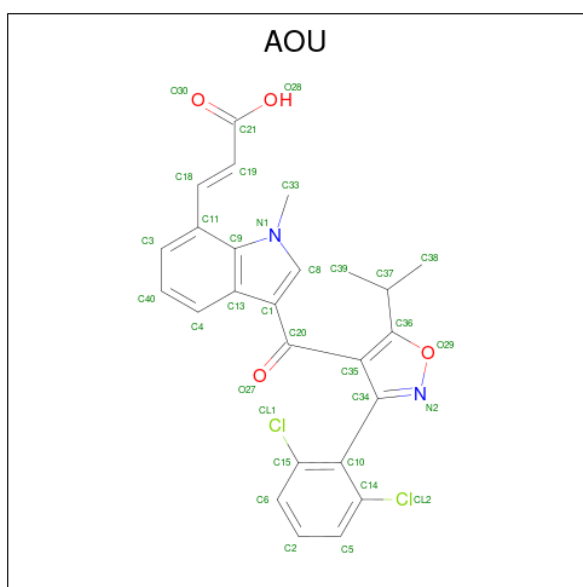
- Molecule 1 is a protein called Isocitrate dehydrogenase [NADP] cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	400	Total	C	N	O	S	0	1	0
			3080	1968	511	582	19			
1	B	400	Total	C	N	O	S	0	1	0
			3095	1975	514	587	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	132	CYS	ARG	engineered mutation	UNP O75874
B	132	CYS	ARG	engineered mutation	UNP O75874

- Molecule 2 is (2E)-3-{3-[3-(2,6-dichlorophenyl)-5-(propan-2-yl)-1,2-oxazole-4-carbonyl]-1-methyl-1H-indol-7-yl}prop-2-enoic acid (CCD ID: AOU) (formula: C₂₅H₂₀Cl₂N₂O₄).



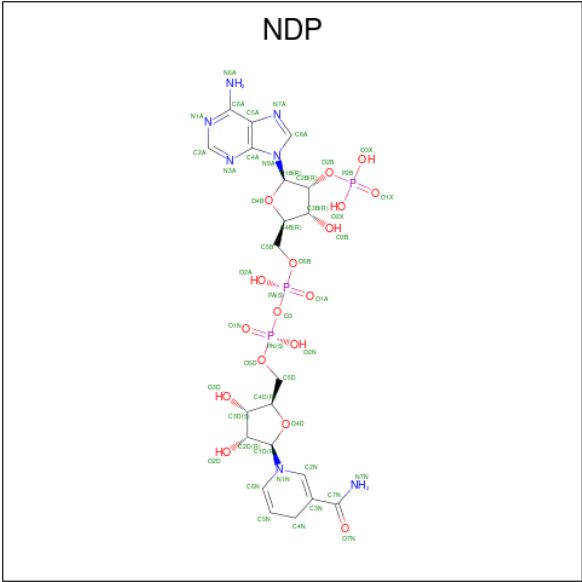
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			33	25	2	2	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
2	B	1	33	25	2	2	4	0	0

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	48	21	7	17	3	0	0
3	B	1	48	21	7	17	3	0	0

- Molecule 4 is CITRIC ACID (CCD ID: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	6	7		
4	A	1	Total	C	O	0	0
			13	6	7		
4	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 6	C 3	O 3	0	0
5	B	1	Total 6	C 3	O 3	0	0
5	B	1	Total 6	C 3	O 3	0	0
5	B	1	Total 6	C 3	O 3	0	0
5	B	1	Total 6	C 3	O 3	0	0
5	B	1	Total 6	C 3	O 3	0	0

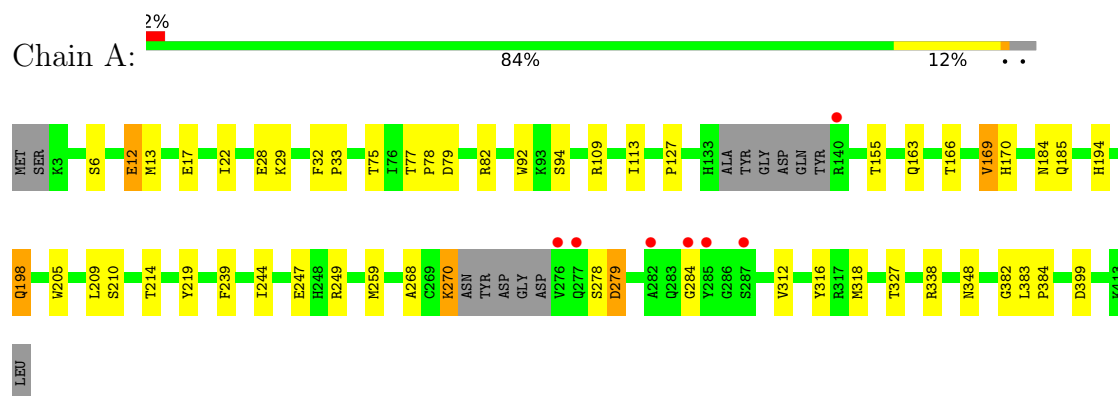
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	121	Total 121	O 121	0	0
6	B	128	Total 128	O 128	0	0

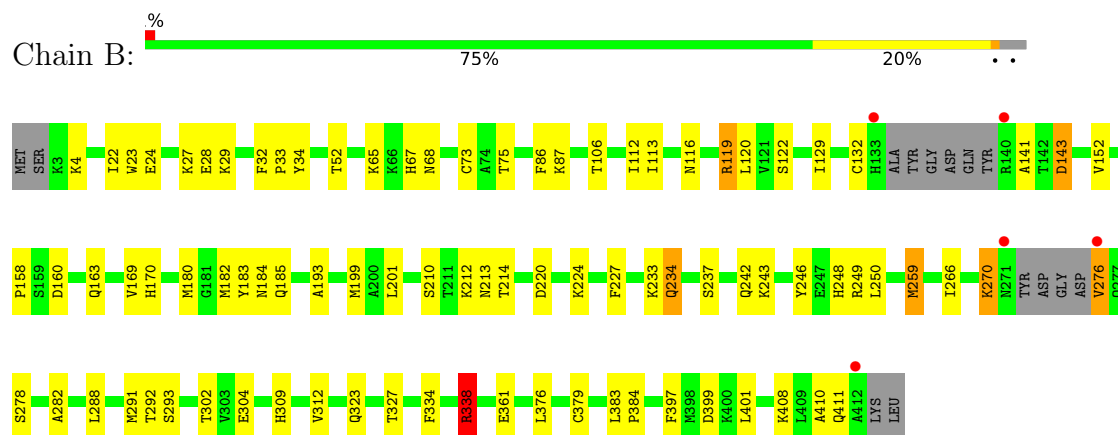
3 Residue-property plots

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 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: Isocitrate dehydrogenase [NADP] cytoplasmic



- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	82.75Å 82.75Å 296.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.20 25.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	94.3 (25.00-2.20) 94.3 (25.00-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.190 , 0.255 0.190 , 0.254	Depositor DCC
R_{free} test set	2526 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	40.3	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6667	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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: NDP, AOU, CIT, GOL

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	0.54	0/3148	1.11	4/4259 (0.1%)
1	B	0.55	0/3163	1.12	4/4279 (0.1%)
All	All	0.55	0/6311	1.12	8/8538 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	338	ARG	CG-CD-NE	6.48	126.26	112.00
1	A	198	GLN	CB-CA-C	-5.80	101.77	110.88
1	B	143	ASP	CA-CB-CG	5.79	118.39	112.60
1	A	348	ASN	CB-CA-C	-5.58	103.29	112.06
1	B	52	THR	CA-CB-OG1	-5.32	101.61	109.60
1	A	166	THR	CA-CB-OG1	-5.16	101.85	109.60
1	A	169	VAL	N-CA-C	-5.13	106.14	111.58
1	B	119	ARG	CD-NE-CZ	-5.06	117.32	124.40

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	3080	0	2968	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3095	0	2980	66	0
2	A	33	0	0	1	0
2	B	33	0	0	1	0
3	A	48	0	26	3	0
3	B	48	0	26	2	0
4	A	26	0	10	3	0
4	B	13	0	5	1	0
5	A	12	0	16	2	0
5	B	30	0	40	7	0
6	A	121	0	0	3	0
6	B	128	0	0	4	0
All	All	6667	0	6071	98	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 8.

All (98) 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:29:LYS:NZ	1:A:399:ASP:OD1	1.67	1.27
1:A:109:ARG:NH1	1:A:279:ASP:OD1	1.95	1.00
1:B:112:ILE:HA	5:B:502:GOL:H12	1.47	0.94
3:A:502:NDP:H42N	4:A:503:CIT:H22	1.50	0.93
1:B:113:ILE:HG12	5:B:502:GOL:H11	1.51	0.92
1:B:259:MET:HE1	2:B:506:AOU:C6	2.08	0.83
1:B:129:ILE:HB	1:B:266:ILE:HD12	1.74	0.70
1:B:410:ALA:O	1:B:411:GLN:HG3	1.91	0.70
1:A:185:GLN:HG2	6:A:683:HOH:O	1.91	0.70
1:A:6:SER:HB3	5:A:505:GOL:H31	1.72	0.70
1:B:323:GLN:O	5:B:504:GOL:H32	1.91	0.70
1:A:284:GLY:HA2	1:B:259:MET:HE3	1.76	0.67
1:A:17:GLU:HG2	1:A:316:TYR:CD2	2.34	0.63
1:B:116:ASN:HB3	6:B:702:HOH:O	2.00	0.62
1:B:158:PRO:HG2	1:B:163:GLN:HG2	1.82	0.62
1:A:210:SER:HA	1:A:249:ARG:O	2.01	0.61
1:B:338:ARG:HH11	1:B:338:ARG:HG3	1.67	0.60
1:A:127:PRO:HD2	1:A:205:TRP:CH2	2.37	0.59
1:B:132:CYS:SG	1:B:276:VAL:HG21	2.43	0.58
1:B:113:ILE:H	5:B:502:GOL:C1	2.17	0.57
1:B:292[B]:THR:HG22	1:B:293:SER:H	1.68	0.57
1:A:194:HIS:O	1:A:198:GLN:HG2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:507:NDP:H42N	4:B:508:CIT:H22	1.86	0.57
1:B:220:ASP:OD1	1:B:270:LYS:HE3	2.05	0.57
1:B:22:ILE:HD11	1:B:327:THR:HB	1.87	0.56
1:A:6:SER:CB	5:A:505:GOL:H31	2.35	0.56
1:B:106:THR:HG23	1:B:132:CYS:O	2.06	0.56
1:A:239:PHE:CD2	1:A:244:ILE:HG13	2.41	0.55
1:B:233:LYS:C	1:B:234:GLN:HG2	2.32	0.55
1:B:383:LEU:N	1:B:384:PRO:CD	2.69	0.55
1:A:12:GLU:HG2	1:A:13:MET:N	2.21	0.54
1:B:210:SER:HA	1:B:249:ARG:O	2.07	0.54
3:A:502:NDP:C4N	4:A:503:CIT:H22	2.32	0.53
1:B:141:ALA:HB1	1:B:180:MET:HE3	1.90	0.53
1:A:79:ASP:H	1:A:82:ARG:HB2	1.74	0.53
1:A:127:PRO:HG2	1:A:205:TRP:HH2	1.75	0.52
1:A:163:GLN:HA	6:A:658:HOH:O	2.09	0.52
1:B:112:ILE:CA	5:B:502:GOL:H12	2.30	0.51
1:A:75:THR:O	3:A:502:NDP:H2N	2.11	0.51
1:A:338:ARG:HG3	1:A:338:ARG:HH11	1.75	0.51
1:B:361:GLU:OE1	1:B:408:LYS:NZ	2.32	0.51
1:B:224:LYS:HG3	1:B:248:HIS:CD2	2.46	0.50
1:B:113:ILE:H	5:B:502:GOL:H12	1.77	0.50
1:A:383:LEU:N	1:A:384:PRO:CD	2.75	0.49
1:B:158:PRO:HD2	1:B:163:GLN:O	2.12	0.49
1:B:4:LYS:HB2	1:B:34:TYR:O	2.12	0.49
1:B:132:CYS:SG	1:B:276:VAL:CG2	3.01	0.49
1:B:212:LYS:O	1:B:214:THR:N	2.46	0.49
1:B:24:GLU:OE1	1:B:27:LYS:NZ	2.46	0.48
1:B:397:PHE:CE2	1:B:401:LEU:HD11	2.47	0.48
1:B:183:TYR:CD1	1:B:183:TYR:C	2.92	0.48
1:B:32:PHE:N	1:B:33:PRO:CD	2.76	0.48
1:B:180:MET:HE2	1:B:182:MET:HG3	1.95	0.47
1:B:233:LYS:C	1:B:234:GLN:CG	2.86	0.47
1:A:169:VAL:O	1:A:170:HIS:HB2	2.14	0.47
1:B:242:GLN:O	1:B:243:LYS:HB2	2.13	0.47
1:A:113:ILE:HD11	1:A:127:PRO:HA	1.96	0.47
1:B:160:ASP:OD1	1:B:160:ASP:C	2.58	0.47
1:B:334:PHE:O	1:B:338:ARG:HG2	2.15	0.47
1:A:284:GLY:HA2	1:B:259:MET:CE	2.44	0.46
1:A:318:MET:HE1	6:A:716:HOH:O	2.13	0.46
1:B:201:LEU:HD23	1:B:201:LEU:HA	1.77	0.46
1:B:224:LYS:HG3	1:B:248:HIS:CG	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:TYR:CD1	1:B:246:TYR:C	2.94	0.46
1:A:155:THR:HG22	6:B:636:HOH:O	2.16	0.46
1:A:32:PHE:N	1:A:33:PRO:CD	2.80	0.45
1:B:113:ILE:N	5:B:502:GOL:H12	2.31	0.45
1:B:376:LEU:O	1:B:379:CYS:HB2	2.16	0.45
1:A:219:TYR:HB2	1:B:143:ASP:HB2	1.97	0.45
1:B:180:MET:CE	1:B:182:MET:HG3	2.47	0.45
1:B:291:MET:HE2	1:B:291:MET:HB2	1.86	0.44
1:B:185:GLN:HB2	6:B:695:HOH:O	2.17	0.44
1:A:22:ILE:HD11	1:A:327:THR:HB	2.00	0.44
1:B:119:ARG:O	1:B:120:LEU:C	2.61	0.44
1:B:383:LEU:HB3	1:B:384:PRO:HD3	1.99	0.44
1:A:270:LYS:HB3	1:A:270:LYS:HE2	1.72	0.43
1:B:67:HIS:O	1:B:68:ASN:HB2	2.18	0.43
1:B:282:ALA:HB2	1:B:291:MET:HE3	1.99	0.43
1:B:24:GLU:O	1:B:28:GLU:HG2	2.19	0.43
1:B:75:THR:O	3:B:507:NDP:H2N	2.18	0.43
1:B:288:LEU:HG	1:B:309:HIS:HB3	2.00	0.43
1:B:129:ILE:HB	1:B:266:ILE:CD1	2.44	0.43
1:A:259:MET:HE1	2:A:501:AOU:C6	2.48	0.43
1:B:29:LYS:HE3	1:B:399:ASP:OD1	2.19	0.43
1:A:77:THR:OG1	4:A:503:CIT:O5	2.32	0.43
1:A:155:THR:O	1:B:152:VAL:HA	2.19	0.42
1:B:122:SER:HB2	6:B:685:HOH:O	2.19	0.42
1:B:233:LYS:O	1:B:234:GLN:HG2	2.19	0.42
1:A:209:LEU:HA	1:A:268:ALA:O	2.19	0.42
1:B:193:ALA:HB2	1:B:227:PHE:CE1	2.55	0.42
1:A:382:GLY:C	1:A:384:PRO:HD2	2.46	0.41
1:B:193:ALA:HA	1:B:227:PHE:CZ	2.56	0.41
1:B:23:TRP:CD2	1:B:73:CYS:HB2	2.56	0.41
1:A:78:PRO:HD2	1:A:92:TRP:O	2.21	0.41
1:B:68:ASN:O	1:B:302:THR:HA	2.21	0.41
1:B:86:PHE:O	1:B:87:LYS:C	2.64	0.41
1:B:169:VAL:O	1:B:170:HIS:HB2	2.21	0.40
1:B:383:LEU:N	1:B:384:PRO:HD2	2.37	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	395/414 (95%)	382 (97%)	13 (3%)	0	100	100
1	B	395/414 (95%)	377 (95%)	17 (4%)	1 (0%)	36	42
All	All	790/828 (95%)	759 (96%)	30 (4%)	1 (0%)	48	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	213	ASN

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	314/350 (90%)	304 (97%)	10 (3%)	34	47
1	B	316/350 (90%)	303 (96%)	13 (4%)	27	37
All	All	630/700 (90%)	607 (96%)	23 (4%)	30	41

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	GLU
1	A	28	GLU
1	A	94	SER
1	A	184	ASN
1	A	214	THR

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Mol	Chain	Res	Type
1	A	247	GLU
1	A	270	LYS
1	A	278	SER
1	A	279	ASP
1	A	312	VAL
1	B	65	LYS
1	B	184	ASN
1	B	199	MET
1	B	234	GLN
1	B	237	SER
1	B	250	LEU
1	B	259	MET
1	B	270	LYS
1	B	276	VAL
1	B	278	SER
1	B	304	GLU
1	B	312	VAL
1	B	338	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	ASN
1	A	198	GLN
1	A	213	ASN
1	A	323	GLN
1	A	404	ASN
1	B	14	GLN
1	B	68	ASN
1	B	90	GLN
1	B	163	GLN
1	B	234	GLN
1	B	283	GLN
1	B	323	GLN
1	B	357	ASN
1	B	404	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

14 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	$\# Z > 2$
4	CIT	A	504	-	12,12,12	1.37	1 (8%)	17,17,17	1.46	2 (11%)
5	GOL	A	505	-	5,5,5	0.12	0	5,5,5	0.41	0
4	CIT	B	508	-	12,12,12	1.18	0	17,17,17	1.08	0
2	AOU	A	501	-	36,36,36	1.36	4 (11%)	47,53,53	1.60	9 (19%)
5	GOL	B	503	-	5,5,5	0.10	0	5,5,5	0.35	0
5	GOL	B	504	-	5,5,5	0.20	0	5,5,5	0.65	0
2	AOU	B	506	-	36,36,36	1.58	7 (19%)	47,53,53	1.61	7 (14%)
5	GOL	A	506	-	5,5,5	0.10	0	5,5,5	0.36	0
3	NDP	A	502	-	51,52,52	0.73	0	71,80,80	0.91	3 (4%)
5	GOL	B	502	-	5,5,5	0.17	0	5,5,5	0.56	0
5	GOL	B	505	-	5,5,5	0.15	0	5,5,5	0.45	0
4	CIT	A	503	-	12,12,12	1.16	1 (8%)	17,17,17	1.24	2 (11%)
3	NDP	B	507	-	51,52,52	0.63	1 (1%)	71,80,80	0.89	4 (5%)
5	GOL	B	501	-	5,5,5	0.08	0	5,5,5	0.48	0

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	CIT	A	504	-	-	3/16/16/16	-
5	GOL	A	505	-	-	4/4/4/4	-
4	CIT	B	508	-	-	4/16/16/16	-
2	AOU	A	501	-	-	4/21/21/21	0/4/4/4
5	GOL	B	503	-	-	2/4/4/4	-
5	GOL	B	504	-	-	3/4/4/4	-
2	AOU	B	506	-	-	5/21/21/21	0/4/4/4
5	GOL	A	506	-	-	0/4/4/4	-
3	NDP	A	502	-	-	8/34/77/77	0/5/5/5
5	GOL	B	502	-	-	2/4/4/4	-
5	GOL	B	505	-	-	4/4/4/4	-
4	CIT	A	503	-	-	10/16/16/16	-
3	NDP	B	507	-	-	4/34/77/77	0/5/5/5
5	GOL	B	501	-	-	2/4/4/4	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	506	AOU	C9-N1	4.56	1.44	1.39
2	A	501	AOU	C9-N1	3.53	1.42	1.39
4	A	504	CIT	C3-C6	3.29	1.56	1.53
2	B	506	AOU	C11-C9	3.27	1.45	1.41
2	A	501	AOU	C11-C9	2.79	1.44	1.41
2	A	501	AOU	C8-N1	2.74	1.41	1.37
2	B	506	AOU	C8-N1	2.41	1.40	1.37
2	B	506	AOU	O28-C21	2.39	1.36	1.30
2	B	506	AOU	C4-C13	2.33	1.43	1.39
3	B	507	NDP	PA-O3	2.29	1.62	1.59
2	A	501	AOU	C13-C9	2.28	1.44	1.41
2	B	506	AOU	C10-C14	2.26	1.43	1.39
4	A	503	CIT	C3-C6	2.19	1.55	1.53
2	B	506	AOU	C13-C9	2.05	1.44	1.41

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	506	AOU	C13-C9-N1	-6.41	104.98	107.18
2	A	501	AOU	C13-C9-N1	-5.95	105.14	107.18
2	B	506	AOU	C33-N1-C8	-3.70	121.80	125.70
2	A	501	AOU	O29-C36-C35	-3.40	107.11	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	AOU	C14-C10-C34	-3.38	117.95	121.58
2	B	506	AOU	O29-C36-C35	-3.35	107.16	109.98
2	A	501	AOU	C33-N1-C8	-3.21	122.32	125.70
4	A	504	CIT	O6-C6-C3	3.11	119.10	113.14
4	A	504	CIT	O5-C6-C3	-2.86	116.55	122.09
2	B	506	AOU	C39-C37-C36	2.78	115.65	111.05
4	A	503	CIT	O5-C6-C3	-2.72	116.82	122.09
2	B	506	AOU	O29-C36-C37	-2.69	113.52	116.87
3	A	502	NDP	O2B-P2B-O1X	-2.52	100.34	109.33
3	A	502	NDP	P2B-O2B-C2B	-2.50	116.77	123.43
4	A	503	CIT	O6-C6-C3	2.49	117.91	113.14
3	B	507	NDP	C3N-C7N-N7N	-2.44	113.33	117.67
2	A	501	AOU	C35-C34-N2	-2.41	108.89	111.43
3	B	507	NDP	C3B-C2B-C1B	-2.27	98.46	102.81
3	B	507	NDP	O3D-C3D-C4D	-2.21	104.73	111.08
2	A	501	AOU	C10-C34-C35	2.18	131.61	129.12
3	B	507	NDP	O3B-C3B-C2B	2.17	117.26	111.19
2	A	501	AOU	C18-C19-C21	-2.08	116.93	122.32
2	A	501	AOU	C10-C14-CL2	-2.06	116.96	119.62
2	B	506	AOU	O30-C21-C19	2.06	127.38	121.06
2	B	506	AOU	C10-C34-C35	2.06	131.47	129.12
2	A	501	AOU	C11-C18-C19	-2.04	122.90	126.91
3	A	502	NDP	O2A-PA-O1A	2.00	121.76	112.44

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	AOU	C35-C36-C37-C39
2	A	501	AOU	O29-C36-C37-C39
2	A	501	AOU	O29-C36-C37-C38
2	B	506	AOU	C35-C36-C37-C38
2	B	506	AOU	O29-C36-C37-C39
2	B	506	AOU	O29-C36-C37-C38
3	A	502	NDP	C5D-O5D-PN-O3
3	A	502	NDP	C5D-O5D-PN-O1N
3	A	502	NDP	C5D-O5D-PN-O2N
4	A	503	CIT	O7-C3-C6-O5
4	A	503	CIT	O7-C3-C6-O6
5	A	505	GOL	O1-C1-C2-C3
5	A	505	GOL	C1-C2-C3-O3
5	B	501	GOL	O1-C1-C2-C3

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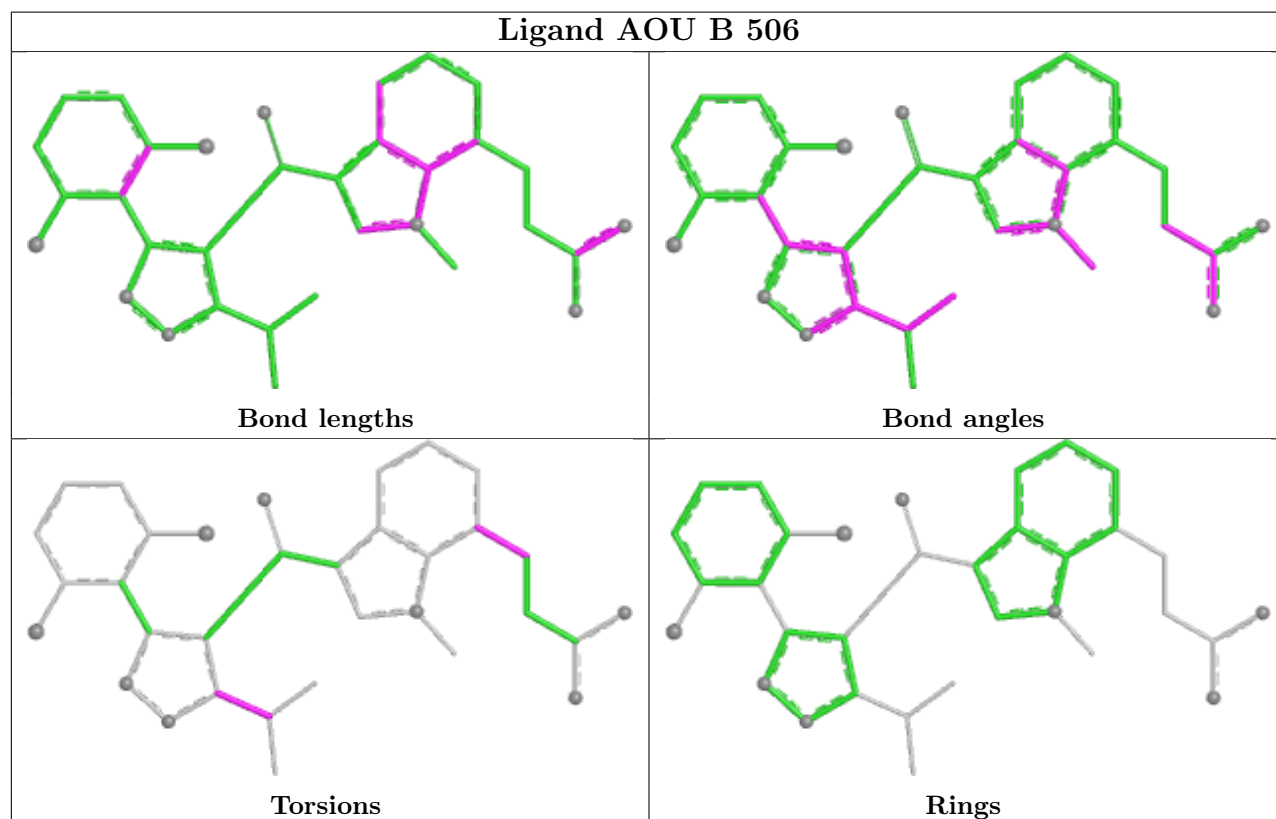
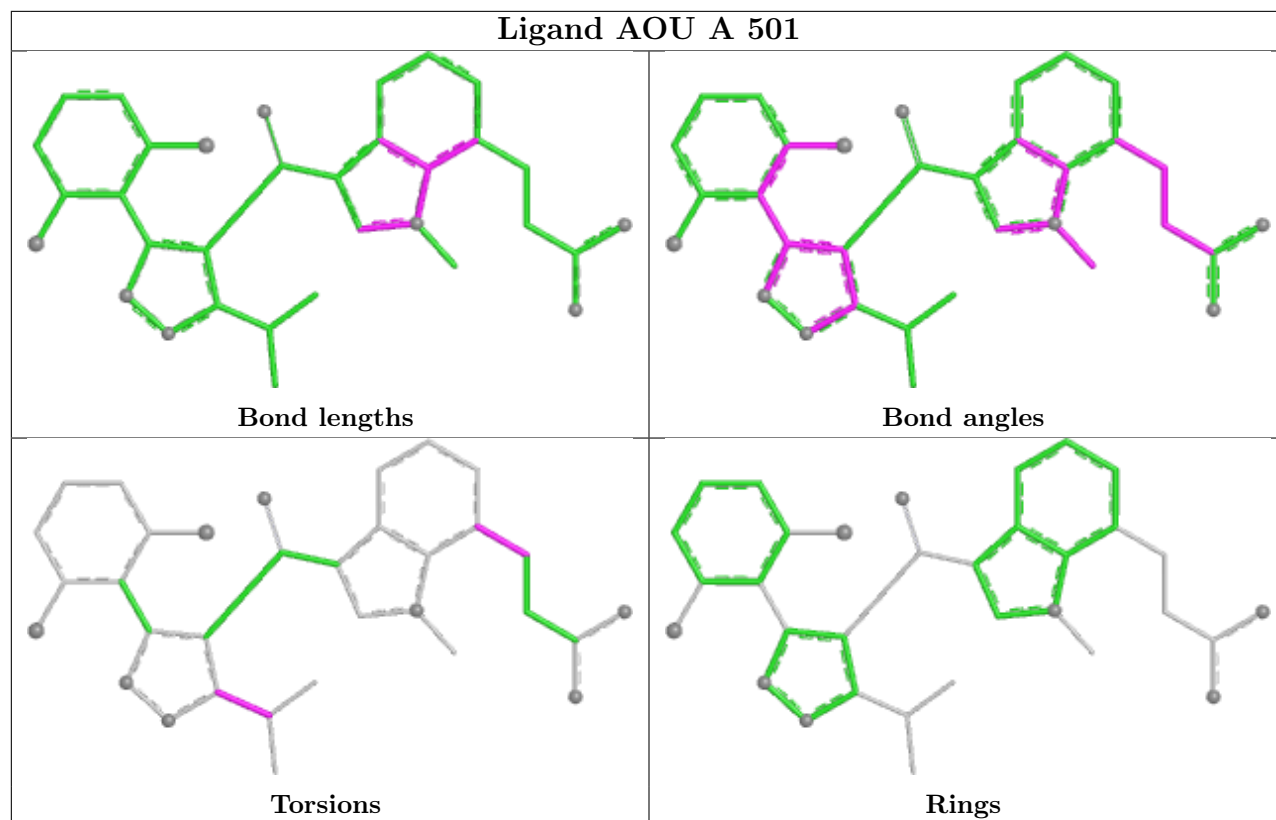
Mol	Chain	Res	Type	Atoms
5	B	502	GOL	C1-C2-C3-O3
5	B	503	GOL	C1-C2-C3-O3
5	B	505	GOL	O1-C1-C2-O2
5	B	505	GOL	O1-C1-C2-C3
5	B	505	GOL	C1-C2-C3-O3
5	B	504	GOL	O1-C1-C2-C3
4	A	503	CIT	C4-C3-C6-O5
4	A	503	CIT	C4-C3-C6-O6
5	A	505	GOL	O2-C2-C3-O3
5	B	502	GOL	O2-C2-C3-O3
5	B	504	GOL	O1-C1-C2-O2
5	B	505	GOL	O2-C2-C3-O3
5	A	505	GOL	O1-C1-C2-O2
5	B	503	GOL	O2-C2-C3-O3
5	B	504	GOL	O2-C2-C3-O3
3	A	502	NDP	O4B-C4B-C5B-O5B
3	A	502	NDP	C3B-C4B-C5B-O5B
4	A	503	CIT	C2-C3-C6-O6
4	B	508	CIT	C2-C3-C6-O6
2	A	501	AOU	C9-C11-C18-C19
2	B	506	AOU	C9-C11-C18-C19
4	B	508	CIT	O7-C3-C6-O6
3	B	507	NDP	C3B-C4B-C5B-O5B
4	A	503	CIT	C2-C3-C6-O5
4	B	508	CIT	C4-C3-C6-O6
3	A	502	NDP	C2D-C1D-N1N-C2N
3	A	502	NDP	O4D-C1D-N1N-C2N
3	B	507	NDP	O4D-C1D-N1N-C2N
3	B	507	NDP	C2D-C1D-N1N-C2N
4	A	503	CIT	O2-C1-C2-C3
4	A	504	CIT	C1-C2-C3-O7
4	B	508	CIT	O7-C3-C6-O5
3	B	507	NDP	C1B-C2B-O2B-P2B
4	A	503	CIT	O1-C1-C2-C3
2	B	506	AOU	C3-C11-C18-C19
3	A	502	NDP	O4D-C1D-N1N-C6N
4	A	504	CIT	C3-C4-C5-O3
5	B	501	GOL	O1-C1-C2-O2
4	A	504	CIT	C3-C4-C5-O4
4	A	503	CIT	O7-C3-C4-C5
4	A	503	CIT	C6-C3-C4-C5

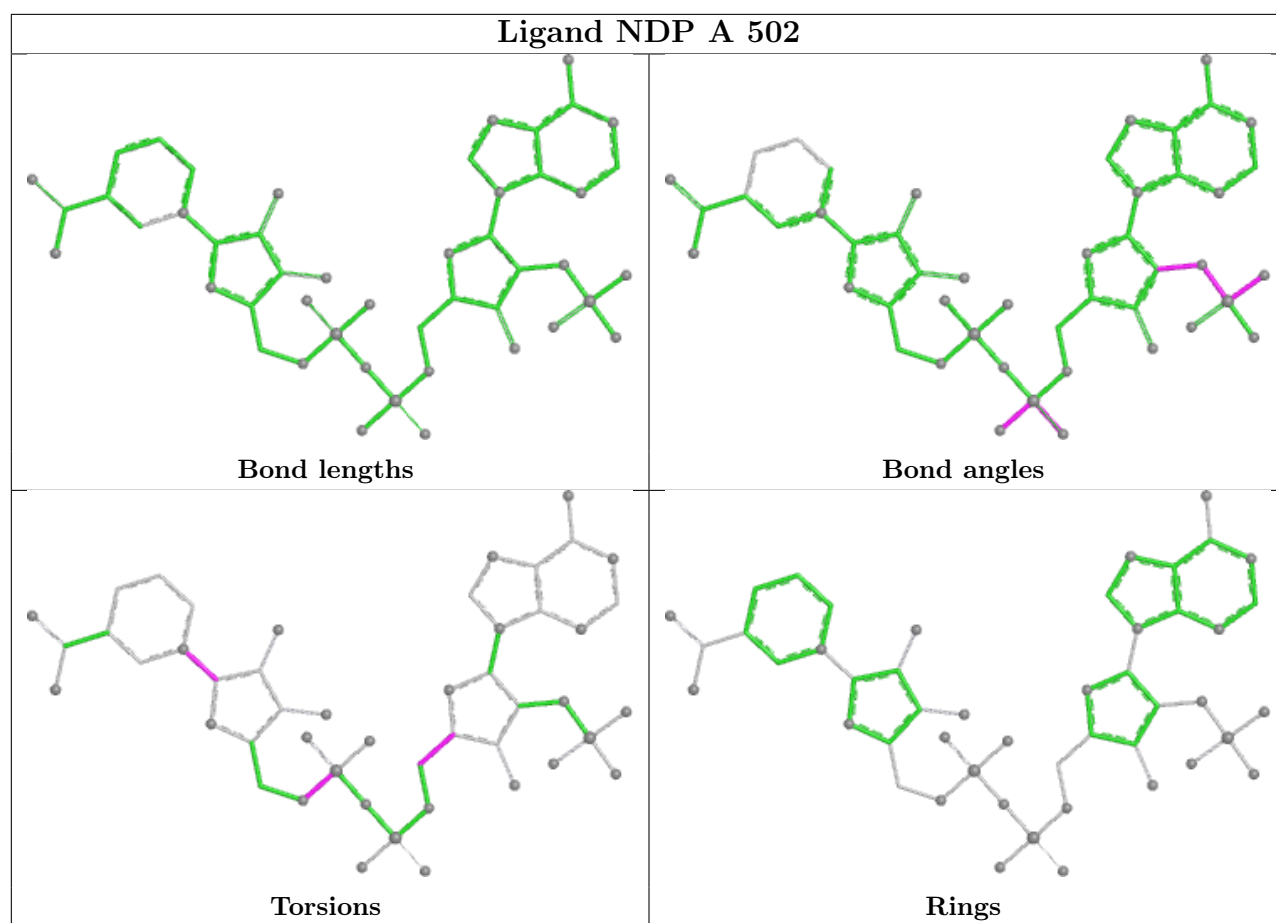
There are no ring outliers.

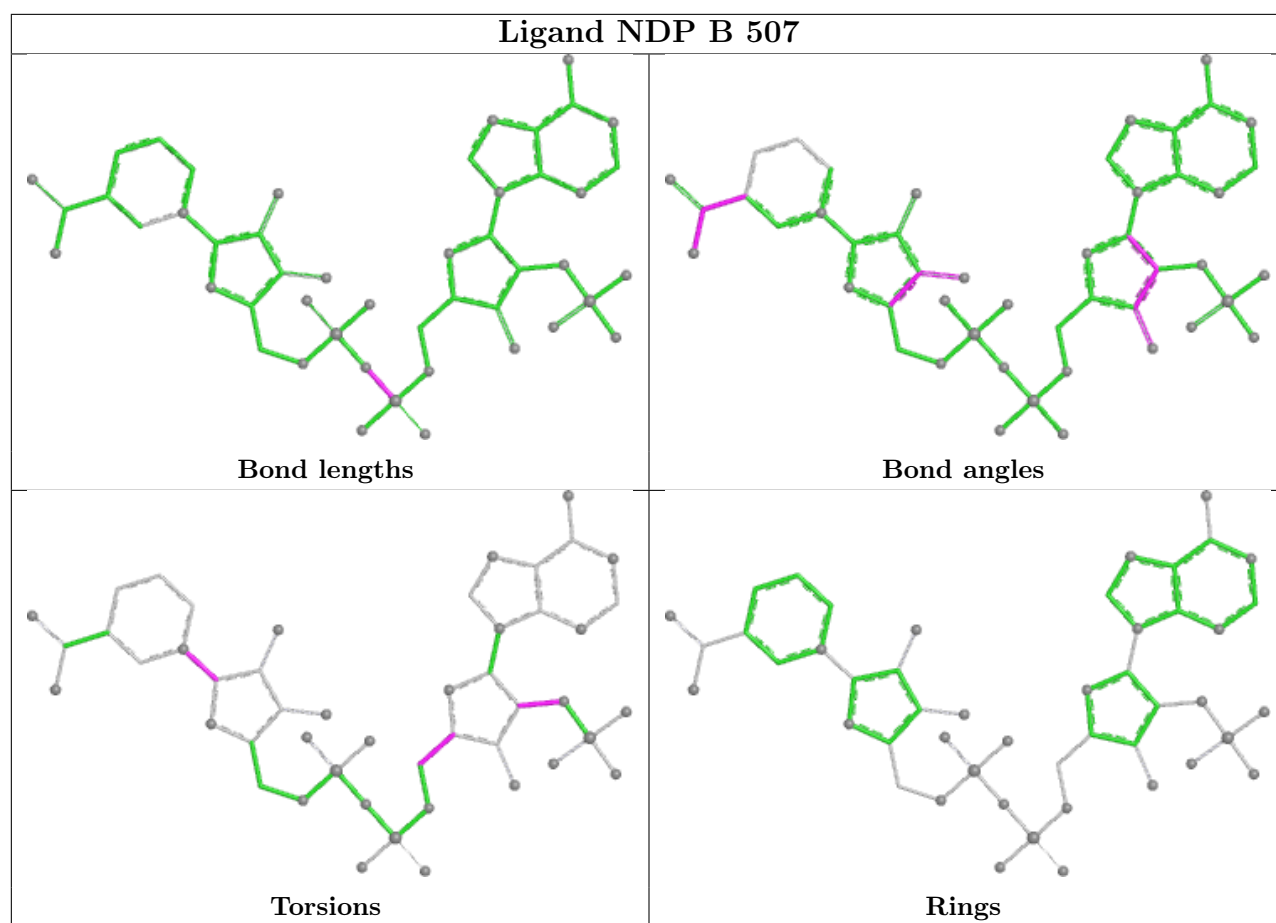
9 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	505	GOL	2	0
4	B	508	CIT	1	0
2	A	501	AOU	1	0
5	B	504	GOL	1	0
2	B	506	AOU	1	0
3	A	502	NDP	3	0
5	B	502	GOL	6	0
4	A	503	CIT	3	0
3	B	507	NDP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	400/414 (96%)	-0.39	7 (1%) 67 64	27, 41, 69, 106	1 (0%)
1	B	400/414 (96%)	-0.49	5 (1%) 75 73	23, 39, 66, 100	1 (0%)
All	All	800/828 (96%)	-0.44	12 (1%) 72 69	23, 41, 69, 106	2 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	276	VAL	5.2
1	A	285	TYR	3.6
1	B	412	ALA	3.6
1	B	133	HIS	3.4
1	B	276	VAL	3.2
1	B	271	ASN	3.0
1	B	140	ARG	2.9
1	A	284	GLY	2.2
1	A	277	GLN	2.2
1	A	282	ALA	2.0
1	A	140	ARG	2.0
1	A	287	SER	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

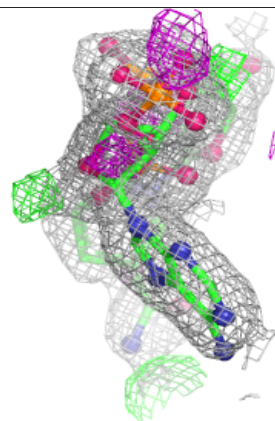
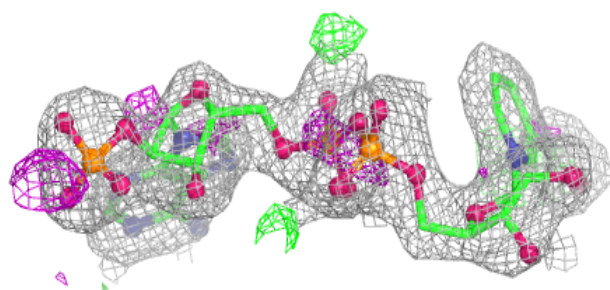
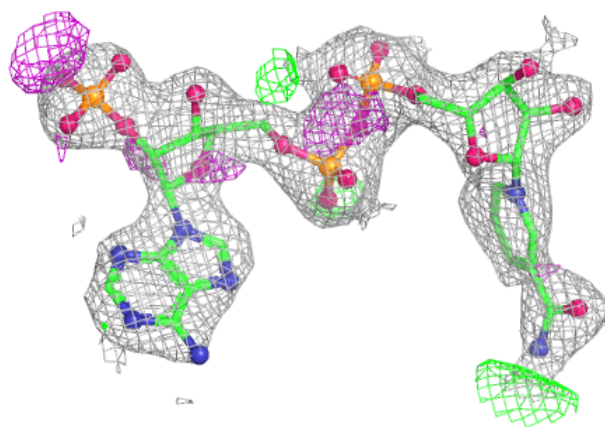
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CIT	A	504	13/13	0.77	0.15	56,80,103,115	0
5	GOL	A	506	6/6	0.82	0.13	69,81,82,85	0
5	GOL	B	502	6/6	0.82	0.15	55,61,64,64	0
5	GOL	B	504	6/6	0.83	0.17	58,63,71,72	0
5	GOL	B	505	6/6	0.83	0.13	60,74,75,77	0
4	CIT	A	503	13/13	0.85	0.10	89,93,96,97	0
3	NDP	A	502	48/48	0.90	0.09	45,59,69,80	0
4	CIT	B	508	13/13	0.90	0.11	67,78,87,111	0
5	GOL	B	501	6/6	0.92	0.11	57,60,61,61	0
5	GOL	B	503	6/6	0.92	0.09	37,64,67,71	0
5	GOL	A	505	6/6	0.93	0.12	49,64,72,74	0
2	AOU	A	501	33/33	0.96	0.07	40,50,58,64	0
2	AOU	B	506	33/33	0.97	0.06	31,41,48,65	0
3	NDP	B	507	48/48	0.99	0.04	25,31,35,38	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.

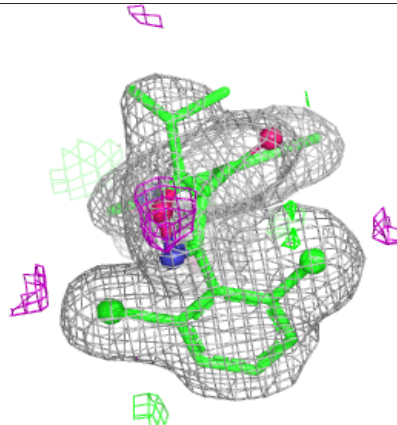
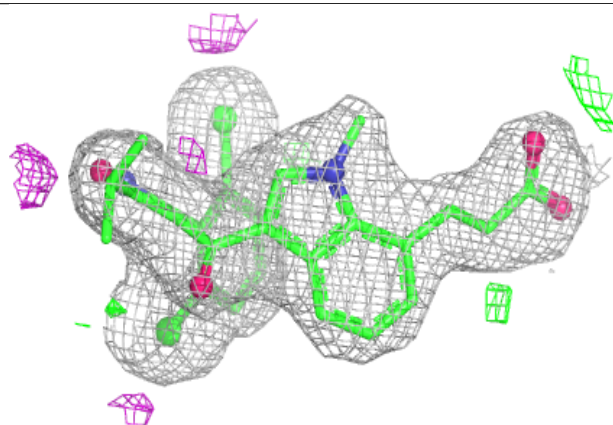
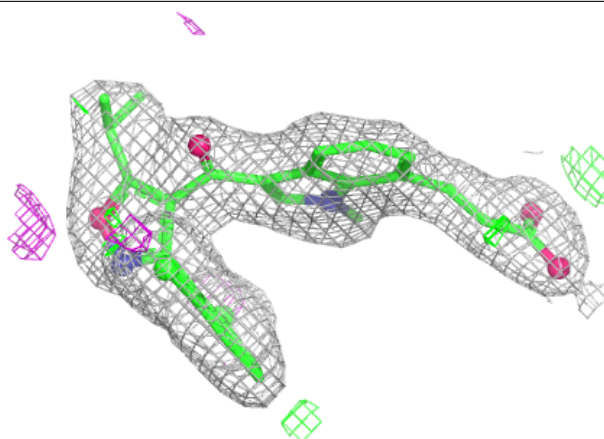
Electron density around NDP A 502:

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



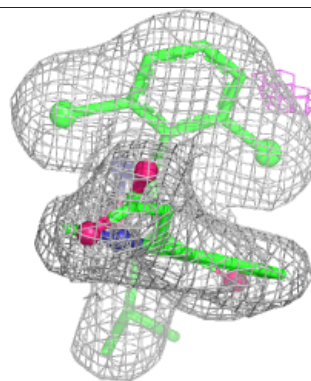
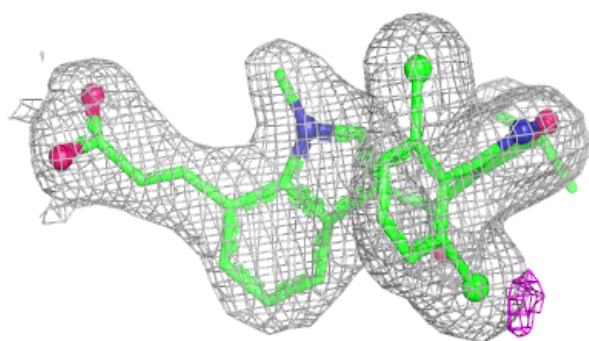
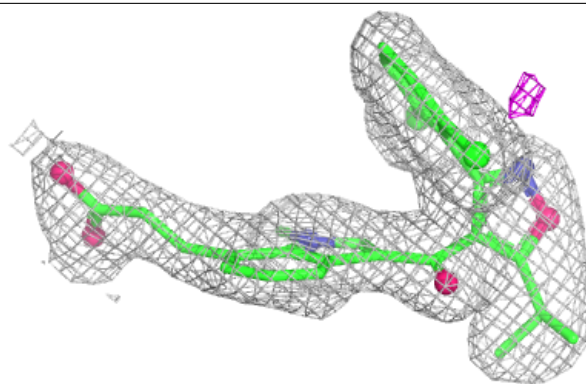
Electron density around AOU A 501:

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



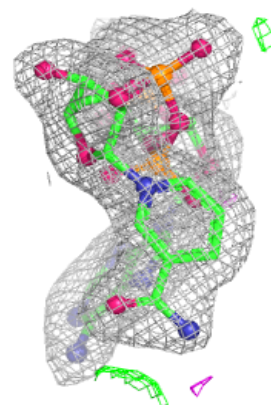
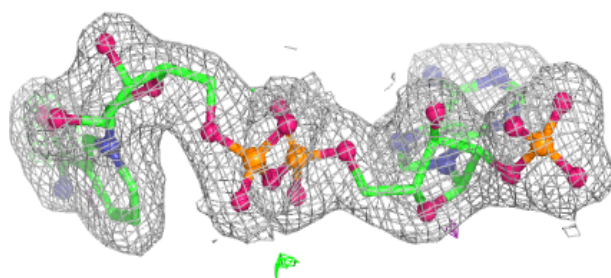
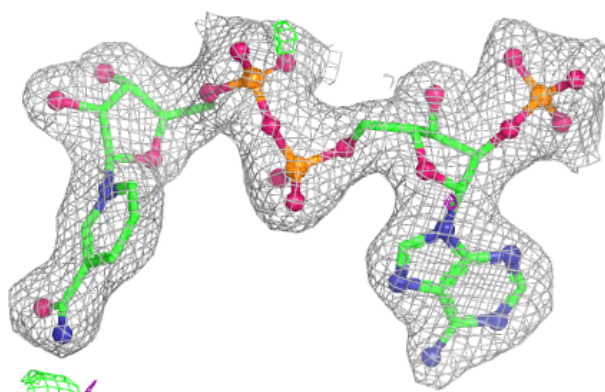
Electron density around AOU B 506:

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



Electron density around NDP B 507:

$2mF_o-DF_c$ (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.