



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:23 PM UTC

PDB ID : 6AJ8 / pdb_00006aj8
Title : Crystal structure of Trypanosoma brucei glycosomal isocitrate dehydrogenase in complex with NADP⁺, alpha-ketoglutarate and ca²⁺
Authors : Wang, X.; Inaoka, D.K.; Shiba, T.; Balogun, E.O.; Ziebart, N.; Allman, S.; Watanabe, Y.; Nozaki, T.; Boshart, M.; Bringaud, F.; Harada, S.; Kita, K.
Deposited on : 2018-08-27
Resolution : 2.40 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

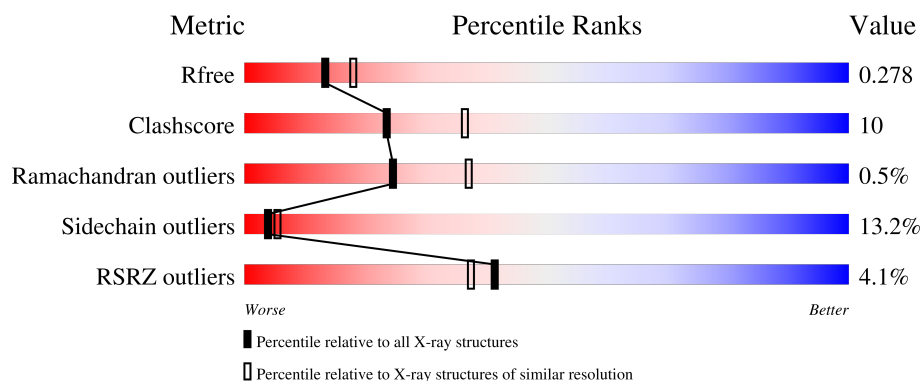
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	413	76% 21% .
1	B	413	7% 74% 20% 6%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 6928 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.

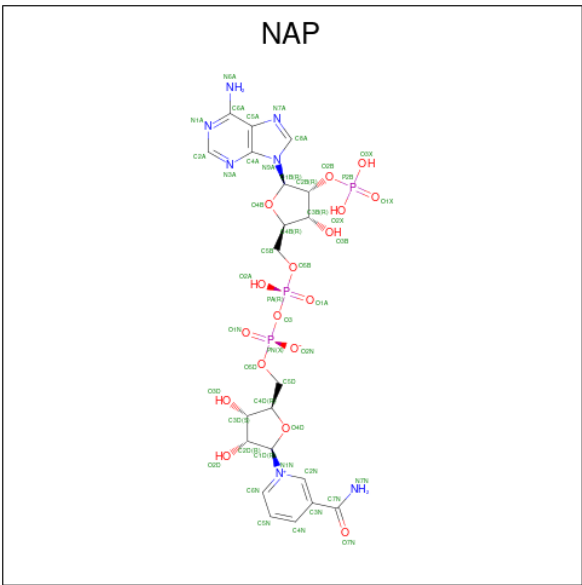
- Molecule 1 is a protein called Isocitrate dehydrogenase [NADP].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	413	3282	2084	563	613	22	0	0	0
1	B	413	3306	2097	566	621	22	0	3	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	MET	engineered mutation	UNP Q387G0
B	1	SER	MET	engineered mutation	UNP Q387G0

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



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

Continued on next page...

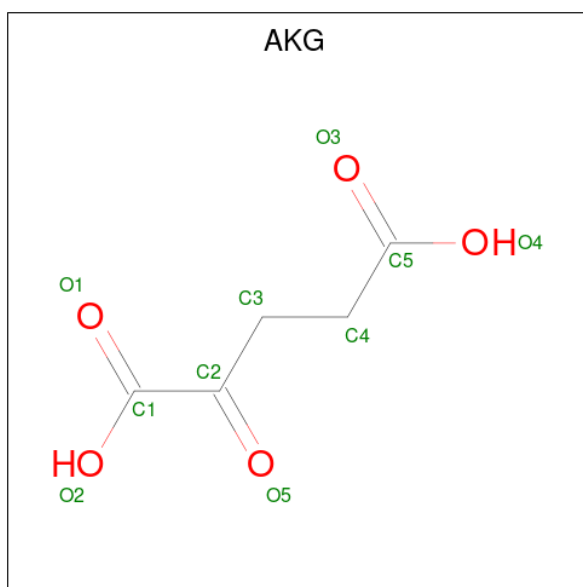
Continued from previous page...

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

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ca	0	0
			2	2		

- Molecule 4 is 2-OXOGLUTARIC ACID (CCD ID: AKG) (formula: C₅H₆O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			10	5	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	127	Total	O	0	0
			127	127		
5	B	105	Total	O	0	0
			105	105		

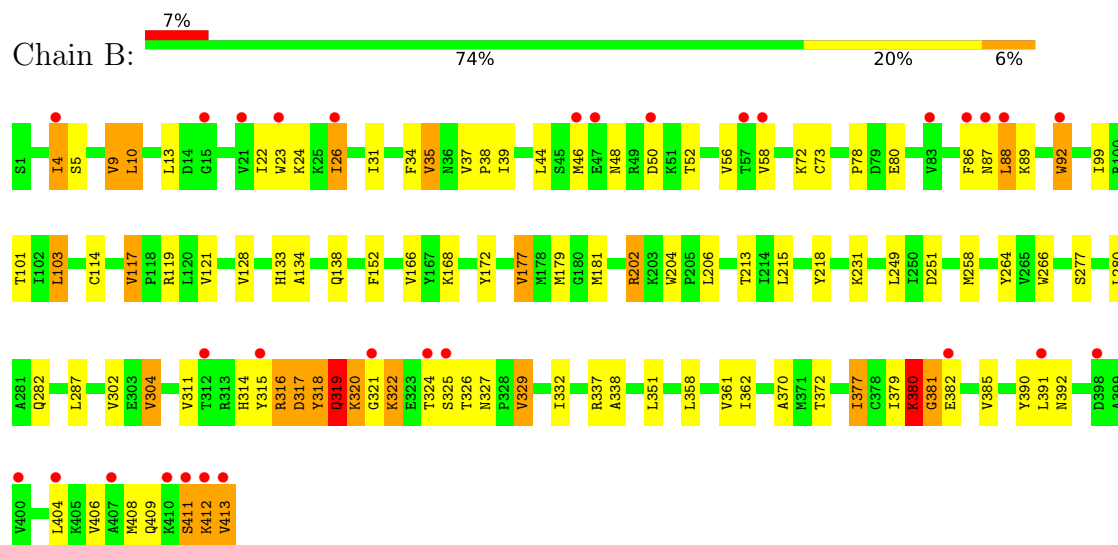
3 Residue-property plots

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]



• Molecule 1: Isocitrate dehydrogenase [NADP]



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.47Å 112.02Å 132.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 20.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.7 (20.00-2.40) 93.7 (20.00-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.36 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.217 , 0.271 0.222 , 0.278	Depositor DCC
R_{free} test set	1596 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å ²)	33.9	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6928	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.19 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.0383e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AKG, CA, NAP

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	0.87	0/3350	1.09	7/4522 (0.2%)
1	B	0.89	0/3374	1.13	11/4555 (0.2%)
All	All	0.88	0/6724	1.11	18/9077 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	320	LYS	N-CA-C	-12.59	93.18	110.68
1	A	4	ILE	N-CA-C	11.27	122.11	110.62
1	B	86	PHE	N-CA-C	-9.02	96.19	109.63
1	B	411	SER	N-CA-C	-8.49	94.41	108.76
1	B	316	ARG	N-CA-C	-7.91	102.66	111.28
1	A	16	ASP	N-CA-C	7.57	120.91	109.41
1	B	318	TYR	N-CA-C	6.40	119.49	109.96
1	B	319	GLN	N-CA-C	6.18	120.06	111.90
1	A	18	MET	N-CA-C	5.63	117.41	111.28
1	B	380	LYS	N-CA-C	5.60	116.72	107.20
1	B	87	ASN	N-CA-C	5.50	118.59	109.46
1	A	2	ASN	N-CA-C	-5.47	100.39	107.73
1	A	170	PHE	CA-C-N	5.32	130.15	122.44
1	A	170	PHE	C-N-CA	5.32	130.15	122.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	92	TRP	N-CA-C	5.14	117.68	110.23
1	B	390	TYR	N-CA-C	5.13	115.82	108.74
1	B	35	VAL	N-CA-C	5.09	115.30	107.77
1	A	137	ASP	N-CA-C	-5.00	100.15	110.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	379	ILE	Peptide
1	B	380	LYS	Peptide

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	3282	0	3273	66	1
1	B	3306	0	3289	84	0
2	A	48	0	25	0	0
2	B	48	0	25	0	0
3	A	2	0	0	0	0
4	B	10	0	4	0	0
5	A	127	0	0	0	0
5	B	105	0	0	1	0
All	All	6928	0	6616	136	1

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 10.

All (136) 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:3:LYS:HZ3	1:A:33:PRO:C	1.11	1.53
1:A:3:LYS:NZ	1:A:33:PRO:C	1.91	1.26
1:A:3:LYS:HE2	1:A:33:PRO:O	1.41	1.18

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:LYS:HG3	1:B:413:VAL:OXT	1.43	1.15
1:A:3:LYS:HB3	1:A:36:ASN:HB2	1.27	1.13
1:A:3:LYS:HZ3	1:A:33:PRO:CA	1.68	1.06
1:A:3:LYS:NZ	1:A:33:PRO:CA	2.23	1.01
1:A:3:LYS:HZ3	1:A:34:PHE:N	1.60	0.99
1:B:88:LEU:HD22	1:B:88:LEU:H	1.31	0.95
1:A:3:LYS:CE	1:A:33:PRO:O	2.16	0.93
1:B:4:ILE:HG23	1:B:34:PHE:O	1.74	0.87
1:A:3:LYS:CE	1:A:33:PRO:C	2.49	0.85
1:A:18:MET:CE	1:A:324:THR:HG21	2.07	0.85
1:B:408:MET:HE3	1:B:408:MET:HA	1.59	0.84
1:A:354:PHE:HD1	1:A:408:MET:CE	1.92	0.82
1:B:408:MET:HE3	1:B:408:MET:CA	2.13	0.78
1:B:412:LYS:CG	1:B:413:VAL:OXT	2.29	0.77
1:A:177:VAL:HG13	1:B:218:TYR:CE2	2.21	0.76
1:B:179:MET:HE2	1:B:181:MET:HE2	1.67	0.76
1:B:4:ILE:CG2	1:B:34:PHE:O	2.34	0.76
1:A:3:LYS:HE2	1:A:33:PRO:C	2.13	0.72
1:A:18:MET:HE2	1:A:324:THR:HG21	1.71	0.71
1:A:354:PHE:HD1	1:A:408:MET:HE2	1.56	0.70
1:A:18:MET:HE1	1:A:324:THR:HG21	1.73	0.70
1:B:88:LEU:HD22	1:B:88:LEU:N	2.06	0.70
1:A:20:ARG:NH2	1:A:43:ASP:OD1	2.27	0.68
1:B:325:SER:OG	1:B:391:LEU:O	2.12	0.66
1:B:316:ARG:O	1:B:320:LYS:HD3	1.95	0.65
1:B:317:ASP:OD2	1:B:322:LYS:HD2	1.99	0.63
1:B:408:MET:HA	1:B:408:MET:CE	2.23	0.62
1:B:88:LEU:H	1:B:88:LEU:CD2	2.03	0.62
1:A:218:TYR:CE2	1:B:177:VAL:HG13	2.34	0.62
1:B:332:ILE:HG21	1:B:362:ILE:HD11	1.81	0.61
1:A:121:VAL:CG2	1:B:258:MET:HE1	2.30	0.61
1:B:320:LYS:C	1:B:322:LYS:H	2.09	0.60
1:B:412:LYS:HG3	1:B:413:VAL:N	2.16	0.60
1:B:114:CYS:HB2	1:B:117:VAL:HG12	1.85	0.59
1:A:133:HIS:O	1:A:134:ALA:HB3	2.02	0.59
1:A:3:LYS:NZ	1:A:33:PRO:HA	2.17	0.57
1:A:354:PHE:CD1	1:A:408:MET:CE	2.83	0.56
1:B:80[A]:GLU:OE1	1:B:80[A]:GLU:N	2.31	0.56
1:A:354:PHE:HD1	1:A:408:MET:HE3	1.71	0.56
1:B:377:ILE:O	1:B:381:GLY:N	2.38	0.55
1:A:3:LYS:HZ1	1:A:33:PRO:CA	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:VAL:HG13	1:B:264:TYR:CE1	2.42	0.55
1:A:218:TYR:CD2	1:B:177:VAL:HG13	2.42	0.54
1:B:319:GLN:N	1:B:319:GLN:OE1	2.39	0.54
1:A:7:THR:HG23	1:A:8:GLY:N	2.21	0.53
1:B:72:LYS:HE3	1:B:73:CYS:O	2.08	0.53
1:A:181:MET:HE2	1:B:181:MET:HE3	1.91	0.53
1:A:354:PHE:CD1	1:A:408:MET:HE3	2.45	0.52
1:A:18:MET:HE2	1:A:324:THR:CG2	2.39	0.52
1:A:20:ARG:HH22	1:A:43:ASP:CG	2.17	0.52
1:A:4:ILE:HD12	1:A:4:ILE:N	2.24	0.52
1:B:13:LEU:HD22	1:B:72:LYS:HG3	1.91	0.51
1:A:327:ASN:OD1	1:A:329:VAL:HG13	2.10	0.51
1:A:40:GLU:OE2	1:A:42:TYR:OH	2.24	0.51
1:B:315:TYR:HA	1:B:318:TYR:HB2	1.93	0.51
1:A:114:CYS:HB2	1:A:117:VAL:HG12	1.93	0.51
1:B:99:ILE:HG22	1:B:103:LEU:HD22	1.92	0.50
1:B:315:TYR:HA	1:B:318:TYR:CB	2.41	0.50
1:A:177:VAL:CG2	1:B:218:TYR:HA	2.41	0.50
1:B:35:VAL:CG1	1:B:37:VAL:HG13	2.41	0.50
1:B:319:GLN:C	1:B:321:GLY:N	2.69	0.50
1:A:4:ILE:N	1:A:4:ILE:CD1	2.75	0.50
1:A:332:ILE:HG21	1:A:362:ILE:HD11	1.94	0.50
1:A:177:VAL:HG21	1:B:218:TYR:HA	1.94	0.49
1:B:78:PRO:HG2	1:B:92:TRP:HB2	1.95	0.49
1:A:3:LYS:HZ1	1:A:33:PRO:HA	1.74	0.49
1:B:10:LEU:O	1:B:39:ILE:HA	2.12	0.49
1:A:22:ILE:HD12	1:A:328:PRO:HB3	1.95	0.49
1:B:413:VAL:HG22	1:B:413:VAL:O	2.11	0.49
1:A:20:ARG:NH2	1:A:45:SER:HB3	2.28	0.48
1:A:4:ILE:HB	1:A:35:VAL:HG23	1.95	0.48
1:A:132:ARG:HG3	1:A:273:GLY:HA3	1.95	0.48
1:B:327:ASN:OD1	1:B:329:VAL:HG13	2.14	0.48
1:B:22:ILE:O	1:B:26:ILE:HG23	2.13	0.48
1:A:80:GLU:O	1:A:83:VAL:HG22	2.13	0.48
1:A:55:ARG:NH1	1:A:58:VAL:HG11	2.29	0.47
1:A:405:LYS:O	1:A:406:VAL:C	2.57	0.47
1:B:325:SER:O	1:B:372:THR:HB	2.14	0.47
1:B:35:VAL:HG13	1:B:37:VAL:HG13	1.96	0.47
1:B:311:VAL:HG12	1:B:314:HIS:HB2	1.96	0.47
1:A:77:THR:HB	1:A:94:SER:HA	1.95	0.47
1:B:52:THR:HG21	1:B:56:VAL:HG23	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:LYS:C	1:B:322:LYS:N	2.71	0.47
1:A:121:VAL:CG2	1:B:258:MET:CE	2.93	0.47
1:B:319:GLN:C	1:B:321:GLY:H	2.23	0.46
1:A:7:THR:CG2	1:A:8:GLY:N	2.78	0.46
1:A:177:VAL:HG13	1:B:218:TYR:CD2	2.50	0.46
1:B:48:ASN:O	1:B:52:THR:HG22	2.16	0.46
1:B:39:ILE:HG12	5:B:635:HOH:O	2.15	0.45
1:B:315:TYR:C	1:B:318:TYR:H	2.24	0.45
1:B:50:ASP:HA	1:B:92:TRP:HE1	1.81	0.45
1:B:13:LEU:HD23	1:B:44:LEU:HD22	1.99	0.44
1:A:383:LYS:HA	1:A:383:LYS:HD2	1.84	0.44
1:B:88:LEU:N	1:B:88:LEU:CD2	2.73	0.44
1:B:318:TYR:CD1	1:B:319:GLN:OE1	2.70	0.44
1:A:404:LEU:O	1:A:408:MET:HB2	2.19	0.43
1:B:304:VAL:HG13	1:B:338:ALA:HB2	1.99	0.43
1:B:50:ASP:OD2	1:B:89:LYS:CE	2.66	0.43
1:A:3:LYS:NZ	1:A:34:PHE:N	2.39	0.43
1:A:121:VAL:HG22	1:B:258:MET:HE1	2.00	0.43
1:A:16:ASP:OD1	1:A:76:ILE:HG13	2.18	0.43
1:B:412:LYS:CG	1:B:413:VAL:N	2.82	0.43
1:A:125:LYS:HB2	1:A:261:GLU:HG2	2.00	0.42
1:B:50:ASP:O	1:B:89:LYS:HE3	2.20	0.42
1:B:332:ILE:HG21	1:B:362:ILE:CD1	2.49	0.42
1:B:314:HIS:O	1:B:318:TYR:N	2.52	0.42
1:B:202:ARG:HG2	1:B:204:TRP:CZ3	2.55	0.42
1:A:13:LEU:HD12	1:A:13:LEU:N	2.35	0.41
1:B:319:GLN:OE1	1:B:319:GLN:CA	2.68	0.41
1:B:370:ALA:HB1	1:B:391:LEU:HD11	2.02	0.41
1:B:266:TRP:CD1	1:B:266:TRP:C	2.97	0.41
1:A:258:MET:CE	1:B:121:VAL:CG2	2.98	0.41
1:A:391:LEU:HD22	1:A:395:GLU:HG3	2.01	0.41
1:B:114:CYS:HB2	1:B:117:VAL:CG1	2.50	0.41
1:A:357:ARG:HG2	1:A:410:LYS:HZ2	1.85	0.41
1:B:358:LEU:HD13	1:B:404:LEU:HD22	2.02	0.41
1:A:230:TYR:CE1	1:A:235:GLU:HA	2.56	0.41
1:B:324:THR:O	1:B:392:ASN:HB2	2.20	0.41
1:B:9:VAL:HB	1:B:38:PRO:HB2	2.02	0.41
1:B:377:ILE:HG22	1:B:385:VAL:HG21	2.02	0.41
1:B:4:ILE:HD11	1:B:351:LEU:HB2	2.02	0.41
1:B:99:ILE:CG2	1:B:103:LEU:HD22	2.50	0.41
1:A:181:MET:HE3	1:B:179:MET:SD	2.61	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:HIS:O	1:B:134:ALA:HB3	2.21	0.41
1:B:409:GLN:HE21	1:B:409:GLN:HB3	1.65	0.41
1:A:258:MET:HE1	1:B:121:VAL:CG2	2.50	0.40
1:B:46:MET:HE1	1:B:78:PRO:HG3	2.03	0.40
1:B:152:PHE:HB2	1:B:172:TYR:HE2	1.86	0.40
1:B:23:TRP:CE3	1:B:73:CYS:HB2	2.56	0.40
1:B:52:THR:HG21	1:B:56:VAL:CG2	2.52	0.40
1:A:218:TYR:CD2	1:B:179:MET:HB2	2.57	0.40
1:A:404:LEU:O	1:A:408:MET:N	2.45	0.40
1:A:152:PHE:CG	1:A:178:MET:HE2	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:GLN:O	1:A:413:VAL:CG1[4_464]	2.17	0.03

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	411/413 (100%)	384 (93%)	25 (6%)	2 (0%)	24	37
1	B	414/413 (100%)	395 (95%)	16 (4%)	3 (1%)	18	28
All	All	825/826 (100%)	779 (94%)	41 (5%)	5 (1%)	24	32

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	GLY
1	B	382[A]	GLU
1	B	382[B]	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	149	PRO
1	B	381	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	353/353 (100%)	303 (86%)	50 (14%)	3	4
1	B	356/353 (101%)	313 (88%)	43 (12%)	5	7
All	All	709/706 (100%)	616 (87%)	93 (13%)	4	5

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	9	VAL
1	A	10	LEU
1	A	16	ASP
1	A	22	ILE
1	A	56	VAL
1	A	66	LYS
1	A	71	VAL
1	A	75	THR
1	A	77	THR
1	A	84	LYS
1	A	90	LYS
1	A	103	LEU
1	A	115	SER
1	A	117	VAL
1	A	119	ARG
1	A	132	ARG
1	A	138	GLN
1	A	145	VAL
1	A	166	VAL
1	A	168	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	171	ASP
1	A	174	SER
1	A	177	VAL
1	A	202	ARG
1	A	206	LEU
1	A	215	LEU
1	A	229	MET
1	A	237	LYS
1	A	280	LEU
1	A	302	VAL
1	A	304	VAL
1	A	313	ARG
1	A	322	LYS
1	A	324	THR
1	A	329	VAL
1	A	337	ARG
1	A	347	ASN
1	A	380	LYS
1	A	383	LYS
1	A	387	ARG
1	A	392	ASN
1	A	394	ASP
1	A	400	VAL
1	A	402	GLN
1	A	405	LYS
1	A	406	VAL
1	A	408	MET
1	A	410	LYS
1	A	412	LYS
1	B	4	ILE
1	B	5	SER
1	B	9	VAL
1	B	10	LEU
1	B	24	LYS
1	B	26	ILE
1	B	31	ILE
1	B	58	VAL
1	B	88	LEU
1	B	101	THR
1	B	103	LEU
1	B	117	VAL
1	B	119	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	138	GLN
1	B	166	VAL
1	B	168	LYS
1	B	177	VAL
1	B	202	ARG
1	B	206	LEU
1	B	213	THR
1	B	215	LEU
1	B	231	LYS
1	B	249	LEU
1	B	251	ASP
1	B	277	SER
1	B	280	LEU
1	B	282	GLN
1	B	287	LEU
1	B	302	VAL
1	B	304	VAL
1	B	317	ASP
1	B	319	GLN
1	B	322	LYS
1	B	326	THR
1	B	329	VAL
1	B	337	ARG
1	B	361	VAL
1	B	377	ILE
1	B	380	LYS
1	B	406	VAL
1	B	411	SER
1	B	412	LYS
1	B	413	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	A	133	HIS
1	A	212	ASN
1	B	212	ASN
1	B	256	HIS
1	B	270	ASN
1	B	348	ASN
1	B	402	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	409	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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$
2	NAP	B	501	-	50,52,52	1.26	6 (12%)	71,80,80	1.74	14 (19%)
2	NAP	A	501	-	50,52,52	1.42	10 (20%)	71,80,80	1.60	11 (15%)
4	AKG	B	502	-	9,9,9	1.70	1 (11%)	11,11,11	1.58	3 (27%)

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	NAP	B	501	-	-	14/35/67/67	0/5/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	A	501	-	-	7/35/67/67	0/5/5/5
4	AKG	B	502	-	-	5/9/9/9	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	NAP	C5A-C4A	4.99	1.48	1.39
2	B	501	NAP	C5A-C4A	4.19	1.46	1.39
4	B	502	AKG	C2-C1	-3.86	1.47	1.53
2	A	501	NAP	C8A-N7A	2.97	1.37	1.31
2	B	501	NAP	C5A-C6A	2.96	1.49	1.41
2	A	501	NAP	C5A-N7A	-2.76	1.34	1.39
2	B	501	NAP	O4D-C1D	2.73	1.44	1.40
2	A	501	NAP	O4D-C1D	2.68	1.44	1.40
2	B	501	NAP	C5A-N7A	-2.47	1.34	1.39
2	A	501	NAP	C5A-C6A	2.43	1.47	1.41
2	A	501	NAP	C3N-C7N	2.43	1.54	1.50
2	A	501	NAP	PA-O3	2.31	1.62	1.59
2	A	501	NAP	P2B-O2B	2.28	1.63	1.59
2	B	501	NAP	C4A-N9A	-2.14	1.33	1.37
2	B	501	NAP	P2B-O2B	2.10	1.63	1.59
2	A	501	NAP	PN-O3	2.02	1.61	1.59
2	A	501	NAP	C4N-C3N	2.02	1.42	1.39

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	NAP	C5A-C4A-N3A	-6.41	117.89	126.72
2	B	501	NAP	C5A-C4A-N3A	-6.26	118.10	126.72
2	B	501	NAP	N3A-C4A-N9A	5.12	135.88	127.17
2	A	501	NAP	N3A-C4A-N9A	4.49	134.80	127.17
2	B	501	NAP	C2A-N3A-C4A	4.18	122.04	111.83
2	A	501	NAP	C2A-N3A-C4A	3.88	121.32	111.83
2	B	501	NAP	N3A-C2A-N1A	-3.52	123.25	128.58
2	B	501	NAP	C4A-C5A-N7A	-3.48	106.61	110.58
2	B	501	NAP	C6N-N1N-C2N	-3.34	119.03	121.88
2	A	501	NAP	C4A-C5A-N7A	-3.30	106.81	110.58
2	A	501	NAP	N3A-C2A-N1A	-3.29	123.60	128.58
2	B	501	NAP	C4A-N9A-C8A	3.07	108.96	105.74
2	A	501	NAP	O7N-C7N-N7N	-2.98	118.31	122.62
2	B	501	NAP	C5A-N7A-C8A	2.87	107.96	103.45
4	B	502	AKG	C3-C2-C1	2.78	120.58	115.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	NAP	O7N-C7N-N7N	-2.67	118.75	122.62
2	B	501	NAP	N9A-C8A-N7A	-2.46	110.45	113.94
2	B	501	NAP	O3X-P2B-O2X	2.43	116.91	107.80
2	A	501	NAP	C6N-N1N-C1D	2.43	124.49	119.73
2	A	501	NAP	C3N-C7N-N7N	2.33	120.61	117.74
2	A	501	NAP	O3X-P2B-O2X	2.29	116.40	107.80
4	B	502	AKG	O4-C5-C4	2.26	121.13	114.00
4	B	502	AKG	O2-C1-C2	2.17	119.60	113.59
2	B	501	NAP	O2N-PN-O1N	2.10	122.23	112.44
2	A	501	NAP	C6A-C5A-N7A	2.06	136.07	132.09
2	A	501	NAP	C5A-N7A-C8A	2.06	106.68	103.45
2	B	501	NAP	C3N-C7N-N7N	2.05	120.26	117.74
2	B	501	NAP	C6N-N1N-C1D	2.04	123.72	119.73

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NAP	PN-O3-PA-O5B
2	A	501	NAP	O4D-C1D-N1N-C2N
2	A	501	NAP	O4D-C1D-N1N-C6N
2	B	501	NAP	C5D-O5D-PN-O3
2	B	501	NAP	C5D-O5D-PN-O1N
2	B	501	NAP	C5D-O5D-PN-O2N
2	B	501	NAP	O4D-C1D-N1N-C2N
2	B	501	NAP	O4D-C1D-N1N-C6N
2	B	501	NAP	C2D-C1D-N1N-C2N
2	B	501	NAP	C2D-C1D-N1N-C6N
4	B	502	AKG	C1-C2-C3-C4
2	B	501	NAP	C2N-C3N-C7N-O7N
4	B	502	AKG	C2-C3-C4-C5
2	B	501	NAP	C4N-C3N-C7N-O7N
2	B	501	NAP	O4B-C4B-C5B-O5B
2	B	501	NAP	C3B-C4B-C5B-O5B
2	B	501	NAP	C4N-C3N-C7N-N7N
2	A	501	NAP	O4B-C4B-C5B-O5B
2	B	501	NAP	C2N-C3N-C7N-N7N
2	A	501	NAP	C3B-C4B-C5B-O5B
2	B	501	NAP	C5B-O5B-PA-O1A
4	B	502	AKG	O2-C1-C2-O5
4	B	502	AKG	O2-C1-C2-C3
2	A	501	NAP	C2D-C1D-N1N-C2N

Continued on next page...

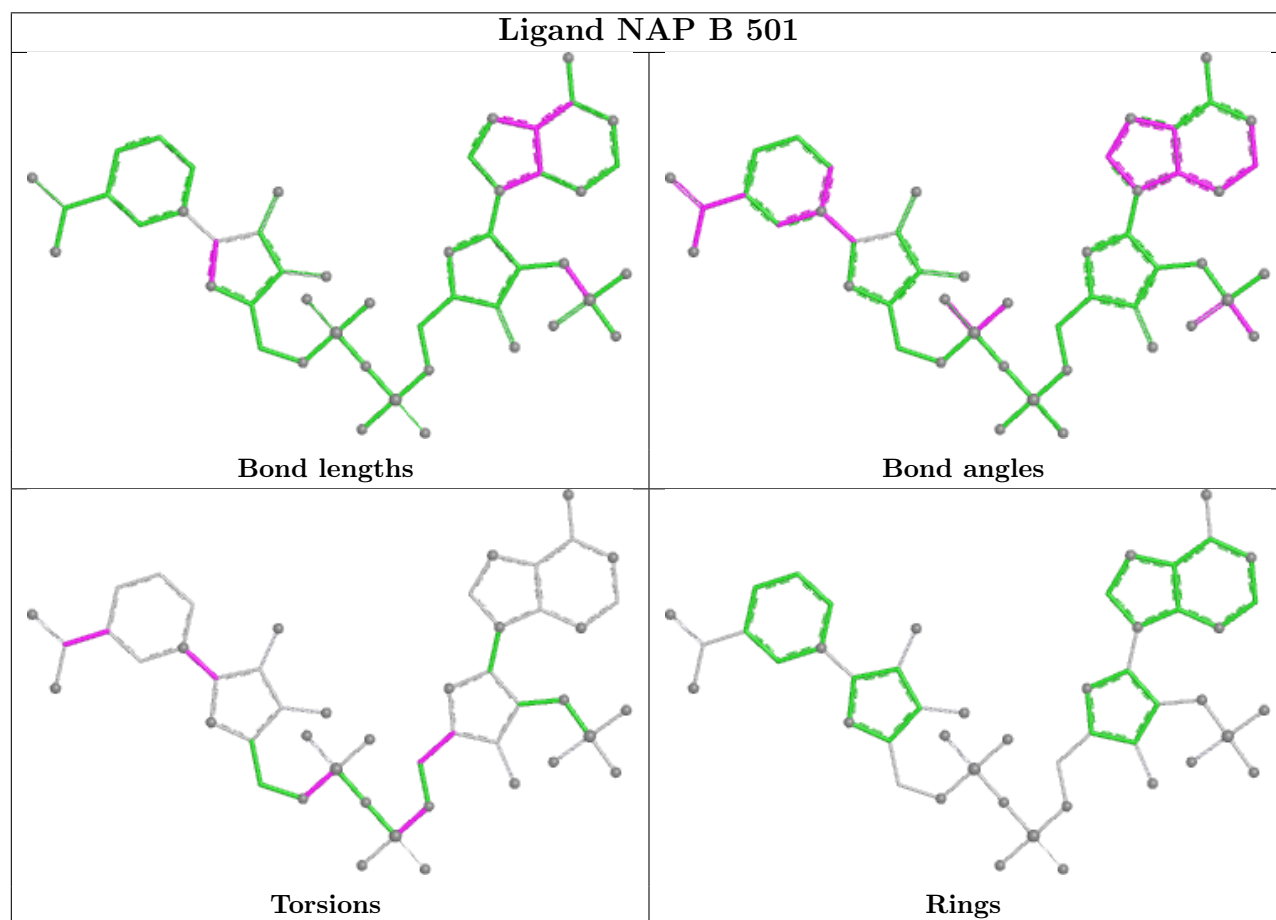
Continued from previous page...

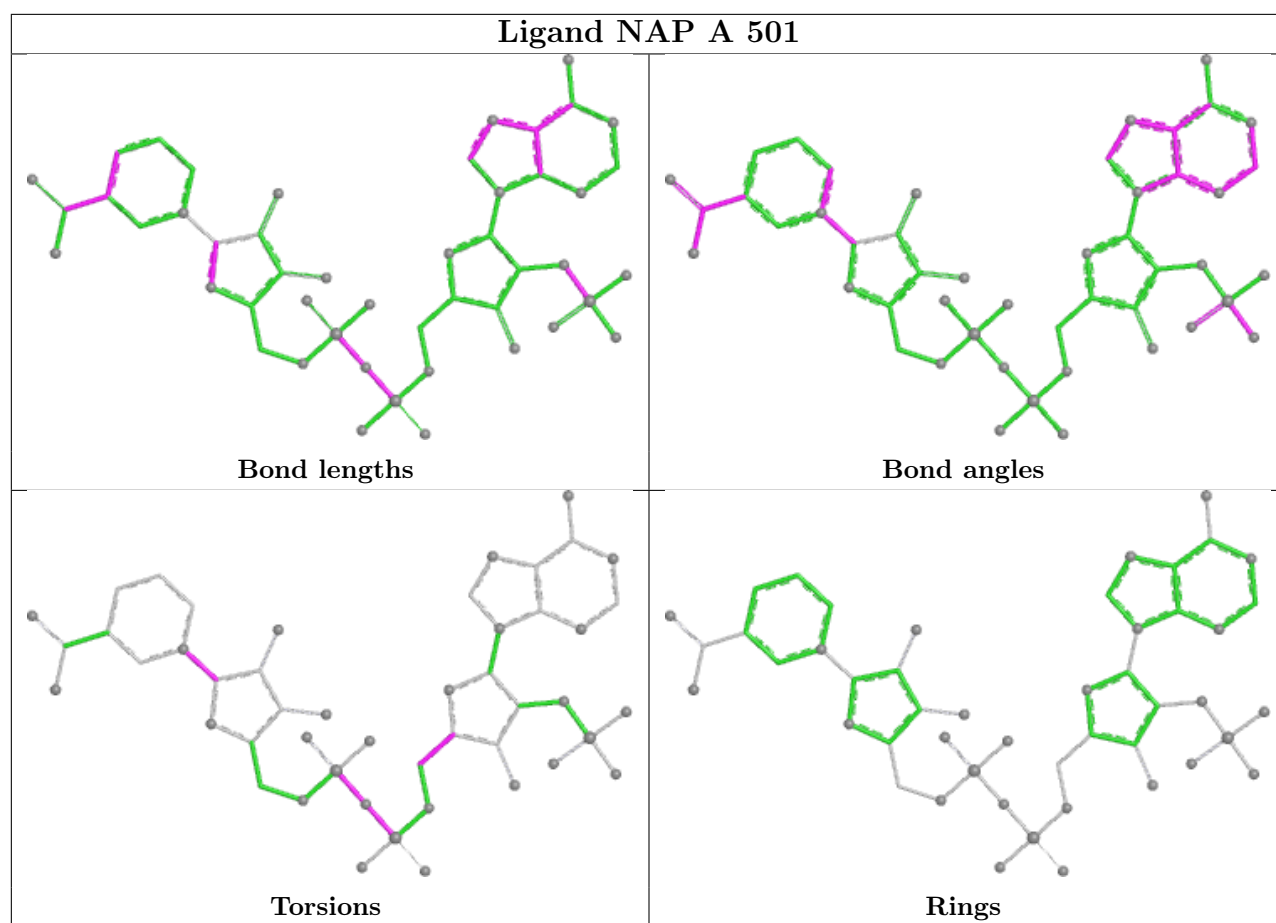
Mol	Chain	Res	Type	Atoms
4	B	502	AKG	O1-C1-C2-C3
2	A	501	NAP	PA-O3-PN-O2N

There are no ring outliers.

No monomer is involved in short contacts.

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	413/413 (100%)	0.15	4 (0%) 79 76	18, 47, 81, 153	0
1	B	413/413 (100%)	0.40	30 (7%) 21 17	19, 47, 106, 162	3 (0%)
All	All	826/826 (100%)	0.28	34 (4%) 41 37	18, 47, 94, 162	3 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	15	GLY	5.1
1	B	413	VAL	3.9
1	B	88	LEU	3.9
1	B	411	SER	3.5
1	B	83	VAL	3.2
1	B	324	THR	3.2
1	A	5	SER	3.0
1	B	315	TYR	2.9
1	B	86	PHE	2.7
1	B	412	LYS	2.5
1	B	382[A]	GLU	2.4
1	B	46	MET	2.4
1	B	4	ILE	2.4
1	B	398	ASP	2.3
1	B	92	TRP	2.3
1	A	410	LYS	2.2
1	B	410	LYS	2.2
1	B	87	ASN	2.2
1	B	321	GLY	2.2
1	B	26	ILE	2.1
1	B	325	SER	2.1
1	A	3	LYS	2.1
1	B	400	VAL	2.1
1	B	312	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	50	ASP	2.1
1	B	391	LEU	2.1
1	B	21	VAL	2.0
1	B	404	LEU	2.0
1	A	161	GLY	2.0
1	B	57	THR	2.0
1	B	58	VAL	2.0
1	B	407	ALA	2.0
1	B	47	GLU	2.0
1	B	23	TRP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

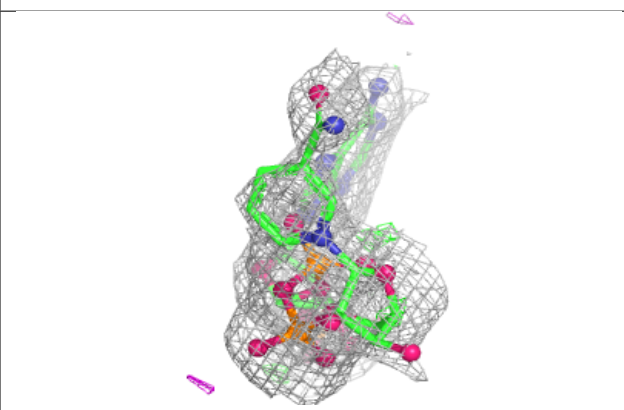
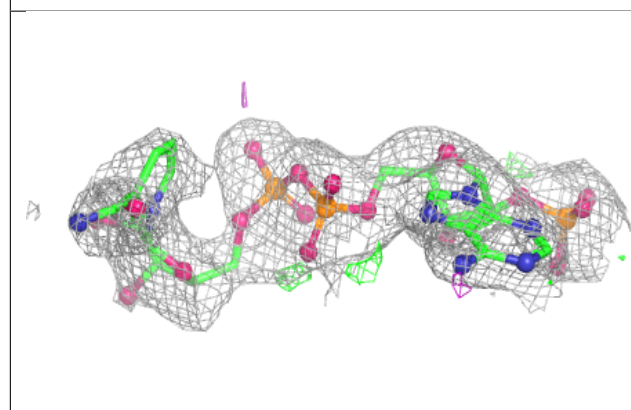
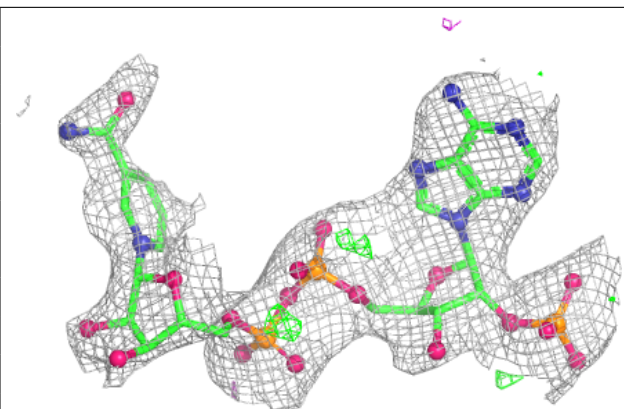
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	AKG	B	502	10/10	0.62	0.14	60,74,84,86	0
2	NAP	B	501	48/48	0.90	0.10	55,60,65,67	0
3	CA	A	503	1/1	0.93	0.04	45,45,45,45	0
2	NAP	A	501	48/48	0.93	0.08	38,42,46,46	0
3	CA	A	502	1/1	0.95	0.05	60,60,60,60	0

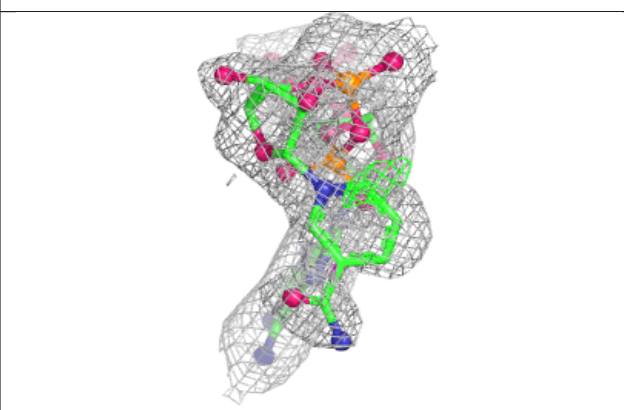
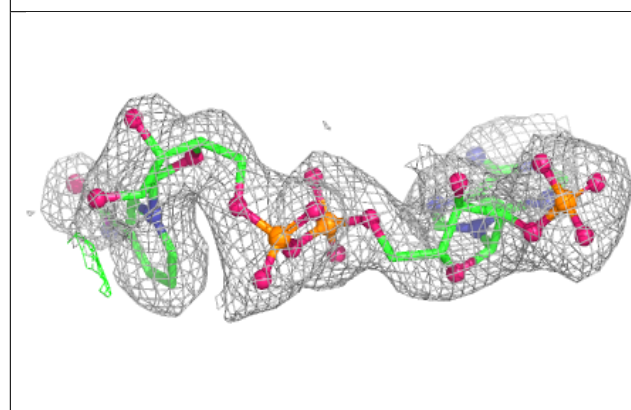
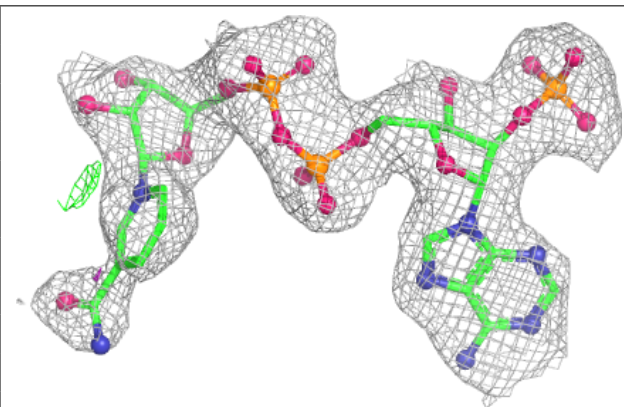
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP B 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 NAP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.