Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2023 – 10:46 PM JST

PDB ID	:	6AJ6
Title	:	Crystal structure of Trypanosoma brucei glycosomal isocitrate dehydrogenase in complex with NADP+
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	:	3.20 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:

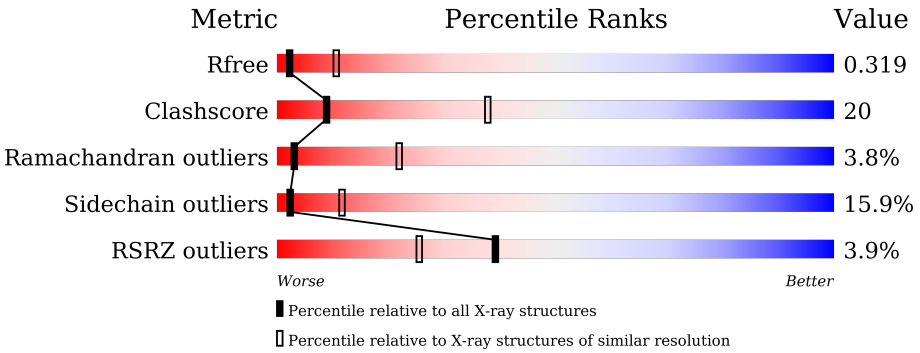
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	413	4% 54% 36% 9%
1	C	413	4% 68% 26% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6660 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.

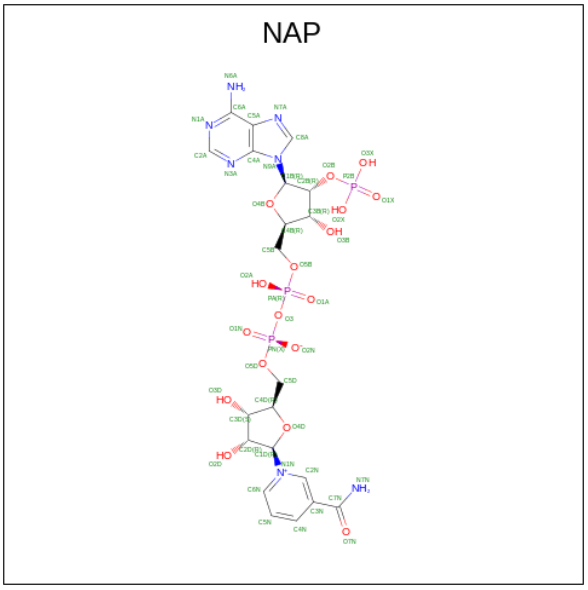
- Molecule 1 is a protein called Isocitrate dehydrogenase [NADP].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	413	Total	C	N	O	S	0	0	0
			3282	2084	563	613	22			
1	C	413	Total	C	N	O	S	0	0	0
			3282	2084	563	613	22			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



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

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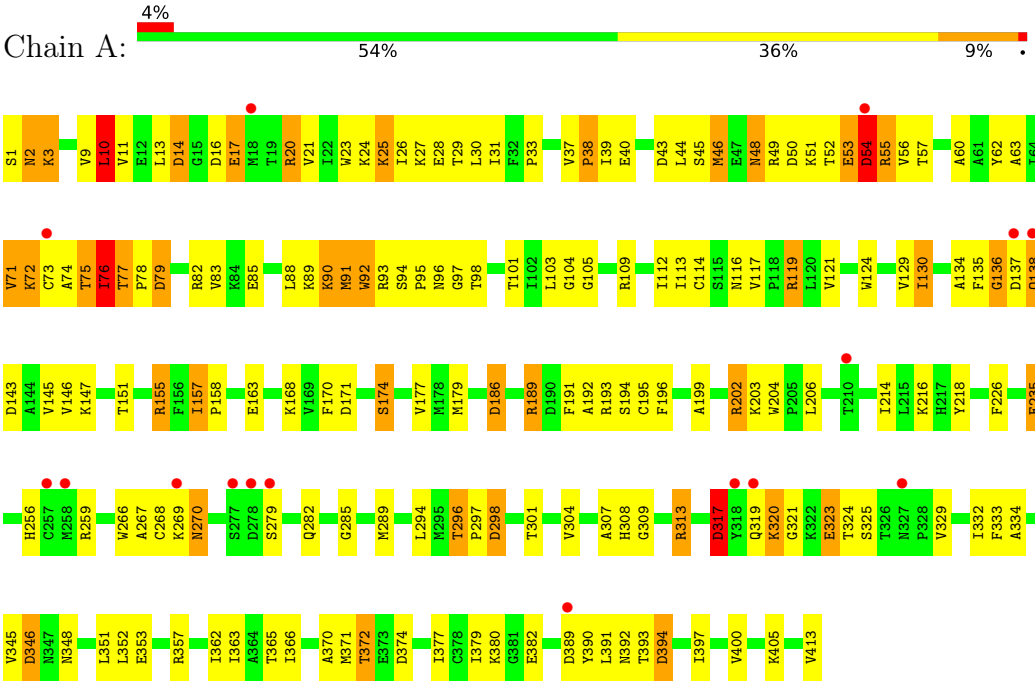
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

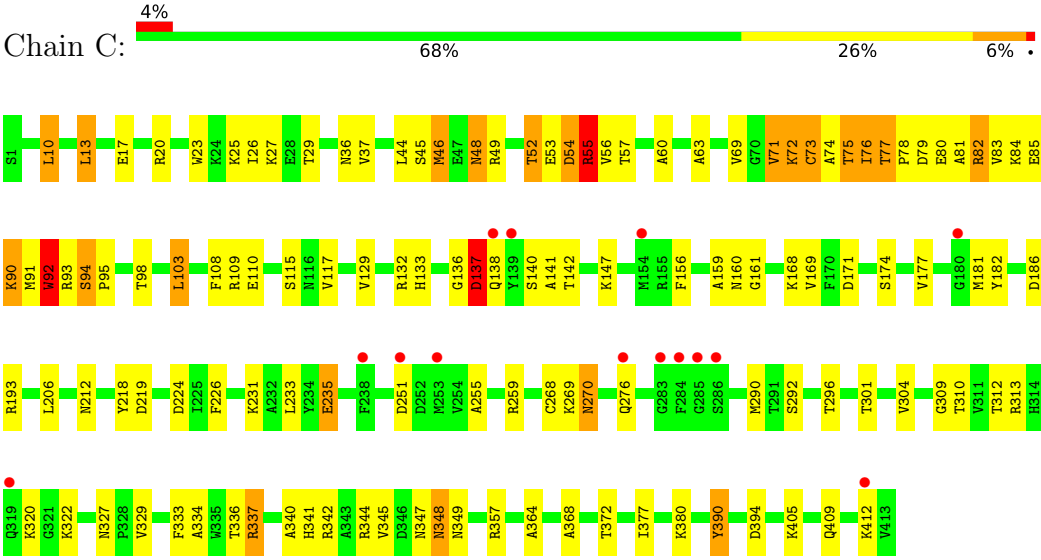
• Molecule 1: Isocitrate dehydrogenase [NADP]

Chain A:



• Molecule 1: Isocitrate dehydrogenase [NADP]

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	62.44Å 109.75Å 64.96Å 90.00° 89.98° 90.00°	Depositor
Resolution (Å)	45.02 – 3.20 45.03 – 3.20	Depositor EDS
% Data completeness (in resolution range)	83.9 (45.02-3.20) 87.0 (45.03-3.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.212 , 0.309 0.228 , 0.319	Depositor DCC
R_{free} test set	582 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å^2)	68.6	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 48.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -l,k,h 0.226 for h,-k,-l 0.008 for -l,-k,-h	Xtriage
Reported twinning fraction	0.609 for H, K, L 0.391 for h,-k,-l	Depositor
Outliers	0 of 12657 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	6660	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: 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	0.78	0/3350	1.05	10/4522 (0.2%)
1	C	0.68	1/3350 (0.0%)	0.88	5/4522 (0.1%)
All	All	0.73	1/6700 (0.0%)	0.97	15/9044 (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	A	0	5
1	C	0	4
All	All	0	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	186	ASP	CB-CG	5.50	1.63	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	137	ASP	N-CA-C	-8.48	88.11	111.00
1	C	55	ARG	N-CA-C	7.20	130.43	111.00
1	A	90	LYS	N-CA-C	6.43	128.37	111.00
1	A	53	GLU	N-CA-C	-6.29	94.02	111.00
1	A	55	ARG	N-CA-C	6.26	127.90	111.00
1	A	193	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	A	10	LEU	CA-CB-CG	5.92	128.92	115.30
1	A	342	ARG	NE-CZ-NH2	-5.67	117.46	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	202	ARG	NE-CZ-NH2	5.50	123.05	120.30
1	C	103	LEU	CA-CB-CG	5.46	127.86	115.30
1	C	94	SER	C-N-CD	5.22	139.36	128.40
1	C	186	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	54	ASP	N-CA-C	-5.04	97.40	111.00
1	A	342	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	A	155	ARG	NE-CZ-NH1	5.01	122.80	120.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	GLY	Peptide
1	A	136	GLY	Peptide
1	A	139	TYR	Peptide
1	A	320	LYS	Peptide
1	A	71	VAL	Peptide
1	C	159	ALA	Peptide
1	C	310	THR	Peptide
1	C	36	ASN	Peptide
1	C	71	VAL	Peptide

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	3282	0	3274	167	0
1	C	3282	0	3271	107	0
2	A	48	0	25	4	0
2	C	48	0	25	3	0
All	All	6660	0	6595	269	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 20.

All (269) 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:C:341:HIS:O	1:C:345:VAL:HG23	1.31	1.25
1:A:79:ASP:O	1:A:83:VAL:HG13	1.61	1.01
1:C:136:GLY:HA3	1:C:140:SER:OG	1.61	1.00
1:C:341:HIS:O	1:C:345:VAL:CG2	2.10	1.00
1:A:79:ASP:CB	1:A:82:ARG:HB2	1.96	0.96
1:A:77:THR:HG23	1:A:94:SER:HB2	1.46	0.95
1:A:85:GLU:O	1:A:88:LEU:HD12	1.67	0.95
1:A:52:THR:OG1	1:A:54:ASP:O	1.85	0.93
1:C:344:ARG:HG3	1:C:344:ARG:HH11	1.36	0.90
1:A:77:THR:CG2	1:A:94:SER:HB2	2.01	0.89
1:C:49:ARG:HH11	1:C:55:ARG:HH12	1.18	0.86
1:C:82:ARG:NH2	2:C:501:NAP:O3D	2.07	0.86
1:C:49:ARG:HH11	1:C:55:ARG:NH1	1.74	0.85
1:A:79:ASP:HB2	1:A:82:ARG:CG	2.08	0.84
1:A:82:ARG:NH1	1:A:85:GLU:OE2	2.11	0.83
1:A:49:ARG:HH11	1:A:55:ARG:NH1	1.76	0.83
1:A:2:ASN:HD22	1:A:3:LYS:H	1.24	0.82
1:C:109:ARG:HB3	1:C:290:MET:HE2	1.63	0.80
1:C:49:ARG:HD2	1:C:55:ARG:NH1	1.96	0.80
1:A:85:GLU:O	1:A:88:LEU:CD1	2.29	0.79
1:C:54:ASP:C	1:C:55:ARG:HG2	2.04	0.78
1:C:83:VAL:HA	1:C:88:LEU:HB2	1.65	0.78
1:C:109:ARG:HB3	1:C:290:MET:CE	2.14	0.78
1:A:317:ASP:OD1	1:A:317:ASP:N	2.17	0.76
1:C:49:ARG:HA	1:C:52:THR:CG2	2.15	0.75
1:C:48:ASN:O	1:C:52:THR:HG22	1.86	0.75
1:A:75:THR:HG22	1:A:95:PRO:HD2	1.68	0.75
1:A:79:ASP:HB3	1:A:82:ARG:HB2	1.66	0.75
1:C:26:ILE:HG13	1:C:27:LYS:N	2.03	0.74
1:C:72:LYS:HE2	1:C:74:ALA:HB3	1.69	0.74
1:C:52:THR:HG21	1:C:56:VAL:HG23	1.69	0.74
1:C:23:TRP:CZ2	1:C:72:LYS:HB2	2.23	0.74
1:C:26:ILE:HG13	1:C:27:LYS:H	1.52	0.74
1:A:79:ASP:CB	1:A:82:ARG:CB	2.67	0.72
1:C:133:HIS:O	1:C:270:ASN:CB	2.38	0.72
1:C:77:THR:HG23	1:C:94:SER:HB2	1.71	0.71
1:C:83:VAL:HG23	1:C:84:LYS:N	2.06	0.71
1:A:138:GLN:HA	1:A:141:ALA:HB3	1.74	0.70
1:A:71:VAL:O	1:A:71:VAL:HG13	1.92	0.70
1:C:49:ARG:NH1	1:C:55:ARG:HH12	1.89	0.70
1:A:10:LEU:O	1:A:39:ILE:HA	1.92	0.69
1:A:79:ASP:O	1:A:83:VAL:CG1	2.38	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:ARG:HG3	1:C:344:ARG:NH1	2.08	0.68
1:A:79:ASP:HB2	1:A:82:ARG:HB2	1.74	0.68
1:A:92:TRP:HE3	1:A:92:TRP:HA	1.59	0.68
1:C:347:ASN:O	1:C:348:ASN:C	2.28	0.68
1:A:83:VAL:HA	1:A:88:LEU:HB2	1.74	0.67
1:C:192:ALA:HA	1:C:226:PHE:CZ	2.30	0.67
1:A:92:TRP:HA	1:A:92:TRP:CE3	2.29	0.67
1:A:26:ILE:HG13	1:A:27:LYS:H	1.60	0.67
1:A:79:ASP:HB3	1:A:82:ARG:CB	2.26	0.66
1:C:255:ALA:O	1:C:259:ARG:HG2	1.96	0.66
1:A:23:TRP:CH2	1:A:72:LYS:HB2	2.30	0.66
1:A:79:ASP:HB2	1:A:82:ARG:HG3	1.77	0.65
1:C:75:THR:HG22	1:C:95:PRO:HD2	1.78	0.65
1:A:79:ASP:HB2	1:A:82:ARG:CB	2.27	0.64
1:C:133:HIS:O	1:C:270:ASN:CG	2.37	0.63
1:A:82:ARG:HH11	1:A:85:GLU:CD	2.01	0.63
1:A:44:LEU:C	1:A:49:ARG:HE	2.01	0.62
1:C:76:ILE:O	1:C:77:THR:C	2.38	0.62
1:C:90:LYS:O	1:C:91:MET:HG3	1.99	0.62
1:A:52:THR:HG21	1:A:56:VAL:HG23	1.82	0.62
1:C:69:VAL:HG23	1:C:342:ARG:NH1	2.15	0.61
1:C:110:GLU:HG3	1:C:129:VAL:HG22	1.82	0.61
1:A:79:ASP:HB3	1:A:82:ARG:N	2.16	0.61
1:A:52:THR:HG23	1:A:52:THR:O	1.99	0.61
1:A:43:ASP:OD2	1:A:45:SER:N	2.34	0.61
1:C:137:ASP:O	1:C:141:ALA:HB2	2.00	0.61
1:C:82:ARG:NH2	2:C:501:NAP:HO3N	1.99	0.61
1:A:49:ARG:HH11	1:A:55:ARG:HH11	1.46	0.61
1:A:79:ASP:CB	1:A:82:ARG:CG	2.77	0.60
1:A:2:ASN:HD22	1:A:3:LYS:N	1.97	0.60
1:C:82:ARG:O	1:C:85:GLU:N	2.33	0.60
1:C:80:GLU:O	1:C:83:VAL:HG22	2.01	0.60
1:C:90:LYS:HG2	1:C:91:MET:HG2	1.84	0.60
1:A:23:TRP:HA	1:A:26:ILE:HG12	1.83	0.59
1:A:92:TRP:O	1:A:93:ARG:HB2	2.01	0.59
1:C:364:ALA:O	1:C:368:ALA:HB2	2.02	0.59
1:A:72:LYS:HE2	1:A:74:ALA:HB3	1.84	0.59
1:C:52:THR:HG23	1:C:52:THR:O	2.03	0.59
1:A:53:GLU:HA	1:A:92:TRP:CH2	2.37	0.59
1:A:366:ILE:HA	1:A:370:ALA:O	2.03	0.59
1:A:9:VAL:HB	1:A:67:HIS:CD2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:HIS:O	1:C:270:ASN:HA	2.02	0.59
1:A:95:PRO:O	1:A:97:GLY:N	2.36	0.58
1:A:49:ARG:NH1	1:A:55:ARG:NH1	2.50	0.58
1:A:186:ASP:OD2	1:A:189:ARG:NH1	2.37	0.58
1:C:49:ARG:O	1:C:52:THR:HG23	2.03	0.58
1:A:95:PRO:O	1:A:96:ASN:C	2.36	0.58
1:C:92:TRP:HA	1:C:92:TRP:CE3	2.38	0.57
1:A:90:LYS:O	1:A:90:LYS:HG3	2.05	0.56
1:C:10:LEU:HD21	1:C:71:VAL:HG12	1.87	0.56
1:A:23:TRP:O	1:A:27:LYS:HB2	2.05	0.56
1:A:76:ILE:O	1:A:77:THR:C	2.43	0.56
1:C:133:HIS:O	1:C:270:ASN:CA	2.54	0.56
1:A:2:ASN:ND2	1:A:3:LYS:H	2.01	0.56
1:C:72:LYS:HE2	1:C:74:ALA:CB	2.34	0.56
1:A:82:ARG:O	1:A:85:GLU:HB3	2.07	0.55
1:C:91:MET:O	1:C:92:TRP:HB2	2.06	0.55
1:A:72:LYS:CE	1:A:74:ALA:HB3	2.36	0.55
1:C:79:ASP:H	1:C:82:ARG:HG3	1.71	0.55
1:A:77:THR:OG1	1:A:94:SER:HB2	2.06	0.54
1:C:81:ALA:O	1:C:84:LYS:HB2	2.08	0.54
1:A:17:GLU:OE2	1:A:82:ARG:NH2	2.32	0.54
1:A:121:VAL:HB	1:A:124:TRP:CH2	2.43	0.54
1:C:83:VAL:HG23	1:C:84:LYS:H	1.72	0.54
1:C:49:ARG:O	1:C:52:THR:O	2.26	0.54
1:A:78:PRO:HD2	1:A:93:ARG:O	2.08	0.53
1:A:214:ILE:HG22	1:A:214:ILE:O	2.08	0.53
1:A:49:ARG:HD2	1:A:55:ARG:NH1	2.23	0.53
1:C:231:LYS:HA	1:C:235:GLU:HB2	1.88	0.53
1:A:218:TYR:HA	1:C:177:VAL:HG21	1.91	0.53
1:A:394:ASP:OD2	1:A:394:ASP:N	2.42	0.53
1:C:317:ASP:O	1:C:320:LYS:N	2.40	0.53
1:C:49:ARG:HB3	1:C:55:ARG:HH11	1.72	0.53
1:C:92:TRP:HA	1:C:92:TRP:HE3	1.73	0.53
1:A:82:ARG:O	1:A:85:GLU:N	2.41	0.53
1:A:266:TRP:CD1	1:A:267:ALA:N	2.77	0.53
1:A:9:VAL:HG22	1:A:38:PRO:HB2	1.89	0.52
1:A:53:GLU:HA	1:A:92:TRP:HH2	1.72	0.52
1:A:309:GLY:CA	2:A:501:NAP:H6N	2.40	0.52
1:A:26:ILE:HG13	1:A:27:LYS:N	2.24	0.52
1:A:199:ALA:HB1	1:A:204:TRP:O	2.09	0.52
1:A:137:ASP:O	1:A:141:ALA:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:GLN:C	1:A:321:GLY:N	2.63	0.52
1:C:83:VAL:CG2	1:C:84:LYS:N	2.73	0.52
1:C:136:GLY:HA2	1:C:140:SER:H	1.74	0.52
1:A:26:ILE:CG1	1:A:27:LYS:N	2.72	0.52
1:A:317:ASP:HA	1:A:320:LYS:HB3	1.91	0.51
1:C:92:TRP:O	1:C:93:ARG:HB2	2.10	0.51
1:A:77:THR:CB	1:A:94:SER:HB2	2.40	0.51
1:A:170:PHE:CD1	1:C:182:TYR:CD1	2.99	0.50
1:C:23:TRP:CZ3	1:C:72:LYS:HG3	2.46	0.50
1:C:46:MET:SD	1:C:78:PRO:HG3	2.51	0.50
1:A:296:THR:OG1	1:A:301:THR:HB	2.11	0.50
1:C:190:ASP:OD2	1:C:193:ARG:NH1	2.44	0.50
1:A:346:ASP:OD1	1:A:346:ASP:N	2.45	0.50
1:A:23:TRP:CZ2	1:A:72:LYS:HB2	2.46	0.50
1:A:23:TRP:HA	1:A:26:ILE:CG1	2.42	0.49
1:C:26:ILE:CG1	1:C:27:LYS:H	2.23	0.49
1:C:364:ALA:O	1:C:368:ALA:CB	2.60	0.49
1:A:49:ARG:HB3	1:A:55:ARG:HD2	1.93	0.49
1:A:296:THR:HB	1:A:298:ASP:OD1	2.12	0.49
1:A:323:GLU:HB3	1:A:392:ASN:HD21	1.77	0.49
1:A:1:SER:O	1:A:1:SER:OG	2.29	0.48
1:C:344:ARG:NH1	1:C:344:ARG:CG	2.73	0.48
1:C:44:LEU:HD13	1:C:57:THR:HG22	1.95	0.48
1:A:10:LEU:HD22	1:A:11:VAL:H	1.79	0.48
1:A:49:ARG:NH1	1:A:55:ARG:HH12	2.11	0.48
1:A:397:ILE:O	1:A:400:VAL:CG2	2.62	0.48
1:A:341:HIS:O	1:A:345:VAL:HG23	2.13	0.48
1:C:54:ASP:H	1:C:92:TRP:HH2	1.59	0.48
1:C:60:ALA:O	1:C:63:ALA:HB3	2.13	0.48
1:A:77:THR:OG1	1:A:94:SER:CB	2.61	0.48
1:A:43:ASP:OD2	1:A:43:ASP:C	2.52	0.48
1:A:143:ASP:HB3	1:A:179:MET:HG3	1.95	0.48
1:A:329:VAL:HA	1:A:332:ILE:HD12	1.95	0.47
1:A:202:ARG:O	1:A:203:LYS:HB2	2.13	0.47
1:C:23:TRP:CE2	1:C:72:LYS:HD2	2.50	0.47
1:A:71:VAL:CG2	1:A:334:ALA:O	2.62	0.47
1:A:157:ILE:HD12	1:A:158:PRO:O	2.14	0.47
1:C:110:GLU:CG	1:C:129:VAL:HG22	2.45	0.47
1:A:109:ARG:O	1:A:129:VAL:HA	2.14	0.47
1:A:117:VAL:HA	1:A:379:ILE:HD13	1.97	0.47
1:A:146:VAL:HG13	1:C:156:PHE:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:ARG:HD3	2:A:501:NAP:O1X	2.15	0.47
1:C:390:TYR:CD1	1:C:390:TYR:C	2.87	0.47
1:A:26:ILE:HD12	1:A:27:LYS:N	2.30	0.47
1:A:393:THR:HB	1:A:394:ASP:OD2	2.14	0.47
1:C:304:VAL:HG21	1:C:334:ALA:O	2.14	0.47
1:A:116:ASN:OD1	1:A:116:ASN:N	2.48	0.46
1:A:49:ARG:O	1:A:52:THR:HG23	2.15	0.46
1:A:98:THR:O	1:A:101:THR:HB	2.16	0.46
1:A:24:LYS:O	1:A:28:GLU:N	2.48	0.46
1:A:113:ILE:HG23	1:A:113:ILE:O	2.15	0.46
1:A:289:MET:SD	1:A:329:VAL:HG21	2.55	0.46
1:A:29:THR:HB	1:A:30:LEU:HG	1.98	0.46
1:A:266:TRP:HD1	1:A:267:ALA:N	2.14	0.46
1:C:10:LEU:HD21	1:C:71:VAL:CG1	2.46	0.46
1:A:46:MET:O	1:A:50:ASP:N	2.42	0.46
1:A:371:MET:O	1:A:391:LEU:N	2.49	0.46
1:A:28:GLU:O	1:A:33:PRO:CD	2.64	0.45
1:C:26:ILE:CG1	1:C:27:LYS:N	2.76	0.45
1:A:16:ASP:OD1	1:A:49:ARG:NH2	2.49	0.45
1:A:348:ASN:OD1	1:A:351:LEU:N	2.35	0.45
1:C:327:ASN:OD1	1:C:329:VAL:HG22	2.16	0.45
1:A:92:TRP:CE3	1:A:92:TRP:CA	2.97	0.45
1:C:46:MET:HG2	1:C:76:ILE:HG12	1.97	0.45
1:A:23:TRP:CH2	1:A:72:LYS:CB	2.98	0.45
1:A:76:ILE:N	1:A:76:ILE:HD12	2.32	0.45
1:A:45:SER:O	1:A:48:ASN:N	2.49	0.45
1:A:309:GLY:HA3	2:A:501:NAP:H6N	1.99	0.45
1:C:25:LYS:O	1:C:29:THR:N	2.36	0.45
1:C:82:ARG:C	1:C:85:GLU:H	2.20	0.45
1:A:79:ASP:CA	1:A:82:ARG:HB2	2.47	0.45
1:A:20:ARG:NH2	1:A:43:ASP:OD1	2.49	0.44
1:A:179:MET:O	1:C:181:MET:N	2.50	0.44
1:A:397:ILE:O	1:A:400:VAL:HG22	2.17	0.44
1:C:13:LEU:O	1:C:72:LYS:HB3	2.17	0.44
1:A:95:PRO:C	1:A:97:GLY:N	2.68	0.44
1:C:46:MET:HE3	1:C:49:ARG:HH12	1.82	0.44
1:A:348:ASN:OD1	1:A:351:LEU:HB3	2.18	0.44
1:C:347:ASN:O	1:C:348:ASN:O	2.36	0.44
1:A:23:TRP:CZ3	1:A:72:LYS:HG3	2.53	0.44
1:A:54:ASP:OD2	1:A:54:ASP:N	2.51	0.44
1:A:371:MET:HG3	1:A:372:THR:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:LEU:O	1:A:14:ASP:C	2.57	0.43
1:A:129:VAL:HG12	1:A:130:ILE:N	2.33	0.43
1:C:23:TRP:CH2	1:C:72:LYS:HB2	2.53	0.43
1:A:71:VAL:HG23	1:A:334:ALA:O	2.19	0.43
1:A:134:ALA:H	1:A:270:ASN:CG	2.21	0.43
1:A:39:ILE:HG22	1:A:40:GLU:N	2.34	0.43
1:A:179:MET:HB2	1:C:218:TYR:CD1	2.52	0.43
1:A:256:HIS:HA	1:A:259:ARG:HE	1.83	0.43
1:C:133:HIS:O	1:C:270:ASN:ND2	2.51	0.43
1:A:25:LYS:O	1:A:29:THR:OG1	2.31	0.43
1:A:112:ILE:HD11	1:A:333:PHE:CG	2.53	0.43
1:A:362:ILE:HG12	1:A:400:VAL:HG11	2.01	0.43
1:A:71:VAL:O	1:A:71:VAL:CG1	2.63	0.43
1:A:119:ARG:HG2	1:A:124:TRP:HE3	1.84	0.43
1:A:192:ALA:HA	1:A:226:PHE:CZ	2.54	0.43
1:C:20:ARG:NH2	1:C:45:SER:OG	2.52	0.43
1:A:23:TRP:O	1:A:27:LYS:CB	2.66	0.43
1:A:28:GLU:O	1:A:33:PRO:CG	2.66	0.43
1:A:77:THR:HG23	1:A:94:SER:CB	2.34	0.43
1:C:138:GLN:HA	1:C:141:ALA:HB3	2.01	0.43
1:A:21:VAL:HG12	1:A:25:LYS:HE2	2.00	0.42
1:A:49:ARG:NH2	1:A:76:ILE:HD11	2.34	0.42
1:C:108:PHE:HB3	1:C:129:VAL:CG1	2.49	0.42
1:C:73:CYS:SG	1:C:73:CYS:O	2.77	0.42
1:C:212:ASN:HA	1:C:219:ASP:HB2	2.00	0.42
1:A:195:CYS:O	1:A:196:PHE:C	2.57	0.42
1:C:83:VAL:CG2	1:C:84:LYS:H	2.33	0.42
1:A:23:TRP:CD1	1:A:27:LYS:HE2	2.54	0.42
1:C:49:ARG:NH1	1:C:76:ILE:HD11	2.34	0.42
1:A:151:THR:OG1	1:A:171:ASP:OD1	2.24	0.42
1:C:309:GLY:HA2	2:C:501:NAP:H6N	2.02	0.42
1:A:90:LYS:HD2	1:A:91:MET:HE2	2.02	0.42
1:A:79:ASP:HB3	1:A:82:ARG:H	1.85	0.41
1:A:343:ALA:O	1:A:346:ASP:N	2.53	0.41
1:A:60:ALA:O	1:A:63:ALA:HB3	2.20	0.41
1:A:62:TYR:O	1:A:65:LYS:HB3	2.20	0.41
1:C:317:ASP:HB3	1:C:322:LYS:HB2	2.03	0.41
1:A:45:SER:O	1:A:46:MET:C	2.58	0.41
1:A:72:LYS:HG2	1:A:74:ALA:H	1.86	0.41
1:A:343:ALA:O	1:A:344:ARG:C	2.57	0.41
1:C:133:HIS:O	1:C:270:ASN:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:THR:OG1	1:C:301:THR:HB	2.20	0.41
1:C:342:ARG:HA	1:C:342:ARG:NE	2.36	0.41
1:A:53:GLU:O	1:A:54:ASP:CB	2.68	0.41
1:C:337:ARG:O	1:C:340:ALA:HB3	2.21	0.41
1:A:121:VAL:HB	1:A:124:TRP:CZ2	2.56	0.41
1:A:79:ASP:CB	1:A:82:ARG:HG2	2.50	0.41
1:A:309:GLY:HA2	2:A:501:NAP:H6N	2.03	0.41
1:C:23:TRP:CD2	1:C:72:LYS:HD2	2.55	0.41
1:C:312:THR:O	1:C:315:TYR:N	2.54	0.41
1:A:296:THR:HG22	1:A:297:PRO:HD2	2.03	0.41
1:C:82:ARG:O	1:C:85:GLU:CB	2.69	0.41
1:A:114:CYS:SG	1:A:117:VAL:HG12	2.60	0.40
1:A:45:SER:O	1:A:49:ARG:N	2.53	0.40
1:A:266:TRP:CD1	1:A:266:TRP:C	2.95	0.40
1:C:54:ASP:N	1:C:92:TRP:CH2	2.80	0.40
1:A:50:ASP:O	1:A:51:LYS:C	2.60	0.40
1:C:82:ARG:O	1:C:85:GLU:HB3	2.21	0.40
1:A:191:PHE:CZ	1:A:267:ALA:HB1	2.57	0.40
1:C:49:ARG:HA	1:C:52:THR:HG22	2.00	0.40
1:C:333:PHE:HA	1:C:336:THR:OG1	2.21	0.40
1:A:104:GLY:O	1:A:294:LEU:HD11	2.21	0.40
1:A:119:ARG:HB3	1:A:124:TRP:HE3	1.87	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	411/413 (100%)	318 (77%)	74 (18%)	19 (5%)	2	18
1	C	411/413 (100%)	355 (86%)	44 (11%)	12 (3%)	4	28
All	All	822/826 (100%)	673 (82%)	118 (14%)	31 (4%)	3	22

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	135	PHE
1	A	235	GLU
1	A	308	HIS
1	A	323	GLU
1	C	72	LYS
1	C	235	GLU
1	C	318	TYR
1	C	348	ASN
1	A	31	ILE
1	A	72	LYS
1	A	73	CYS
1	A	307	ALA
1	C	160	ASN
1	A	136	GLY
1	A	285	GLY
1	A	317	ASP
1	A	365	THR
1	C	73	CYS
1	C	92	TRP
1	C	161	GLY
1	A	3	LYS
1	A	65	LYS
1	C	77	THR
1	C	90	LYS
1	C	224	ASP
1	A	14	ASP
1	A	174	SER
1	A	76	ILE
1	C	76	ILE
1	A	77	THR
1	A	38	PRO

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	353/353 (100%)	288 (82%)	65 (18%)	1 8
1	C	353/353 (100%)	306 (87%)	47 (13%)	4 18
All	All	706/706 (100%)	594 (84%)	112 (16%)	2 12

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	10	LEU
1	A	17	GLU
1	A	20	ARG
1	A	25	LYS
1	A	37	VAL
1	A	46	MET
1	A	48	ASN
1	A	54	ASP
1	A	57	THR
1	A	65	LYS
1	A	75	THR
1	A	76	ILE
1	A	79	ASP
1	A	89	LYS
1	A	91	MET
1	A	92	TRP
1	A	103	LEU
1	A	119	ARG
1	A	130	ILE
1	A	138	GLN
1	A	140	SER
1	A	145	VAL
1	A	147	LYS
1	A	155	ARG
1	A	157	ILE
1	A	163	GLU
1	A	168	LYS
1	A	174	SER
1	A	177	VAL
1	A	186	ASP
1	A	189	ARG
1	A	194	SER
1	A	206	LEU
1	A	216	LYS

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Mol	Chain	Res	Type
1	A	235	GLU
1	A	247	HIS
1	A	251	ASP
1	A	268	CYS
1	A	269	LYS
1	A	270	ASN
1	A	279	SER
1	A	282	GLN
1	A	296	THR
1	A	298	ASP
1	A	304	VAL
1	A	313	ARG
1	A	317	ASP
1	A	324	THR
1	A	325	SER
1	A	346	ASP
1	A	352	LEU
1	A	353	GLU
1	A	357	ARG
1	A	363	ILE
1	A	372	THR
1	A	374	ASP
1	A	377	ILE
1	A	380	LYS
1	A	382	GLU
1	A	389	ASP
1	A	390	TYR
1	A	394	ASP
1	A	405	LYS
1	A	413	VAL
1	C	10	LEU
1	C	13	LEU
1	C	17	GLU
1	C	37	VAL
1	C	46	MET
1	C	48	ASN
1	C	52	THR
1	C	53	GLU
1	C	54	ASP
1	C	55	ARG
1	C	75	THR
1	C	82	ARG

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Mol	Chain	Res	Type
1	C	88	LEU
1	C	92	TRP
1	C	98	THR
1	C	103	LEU
1	C	115	SER
1	C	117	VAL
1	C	132	ARG
1	C	137	ASP
1	C	142	THR
1	C	147	LYS
1	C	168	LYS
1	C	169	VAL
1	C	171	ASP
1	C	174	SER
1	C	206	LEU
1	C	233	LEU
1	C	251	ASP
1	C	268	CYS
1	C	269	LYS
1	C	270	ASN
1	C	276	GLN
1	C	292	SER
1	C	313	ARG
1	C	317	ASP
1	C	337	ARG
1	C	349	ASN
1	C	357	ARG
1	C	372	THR
1	C	377	ILE
1	C	380	LYS
1	C	390	TYR
1	C	394	ASP
1	C	405	LYS
1	C	409	GLN
1	C	412	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	67	HIS
1	A	133	HIS

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Mol	Chain	Res	Type
1	A	392	ASN
1	C	270	ASN
1	C	392	ASN

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

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	NAP	A	501	-	45,52,52	0.97	3 (6%)	56,80,80	1.42	7 (12%)
2	NAP	C	501	-	45,52,52	0.93	2 (4%)	56,80,80	1.60	7 (12%)

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	A	501	-	-	6/31/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	C	501	-	-	10/31/67/67	0/5/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	NAP	O4D-C1D	2.90	1.45	1.41
2	C	501	NAP	O4D-C1D	2.79	1.45	1.41
2	A	501	NAP	C5A-C4A	2.58	1.47	1.40
2	C	501	NAP	C5A-C4A	2.19	1.46	1.40
2	A	501	NAP	C2A-N3A	2.06	1.35	1.32

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	NAP	C6N-N1N-C2N	-3.88	118.44	121.97
2	C	501	NAP	PN-O3-PA	-3.76	119.91	132.83
2	C	501	NAP	C3D-C2D-C1D	3.72	106.59	100.98
2	A	501	NAP	C3N-C7N-N7N	3.68	122.17	117.75
2	A	501	NAP	PN-O3-PA	-3.61	120.45	132.83
2	C	501	NAP	O3X-P2B-O2X	3.42	120.71	107.64
2	C	501	NAP	N3A-C2A-N1A	-3.42	123.34	128.68
2	C	501	NAP	C3N-C7N-N7N	3.33	121.75	117.75
2	A	501	NAP	N3A-C2A-N1A	-2.84	124.23	128.68
2	C	501	NAP	O4D-C1D-C2D	-2.67	103.02	106.93
2	A	501	NAP	O3X-P2B-O2X	2.66	117.81	107.64
2	A	501	NAP	C6N-N1N-C2N	-2.61	119.59	121.97
2	A	501	NAP	N6A-C6A-N1A	2.52	123.80	118.57
2	A	501	NAP	O2B-C2B-C1B	-2.12	102.47	110.10

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NAP	C5B-O5B-PA-O1A
2	A	501	NAP	C5D-O5D-PN-O1N
2	A	501	NAP	C5D-O5D-PN-O2N
2	A	501	NAP	O4D-C1D-N1N-C2N
2	C	501	NAP	C5D-O5D-PN-O3
2	C	501	NAP	C5D-O5D-PN-O1N
2	C	501	NAP	C5D-O5D-PN-O2N
2	C	501	NAP	C2D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
2	C	501	NAP	C2D-C1D-N1N-C6N
2	C	501	NAP	C2N-C3N-C7N-N7N
2	C	501	NAP	C2N-C3N-C7N-O7N
2	A	501	NAP	C5D-O5D-PN-O3
2	C	501	NAP	C4N-C3N-C7N-N7N
2	C	501	NAP	C4N-C3N-C7N-O7N
2	A	501	NAP	PA-O3-PN-O2N
2	C	501	NAP	C5B-O5B-PA-O1A

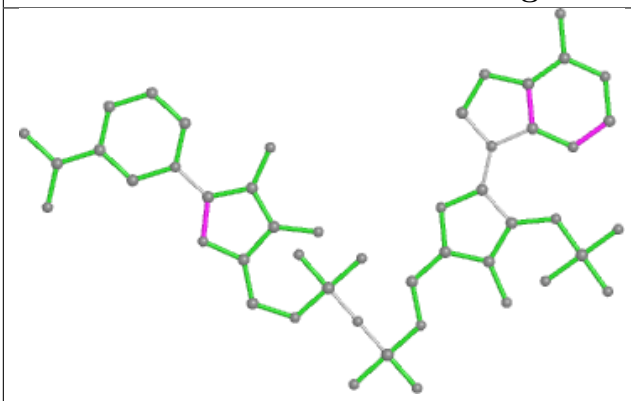
There are no ring outliers.

2 monomers are involved in 7 short contacts:

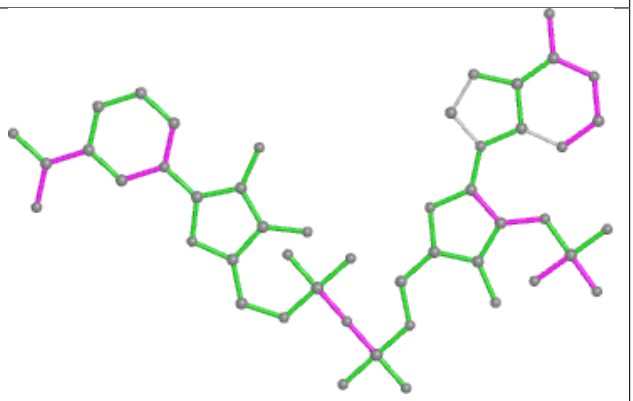
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NAP	4	0
2	C	501	NAP	3	0

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.

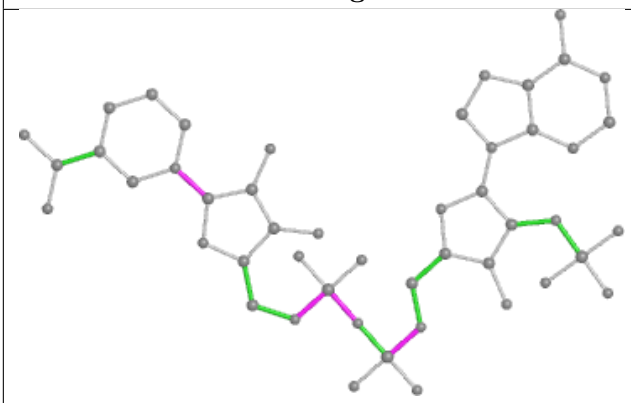
Ligand NAP A 501



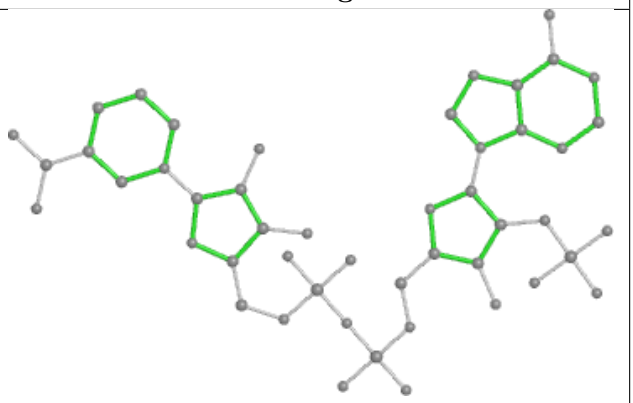
Bond lengths



Bond angles

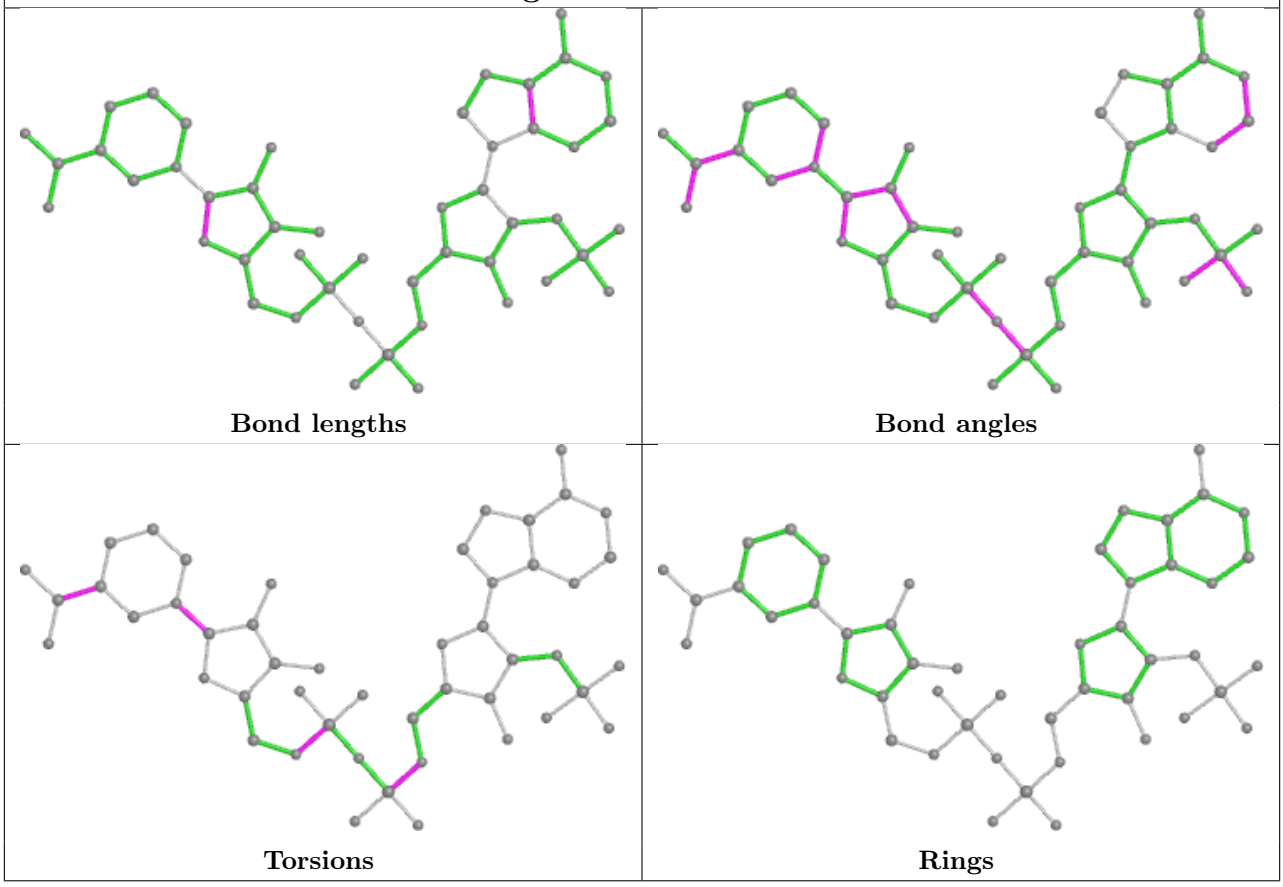


Torsions



Rings

Ligand NAP C 501



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, 95^{th} 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%)	-0.05	17 (4%)	37	24	43, 84, 130, 163	0
1	C	413/413 (100%)	-0.08	15 (3%)	42	27	27, 67, 128, 197	0
All	All	826/826 (100%)	-0.06	32 (3%)	39	25	27, 76, 129, 197	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	319	GLN	8.5
1	C	284	PHE	8.4
1	C	283	GLY	7.1
1	C	139	TYR	6.4
1	A	257	CYS	4.8
1	A	73	CYS	4.7
1	A	277	SER	4.2
1	A	318	TYR	4.1
1	A	258	MET	3.9
1	C	286	SER	3.7
1	C	319	GLN	3.3
1	A	137	ASP	3.3
1	C	86	PHE	3.0
1	A	279	SER	2.9
1	A	210	THR	2.9
1	A	269	LYS	2.8
1	C	285	GLY	2.7
1	C	138	GLN	2.7
1	C	238	PHE	2.6
1	A	138	GLN	2.6
1	A	389	ASP	2.5
1	C	412	LYS	2.5
1	C	253	MET	2.4
1	A	54	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	247	HIS	2.3
1	A	278	ASP	2.3
1	C	180	GLY	2.3
1	C	154	MET	2.3
1	C	251	ASP	2.1
1	A	327	ASN	2.1
1	A	18	MET	2.0
1	C	276	GLN	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 monosaccharides in this entry.

6.4 Ligands (i)

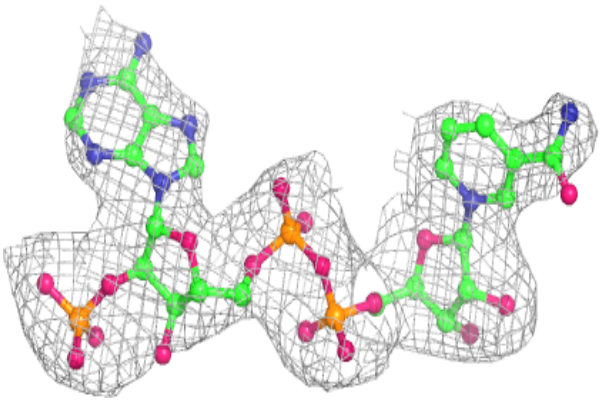
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

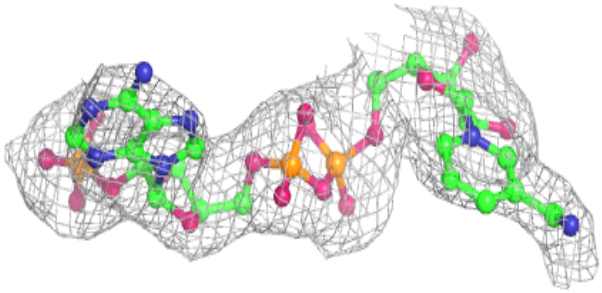
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAP	A	501	48/48	0.93	0.20	56,70,90,97	0
2	NAP	C	501	48/48	0.94	0.19	52,65,81,91	0

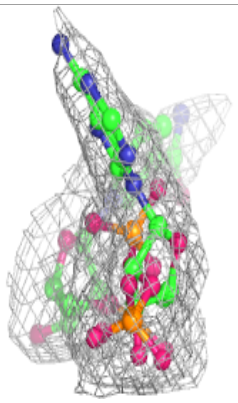
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP 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)

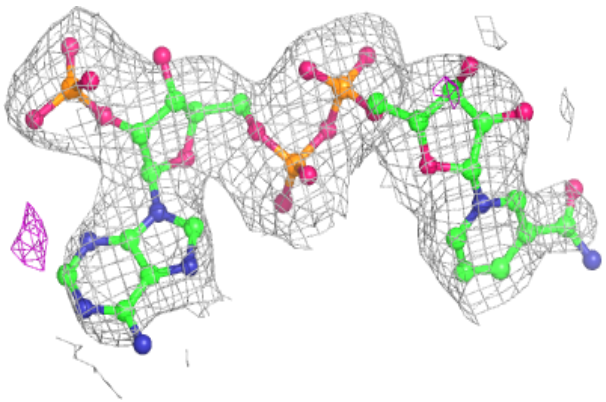


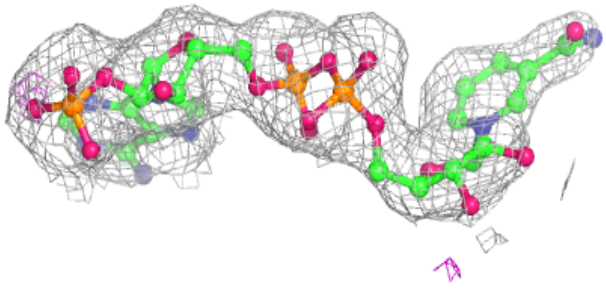


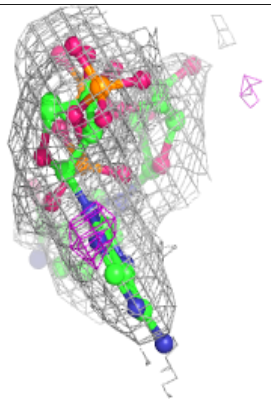


Electron density around NAP C 501:

$2mF_o$-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.