



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 30, 2023 – 10:03 AM EST

PDB ID : 8V15
Title : Human SIRT3 bound to p53-AMC peptide, Carba-NAD, and Honokiol
Authors : Chakrabarti, R.; Ghosh, A.; Guan, X.; Upadhyay, A.; Dumpati, R.K.; Munshi, S.; Roy, S.; Chall, S.; Rahnamoun, A.; Reverdy, C.; Errasti, G.; Delacroix, T.
Deposited on : 2023-11-19
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 : 4.02b-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

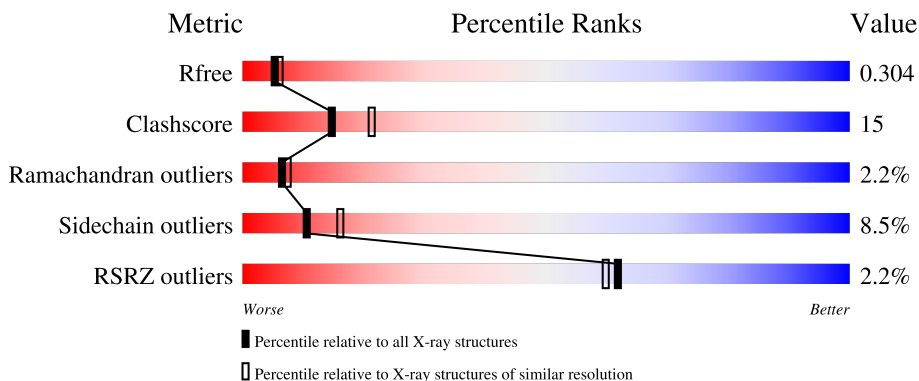
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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	282	
1	C	282	
2	B	4	
2	D	4	

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
4	CNA	A	402	-	-	-	X
4	CNA	C	403	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4442 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 NAD-dependent protein deacetylase sirtuin-3, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	270	Total	C	N	O	S	0	1	0
			2099	1358	356	376	9			
1	C	271	Total	C	N	O	S	0	2	0
			2110	1363	359	379	9			

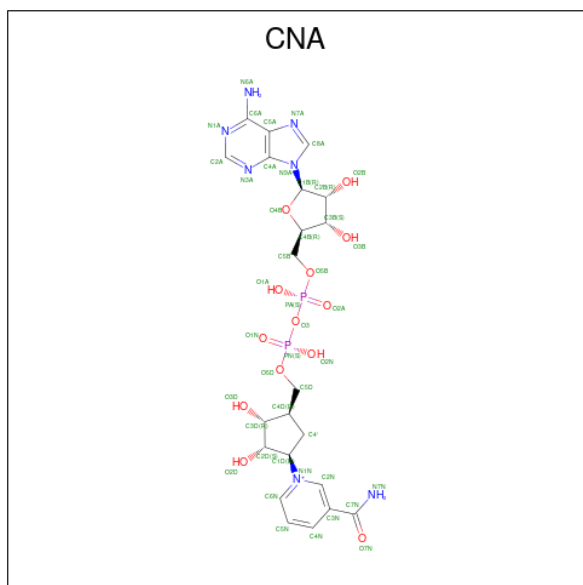
- Molecule 2 is a protein called GLN-PRO-LYS-FDL.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	4	Total	C	N	O	0	0	0
			46	32	7	7			
2	D	4	Total	C	N	O	0	0	0
			46	32	7	7			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

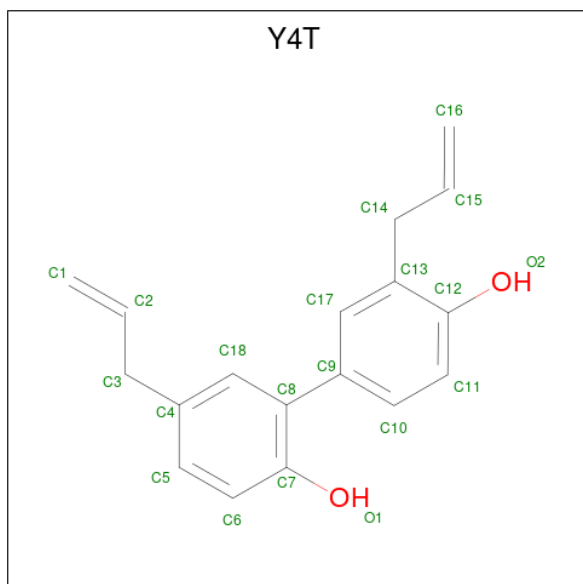
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

- Molecule 4 is CARBA-NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: CNA) (formula: C₂₂H₃₀N₇O₁₃P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
			Total	C	N	O			P	
4	A	1	Total	44	22	7	13	2	0	0
4	C	1	Total	44	22	7	13	2	0	0

- Molecule 5 is (1P)-3',5-di(prop-2-en-1-yl)[1,1'-biphenyl]-2,4'-diol (three-letter code: Y4T) (formula: C₁₈H₁₈O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf		
			Total	C O				
5	C	1	Total	20	18	2	0	0

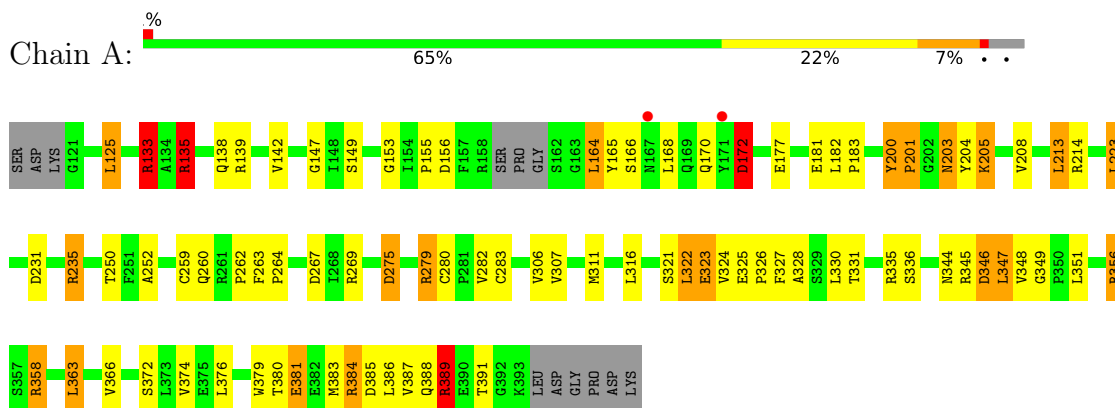
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	16	Total 16	O 16	0	0
6	B	1	Total 1	O 1	0	0
6	C	14	Total 14	O 14	0	0

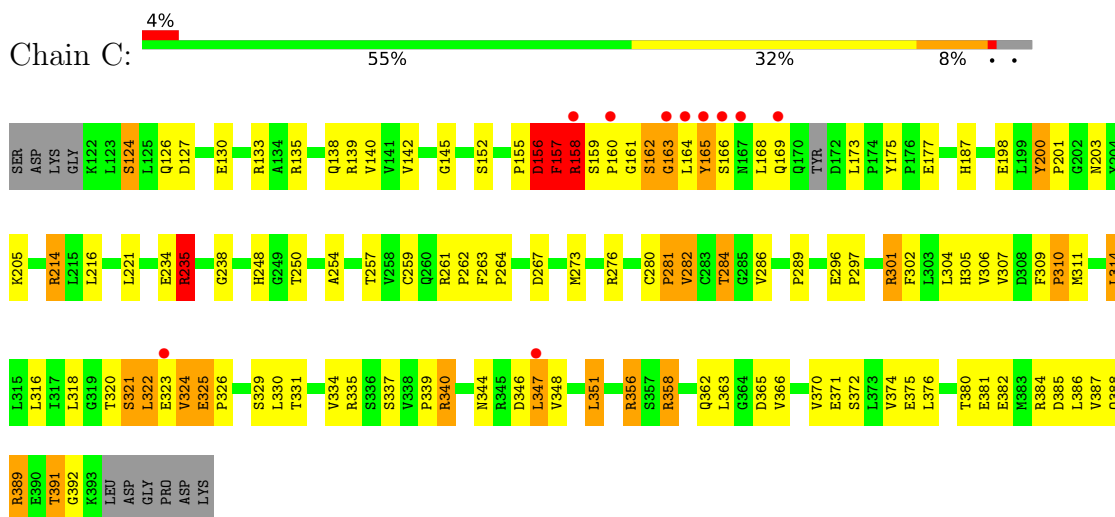
3 Residue-property plots i

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.

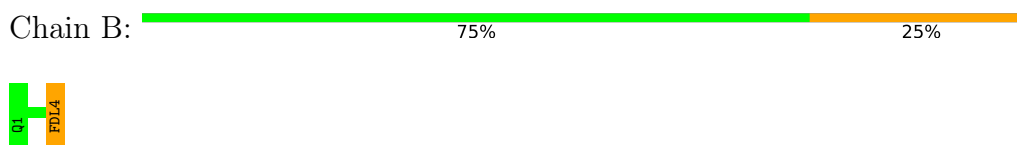
- Molecule 1: NAD-dependent protein deacetylase sirtuin-3, mitochondrial



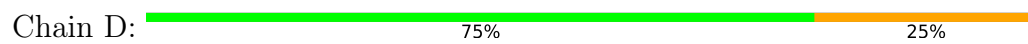
- Molecule 1: NAD-dependent protein deacetylase sirtuin-3, mitochondrial



- Molecule 2: GLN-PRO-LYS-FDL



- Molecule 2: GLN-PRO-LYS-FDL



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	34.68Å 159.43Å 53.05Å 90.00° 90.61° 90.00°	Depositor
Resolution (Å)	44.16 – 2.40 44.16 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.0 (44.16-2.40) 93.3 (44.16-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.39Å)	Xtrriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.194 , 0.303 0.202 , 0.304	Depositor DCC
R_{free} test set	1038 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	49.9	Xtrriage
Anisotropy	0.057	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 20.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.197 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4442	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.62% 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: Y4T, FDL, ZN, CNA

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	0.82	2/2155 (0.1%)	1.56	30/2940 (1.0%)
1	C	0.87	4/2169 (0.2%)	1.51	35/2959 (1.2%)
2	B	0.74	0/21	1.07	0/27
2	D	0.97	0/21	1.12	0/27
All	All	0.84	6/4366 (0.1%)	1.53	65/5953 (1.1%)

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	8
1	C	0	5
All	All	0	13

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	160	PRO	N-CD	11.48	1.64	1.47
1	A	201	PRO	N-CD	7.65	1.58	1.47
1	C	372	SER	CA-CB	-7.31	1.42	1.52
1	A	372	SER	CA-CB	-5.90	1.44	1.52
1	C	152	SER	CA-CB	-5.81	1.44	1.52
1	C	234	GLU	CD-OE2	5.46	1.31	1.25

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	389	ARG	NE-CZ-NH2	-18.14	111.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	389	ARG	NE-CZ-NH1	15.04	127.82	120.30
1	A	356	ARG	NE-CZ-NH2	-12.25	114.18	120.30
1	C	356	ARG	NE-CZ-NH1	10.50	125.55	120.30
1	A	214	ARG	NE-CZ-NH1	10.03	125.31	120.30
1	C	391	THR	CA-CB-OG1	-9.73	88.57	109.00
1	C	331	THR	CA-CB-OG1	-8.82	90.47	109.00
1	A	139	ARG	NE-CZ-NH1	8.59	124.59	120.30
1	C	335	ARG	NE-CZ-NH1	-8.30	116.15	120.30
1	C	356	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	C	139	ARG	NE-CZ-NH1	7.93	124.26	120.30
1	C	358	ARG	NE-CZ-NH1	7.91	124.25	120.30
1	C	358	ARG	NE-CZ-NH2	-7.51	116.55	120.30
1	A	358	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	C	198	GLU	CB-CA-C	7.36	125.13	110.40
1	A	133	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	A	346	ASP	CB-CA-C	-7.14	96.12	110.40
1	C	157	PHE	N-CA-CB	-7.10	97.82	110.60
1	A	389	ARG	CD-NE-CZ	6.94	133.32	123.60
1	A	177	GLU	CB-CA-C	6.87	124.13	110.40
1	A	214	ARG	NE-CZ-NH2	-6.75	116.92	120.30
1	C	325	GLU	CB-CA-C	6.70	123.80	110.40
1	C	389	ARG	NE-CZ-NH1	6.61	123.60	120.30
1	C	273	MET	CG-SD-CE	6.59	110.75	100.20
1	A	213	LEU	CB-CG-CD1	6.55	122.13	111.00
1	A	322	LEU	CB-CG-CD1	-6.41	100.11	111.00
1	C	340	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	363	LEU	CB-CG-CD1	-6.20	100.45	111.00
1	C	177	GLU	CB-CA-C	6.19	122.77	110.40
1	C	311	MET	CG-SD-CE	6.18	110.09	100.20
1	A	358	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	356	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	C	358	ARG	CD-NE-CZ	6.11	132.16	123.60
1	A	279	ARG	CD-NE-CZ	6.06	132.09	123.60
1	A	358	ARG	CB-CA-C	6.03	122.45	110.40
1	C	331	THR	OG1-CB-CG2	5.98	123.75	110.00
1	A	383	MET	CG-SD-CE	-5.94	90.69	100.20
1	A	311	MET	CG-SD-CE	5.93	109.69	100.20
1	C	386	LEU	CB-CG-CD1	5.91	121.05	111.00
1	A	181	GLU	N-CA-CB	-5.89	100.00	110.60
1	A	386	LEU	CB-CG-CD2	-5.84	101.07	111.00
1	A	335	ARG	N-CA-CB	-5.76	100.23	110.60
1	C	235	ARG	NE-CZ-NH1	5.67	123.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	384	ARG	NE-CZ-NH1	-5.59	117.51	120.30
1	A	235	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	C	139	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	C	158	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	205	LYS	CB-CA-C	-5.41	99.58	110.40
1	C	382	GLU	OE1-CD-OE2	5.36	129.74	123.30
1	C	314	LEU	CB-CG-CD1	5.34	120.08	111.00
1	C	234	GLU	OE1-CD-OE2	5.32	129.68	123.30
1	C	261	ARG	N-CA-CB	5.25	120.04	110.60
1	A	335	ARG	CA-CB-CG	5.23	124.91	113.40
1	C	362	GLN	N-CA-CB	-5.23	101.19	110.60
1	A	135	ARG	CD-NE-CZ	5.22	130.91	123.60
1	C	335	ARG	CD-NE-CZ	5.22	130.90	123.60
1	C	310	PRO	N-CA-CB	-5.19	96.89	102.60
1	C	281	PRO	N-CD-CG	-5.17	95.44	103.20
1	A	335	ARG	CD-NE-CZ	5.17	130.83	123.60
1	C	322	LEU	CB-CG-CD1	-5.15	102.25	111.00
1	A	139	ARG	NH1-CZ-NH2	-5.09	113.80	119.40
1	C	326	PRO	N-CA-CB	-5.09	97.00	102.60
1	C	203	ASN	CB-CA-C	5.07	120.55	110.40
1	C	214	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	C	301	ARG	O-C-N	-5.01	114.69	122.70

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	133	ARG	Sidechain
1	A	135	ARG	Sidechain
1	A	172	ASP	Peptide
1	A	279	ARG	Sidechain
1	A	345	ARG	Sidechain
1	A	356	ARG	Sidechain
1	A	358	ARG	Sidechain
1	A	389	ARG	Sidechain
1	C	133	ARG	Sidechain
1	C	156	ASP	Peptide
1	C	157	PHE	Peptide
1	C	163	GLY	Peptide
1	C	276	ARG	Sidechain

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	2099	0	2087	51	0
1	C	2110	0	2113	73	0
2	B	46	0	45	1	0
2	D	46	0	45	3	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	44	0	29	10	0
4	C	44	0	29	7	0
5	C	20	0	0	5	0
6	A	16	0	0	0	0
6	B	1	0	0	0	0
6	C	14	0	0	0	0
All	All	4442	0	4348	134	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 15.

All (134) 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:165:TYR:O	1:A:168:LEU:N	2.03	0.91
1:C:124:SER:HB3	1:C:127:ASP:OD2	1.72	0.90
4:A:402:CNA:H3	4:A:402:CNA:H10	1.53	0.90
1:C:366:VAL:HG23	4:C:403:CNA:C2A	2.02	0.89
1:C:280:CYS:O	1:C:284:THR:HA	1.81	0.79
1:C:126:GLN:HG3	1:C:376:LEU:HD22	1.66	0.78
4:A:402:CNA:O3	4:A:402:CNA:H4	1.84	0.77
1:C:165:TYR:HE1	1:C:173:LEU:HD23	1.52	0.75
1:C:248:HIS:HE1	4:C:403:CNA:H20	1.53	0.73
1:C:316[A]:LEU:HD11	1:C:318:LEU:HD21	1.69	0.73
1:C:140:VAL:HG11	1:C:316[B]:LEU:HD12	1.72	0.72
1:A:321:SER:OG	1:A:323:GLU:OE1	2.10	0.68
1:C:248:HIS:CE1	4:C:403:CNA:H20	2.28	0.68
1:A:323:GLU:H	1:A:323:GLU:CD	1.99	0.66
1:C:314:LEU:CD1	1:C:339:PRO:HB2	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:PRO:O	1:C:282:VAL:C	2.33	0.66
5:C:402:Y4T:C16	2:D:4:FDL:H3	2.26	0.66
1:C:216[A]:LEU:HD12	1:C:221:LEU:HB2	1.78	0.65
1:A:182:LEU:HB2	1:A:183:PRO:HD3	1.78	0.65
1:C:323:GLU:O	1:C:324:VAL:HG23	1.97	0.64
1:A:325:GLU:HB3	1:A:326:PRO:HA	1.80	0.64
1:C:161:GLY:O	1:C:162:SER:O	2.15	0.64
1:C:381:GLU:HB3	1:C:384:ARG:HH21	1.65	0.61
1:C:314:LEU:HD12	1:C:339:PRO:HB2	1.81	0.60
1:A:164:LEU:HG	1:A:165:TYR:N	2.16	0.59
1:A:347:LEU:HD12	1:A:363:LEU:HD21	1.84	0.59
1:C:140:VAL:HG11	1:C:316[B]:LEU:CD1	2.31	0.59
1:C:322:LEU:HA	5:C:402:Y4T:C1	2.33	0.59
1:A:200:TYR:CD2	1:A:201:PRO:HD2	2.38	0.58
1:A:156:ASP:O	1:A:164:LEU:HD22	2.04	0.58
1:C:387:VAL:O	1:C:391:THR:HG23	2.04	0.57
1:C:216[A]:LEU:CD1	1:C:221:LEU:HB2	2.34	0.57
1:C:254:ALA:HB2	1:C:289:PRO:HA	1.86	0.57
1:A:203:ASN:O	1:A:204:TYR:CG	2.58	0.56
1:C:374:VAL:HG12	1:C:380:THR:HG22	1.88	0.56
1:C:161:GLY:C	1:C:162:SER:O	2.43	0.56
1:C:159:SER:OG	1:C:162:SER:HB3	2.06	0.55
1:C:347:LEU:O	1:C:348:VAL:HG13	2.06	0.55
1:A:306:VAL:HG23	1:A:307:VAL:HG13	1.89	0.55
4:C:403:CNA:O3D	2:D:4:FDL:OAY	2.15	0.55
1:C:140:VAL:CG1	1:C:316[B]:LEU:HD12	2.37	0.55
4:A:402:CNA:H3	4:A:402:CNA:C8A	2.33	0.54
1:A:203:ASN:O	1:A:204:TYR:CD2	2.61	0.54
1:C:316[A]:LEU:HD11	1:C:318:LEU:CD2	2.35	0.54
1:A:153:GLY:O	1:A:204:TYR:CE1	2.61	0.54
1:C:165:TYR:CD1	1:C:169:GLN:HB2	2.43	0.54
1:C:337:SER:O	1:C:358:ARG:NH1	2.30	0.54
1:A:147:GLY:HA2	4:A:402:CNA:N7A	2.23	0.53
1:A:347:LEU:O	1:A:349:GLY:N	2.41	0.53
1:A:325:GLU:CB	1:A:326:PRO:HA	2.36	0.52
1:C:321:SER:OG	5:C:402:Y4T:C6	2.58	0.51
1:C:340:ARG:CZ	1:C:351:LEU:HD22	2.40	0.51
1:C:257:THR:HG23	1:C:286:VAL:O	2.10	0.51
1:C:156:ASP:O	1:C:164:LEU:HD23	2.10	0.51
1:C:322:LEU:HA	5:C:402:Y4T:C2	2.41	0.51
4:A:402:CNA:H19	4:A:402:CNA:O1N	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:ASN:O	1:A:363:LEU:HA	2.11	0.51
1:A:147:GLY:HA2	4:A:402:CNA:C5A	2.40	0.50
1:C:165:TYR:O	1:C:166:SER:C	2.48	0.50
1:C:156:ASP:OD2	4:C:403:CNA:H28	2.11	0.50
1:A:328:ALA:O	1:A:331:THR:OG1	2.22	0.50
1:C:309:PHE:N	1:C:310:PRO:HD3	2.27	0.49
1:C:324:VAL:HB	5:C:402:Y4T:C1	2.43	0.49
1:C:370:VAL:O	1:C:374:VAL:HG23	2.11	0.49
1:C:235:ARG:NH1	1:C:250:THR:OG1	2.46	0.49
1:C:280:CYS:O	1:C:284:THR:CA	2.58	0.49
1:C:250:THR:HG23	1:C:250:THR:O	2.13	0.48
1:C:309:PHE:N	1:C:310:PRO:CD	2.76	0.48
1:A:125:LEU:HD13	1:A:376:LEU:HD12	1.95	0.48
1:A:165:TYR:HA	1:A:168:LEU:HB2	1.95	0.48
1:A:381:GLU:HG2	1:A:384:ARG:NH1	2.29	0.48
1:C:340:ARG:NH2	1:C:351:LEU:HD22	2.28	0.48
1:C:262:PRO:C	1:C:263:PHE:CD1	2.87	0.48
1:C:334:VAL:O	1:C:356:ARG:NH1	2.41	0.48
1:A:385:ASP:O	1:A:389:ARG:HG3	2.14	0.47
1:C:385:ASP:O	1:C:389:ARG:HG3	2.15	0.47
1:C:391:THR:OG1	1:C:392:GLY:N	2.45	0.47
1:A:280:CYS:SG	1:A:282:VAL:HB	2.54	0.47
1:C:321:SER:HB2	1:C:348:VAL:HG23	1.97	0.46
1:C:214:ARG:NH1	1:C:238:GLY:HA3	2.30	0.46
1:C:321:SER:HB2	1:C:348:VAL:CG2	2.45	0.46
1:A:223:LEU:HD12	1:A:223:LEU:O	2.15	0.46
1:A:374:VAL:HG12	1:A:380:THR:HG22	1.96	0.46
1:A:142:VAL:HA	1:A:316:LEU:O	2.16	0.46
1:A:264:PRO:HG2	1:A:267:ASP:OD2	2.16	0.45
1:A:321:SER:O	1:A:322:LEU:HB2	2.16	0.45
1:C:296:GLU:HB3	1:C:297:PRO:HD2	1.98	0.45
1:A:262:PRO:C	1:A:263:PHE:CD1	2.90	0.45
1:C:156:ASP:OD1	4:C:403:CNA:O2A	2.35	0.45
1:C:321:SER:CB	1:C:348:VAL:CG2	2.95	0.45
1:A:223:LEU:HD12	1:A:223:LEU:C	2.37	0.45
1:A:259:CYS:HB3	1:A:283:CYS:SG	2.57	0.45
2:D:4:FDL:H6	2:D:4:FDL:H1	1.78	0.45
1:C:337:SER:O	1:C:358:ARG:HD3	2.17	0.45
1:A:201:PRO:O	1:A:269:ARG:NH2	2.38	0.44
1:A:275:ASP:N	1:A:275:ASP:OD1	2.50	0.44
1:C:200:TYR:CD2	1:C:201:PRO:HD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:402:CNA:O3	4:A:402:CNA:C4B	2.59	0.44
1:C:155:PRO:HB2	1:C:164:LEU:HB2	2.00	0.44
1:C:344:ASN:O	1:C:363:LEU:HA	2.18	0.44
1:A:153:GLY:O	1:A:204:TYR:HE1	1.99	0.44
1:A:325:GLU:HB3	1:A:326:PRO:CA	2.46	0.44
4:A:402:CNA:O1N	4:A:402:CNA:C4'	2.66	0.44
1:A:155:PRO:HB2	1:A:164:LEU:HD13	1.99	0.44
1:C:305:HIS:CD2	1:C:330:LEU:HD22	2.53	0.43
1:A:149:SER:CB	4:A:402:CNA:H26	2.31	0.43
2:B:4:FDL:H1	2:B:4:FDL:H6	1.81	0.43
1:C:145:GLY:HA3	1:C:320:THR:HB	2.00	0.43
1:A:149:SER:OG	1:A:231:ASP:OD2	2.29	0.43
1:C:366:VAL:HG23	4:C:403:CNA:H13	1.96	0.43
1:A:170:GLN:C	1:A:172:ASP:H	2.20	0.43
1:C:264:PRO:HG2	1:C:267:ASP:OD2	2.19	0.43
1:A:125:LEU:HD23	1:A:125:LEU:HA	1.93	0.42
1:A:322:LEU:HD22	1:A:327:PHE:HB3	2.01	0.42
1:C:161:GLY:O	1:C:162:SER:C	2.58	0.42
1:C:339:PRO:HD3	1:C:358:ARG:NH1	2.35	0.42
1:A:324:VAL:HG12	1:A:325:GLU:O	2.19	0.42
1:A:374:VAL:HG13	1:A:379:TRP:HB2	2.01	0.42
1:A:250:THR:HG21	1:A:252:ALA:HB3	2.02	0.42
1:C:214:ARG:HH11	1:C:238:GLY:HA3	1.85	0.42
1:A:366:VAL:HG23	4:A:402:CNA:N1A	2.35	0.42
1:A:259:CYS:O	1:A:260:GLN:HB2	2.20	0.42
1:A:330:LEU:HD23	1:A:330:LEU:HA	1.81	0.41
1:A:235:ARG:NH1	1:A:250:THR:OG1	2.51	0.41
1:C:165:TYR:HD1	1:C:165:TYR:HA	1.65	0.41
1:C:301:ARG:O	1:C:302:PHE:C	2.56	0.41
1:A:213:LEU:HA	1:A:213:LEU:HD23	1.88	0.41
1:A:387:VAL:O	1:A:391:THR:HG23	2.20	0.41
1:C:306:VAL:HG23	1:C:307:VAL:HG13	2.03	0.41
1:C:324:VAL:HG12	1:C:325:GLU:O	2.21	0.41
1:C:304:LEU:HD23	1:C:304:LEU:HA	1.76	0.41
1:C:157:PHE:CZ	1:C:164:LEU:HD21	2.57	0.40
1:C:216[A]:LEU:HD12	1:C:216[A]:LEU:HA	1.76	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	267/282 (95%)	240 (90%)	23 (9%)	4 (2%)	10	14
1	C	269/282 (95%)	236 (88%)	25 (9%)	8 (3%)	4	3
2	B	2/4 (50%)	2 (100%)	0	0	100	100
2	D	2/4 (50%)	1 (50%)	1 (50%)	0	100	100
All	All	540/572 (94%)	479 (89%)	49 (9%)	12 (2%)	6	7

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	135	ARG
1	A	172	ASP
1	A	348	VAL
1	C	135	ARG
1	C	158	ARG
1	C	162	SER
1	C	284	THR
1	A	166	SER
1	C	324	VAL
1	C	163	GLY
1	C	175	TYR
1	C	282	VAL

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	227/244 (93%)	210 (92%)	17 (8%)	13	21
1	C	232/244 (95%)	210 (90%)	22 (10%)	8	12
2	B	2/3 (67%)	2 (100%)	0	100	100
2	D	2/3 (67%)	2 (100%)	0	100	100
All	All	463/494 (94%)	424 (92%)	39 (8%)	10	16

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	125	LEU
1	A	133	ARG
1	A	138	GLN
1	A	164	LEU
1	A	200	TYR
1	A	203	ASN
1	A	205	LYS
1	A	208	VAL
1	A	223	LEU
1	A	275	ASP
1	A	323	GLU
1	A	336	SER
1	A	346	ASP
1	A	347	LEU
1	A	351	LEU
1	A	381	GLU
1	A	388	GLN
1	C	124	SER
1	C	130	GLU
1	C	138	GLN
1	C	156	ASP
1	C	157	PHE
1	C	158	ARG
1	C	165	TYR
1	C	168	LEU
1	C	187	HIS
1	C	200	TYR
1	C	205	LYS
1	C	235	ARG
1	C	259	CYS
1	C	321	SER
1	C	329	SER
1	C	346	ASP

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Mol	Chain	Res	Type
1	C	347	LEU
1	C	351	LEU
1	C	365	ASP
1	C	371	GLU
1	C	375	GLU
1	C	388	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	GLN
1	A	354	HIS
1	C	169	GLN
1	C	248	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	FDL	B	4	2	26,26,26	1.91	4 (15%)	34,35,35	1.29	6 (17%)
2	FDL	D	4	2	26,26,26	1.87	5 (19%)	34,35,35	1.60	9 (26%)

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	FDL	B	4	2	-	2/16/16/16	0/2/2/2
2	FDL	D	4	2	-	8/16/16/16	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4	FDL	OAK-CAB	7.57	1.37	1.21
2	D	4	FDL	OAK-CAB	7.23	1.36	1.21
2	B	4	FDL	CAC-CAD	4.12	1.40	1.35
2	D	4	FDL	CAC-CAD	3.19	1.39	1.35
2	D	4	FDL	CAJ-NAM	-2.71	1.36	1.41
2	D	4	FDL	CAE-CAD	-2.69	1.41	1.45
2	B	4	FDL	CAE-CAD	-2.50	1.41	1.45
2	D	4	FDL	CAC-CAB	-2.41	1.39	1.44
2	B	4	FDL	CAJ-NAM	-2.33	1.36	1.41

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4	FDL	CAB-CAC-CAD	-3.68	119.93	123.12
2	B	4	FDL	CAB-CAC-CAD	-3.55	120.04	123.12
2	D	4	FDL	OAK-CAB-CAC	-3.38	118.94	125.84
2	D	4	FDL	OAA-CAF-CAG	3.20	120.60	115.79
2	D	4	FDL	OAA-CAB-OAK	3.14	120.44	116.44
2	D	4	FDL	CAH-CAE-CAD	-3.02	120.02	124.27
2	B	4	FDL	OAK-CAB-CAC	-2.69	120.35	125.84
2	D	4	FDL	OAA-CAB-CAC	2.68	120.62	117.17
2	D	4	FDL	CAJ-NAM-C	-2.58	121.23	127.40
2	B	4	FDL	OAA-CAF-CAG	2.54	119.61	115.79
2	B	4	FDL	OAA-CAB-OAK	2.48	119.60	116.44
2	B	4	FDL	CAH-CAE-CAD	-2.31	121.01	124.27
2	B	4	FDL	OAA-CAB-CAC	2.24	120.05	117.17
2	D	4	FDL	CAF-CAE-CAD	2.22	120.21	118.59
2	D	4	FDL	OAA-CAF-CAE	-2.11	119.55	121.56

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	4	FDL	O-C-NAM-CAJ
2	D	4	FDL	CA-C-NAM-CAJ
2	D	4	FDL	NAM-C-CA-N

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Mol	Chain	Res	Type	Atoms
2	D	4	FDL	O-C-CA-N
2	D	4	FDL	CAG-CAJ-NAM-C
2	D	4	FDL	CAI-CAJ-NAM-C
2	B	4	FDL	CAI-CAJ-NAM-C
2	B	4	FDL	CAG-CAJ-NAM-C
2	D	4	FDL	O-C-CA-CB
2	D	4	FDL	NAM-C-CA-CB

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	4	FDL	1	0
2	D	4	FDL	3	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
4	CNA	A	402	-	42,48,48	0.59	1 (2%)	49,73,73	1.47	7 (14%)
5	Y4T	C	402	-	21,21,21	1.39	3 (14%)	28,28,28	1.05	3 (10%)
4	CNA	C	403	-	42,48,48	0.66	0	49,73,73	1.14	5 (10%)

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	CNA	A	402	-	-	15/24/62/62	0/5/5/5
5	Y4T	C	402	-	-	2/10/10/10	0/2/2/2
4	CNA	C	403	-	-	11/24/62/62	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	402	Y4T	C3-C4	-4.85	1.43	1.52
5	C	402	Y4T	C5-C4	-2.30	1.33	1.38
4	A	402	CNA	C8A-N7A	-2.08	1.31	1.34
5	C	402	Y4T	C6-C7	2.01	1.43	1.39

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	402	CNA	PN-O3-PA	5.31	151.03	132.83
4	C	403	CNA	O7N-C7N-C3N	3.20	123.46	119.63
4	A	402	CNA	O3D-C3D-C4D	-3.17	104.54	112.75
4	A	402	CNA	O2B-C2B-C1B	2.95	121.75	110.85
4	C	403	CNA	C2N-C3N-C7N	2.93	127.97	119.46
4	A	402	CNA	O2D-C2D-C3D	-2.69	103.11	111.82
4	C	403	CNA	C4N-C3N-C7N	-2.58	114.14	121.04
5	C	402	Y4T	C9-C8-C7	2.32	124.39	122.36
5	C	402	Y4T	C4-C3-C2	-2.19	106.72	113.84
4	A	402	CNA	C4N-C3N-C7N	-2.13	115.34	121.04
4	C	403	CNA	O3B-C3B-C4B	2.12	117.17	111.05
4	A	402	CNA	C3N-C2N-N1N	-2.06	118.42	120.43
4	A	402	CNA	O3B-C3B-C2B	2.03	118.40	111.82
4	C	403	CNA	C5A-C6A-N6A	2.02	123.42	120.35
5	C	402	Y4T	C5-C4-C18	2.00	121.34	118.54

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	402	CNA	C4B-C5B-O5B-PA
4	A	402	CNA	C5D-O5D-PN-O1N
4	A	402	CNA	C5D-O5D-PN-O2N
4	A	402	CNA	C4D-C5D-O5D-PN
4	A	402	CNA	C2D-C1D-N1N-C2N
4	A	402	CNA	C2D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
4	A	402	CNA	C2N-C3N-C7N-O7N
4	C	403	CNA	C5B-O5B-PA-O2A
4	C	403	CNA	C5D-O5D-PN-O1N
4	C	403	CNA	C5D-O5D-PN-O2N
4	C	403	CNA	C4'-C4D-C5D-O5D
4	C	403	CNA	C2D-C1D-N1N-C2N
4	C	403	CNA	C2D-C1D-N1N-C6N
4	A	402	CNA	C4N-C3N-C7N-O7N
4	A	402	CNA	O4B-C4B-C5B-O5B
4	A	402	CNA	C3B-C4B-C5B-O5B
4	A	402	CNA	C4N-C3N-C7N-N7N
5	C	402	Y4T	C13-C14-C15-C16
4	A	402	CNA	C2N-C3N-C7N-N7N
5	C	402	Y4T	C1-C2-C3-C4
4	A	402	CNA	PA-O3-PN-O5D
4	C	403	CNA	C5B-O5B-PA-O3
4	C	403	CNA	C5D-O5D-PN-O3
4	C	403	CNA	O4B-C4B-C5B-O5B
4	A	402	CNA	C5D-O5D-PN-O3
4	C	403	CNA	C3D-C4D-C5D-O5D
4	A	402	CNA	C5B-O5B-PA-O2A
4	C	403	CNA	C5B-O5B-PA-O1A

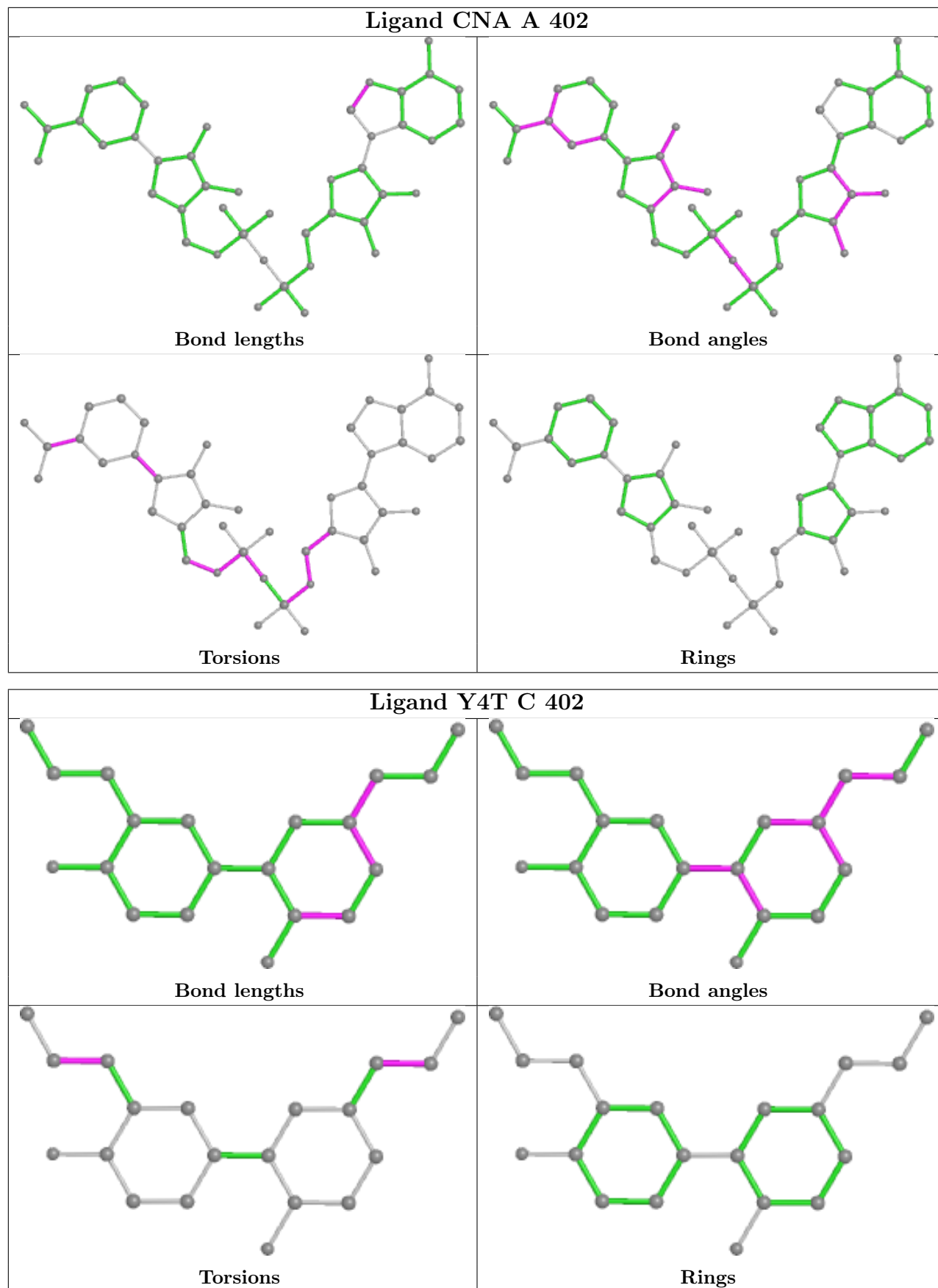
There are no ring outliers.

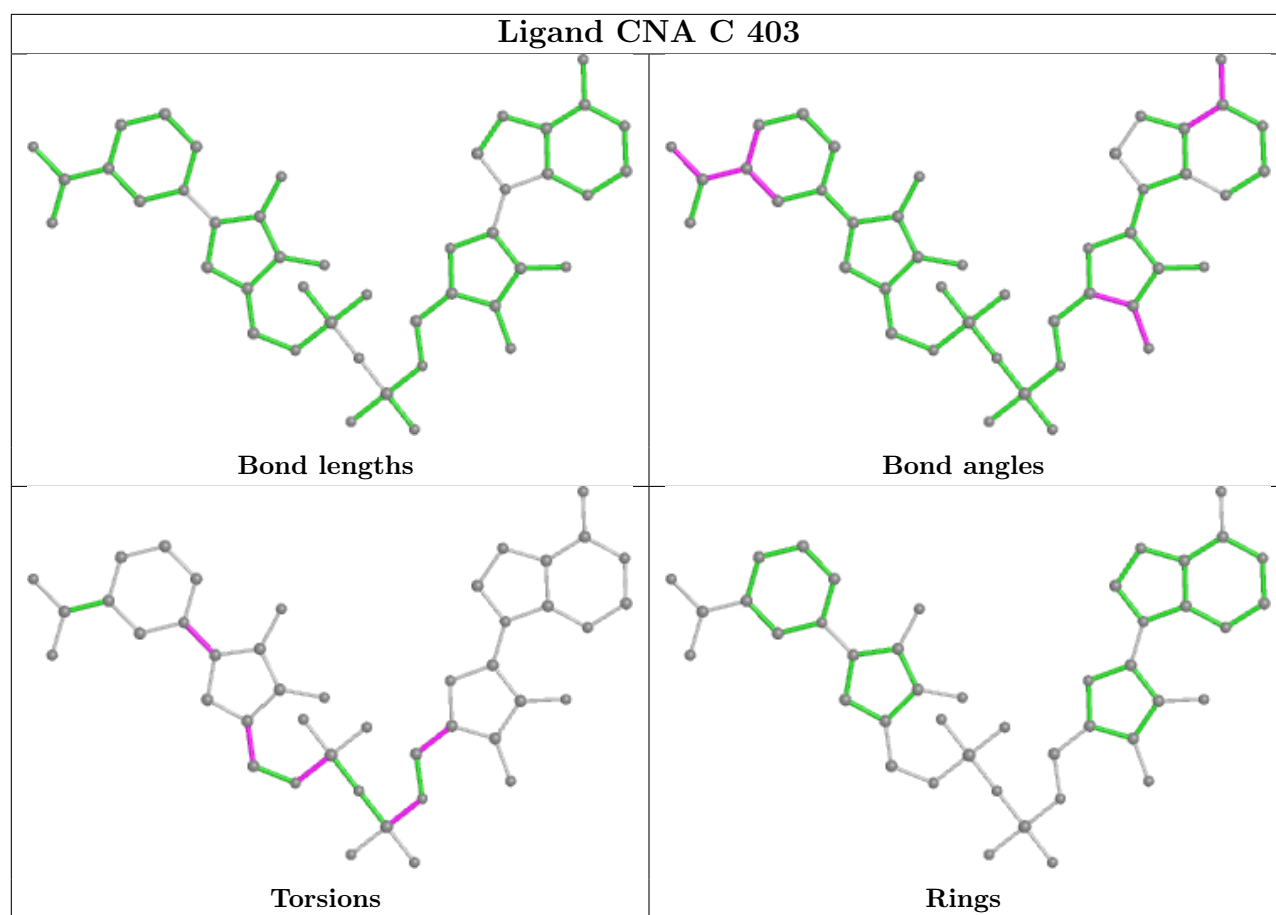
3 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	402	CNA	10	0
5	C	402	Y4T	5	0
4	C	403	CNA	7	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	270/282 (95%)	-0.55	2 (0%) 87 86	32, 53, 96, 143	0
1	C	271/282 (96%)	-0.44	10 (3%) 41 41	32, 52, 110, 179	0
2	B	3/4 (75%)	-0.70	0 100 100	58, 58, 66, 75	0
2	D	3/4 (75%)	-0.56	0 100 100	62, 62, 70, 76	0
All	All	547/572 (95%)	-0.50	12 (2%) 62 60	32, 52, 104, 179	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	160	PRO	9.0
1	A	171	TYR	3.8
1	C	167	ASN	3.4
1	C	165	TYR	3.3
1	C	323	GLU	3.1
1	C	169	GLN	2.8
1	C	347	LEU	2.5
1	C	166	SER	2.5
1	C	163	GLY	2.3
1	C	164	LEU	2.2
1	C	158	ARG	2.1
1	A	167	ASN	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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(\AA^2)	Q<0.9
2	FDL	B	4	25/25	0.88	0.22	32,53,117,148	0
2	FDL	D	4	25/25	0.91	0.15	39,59,100,108	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

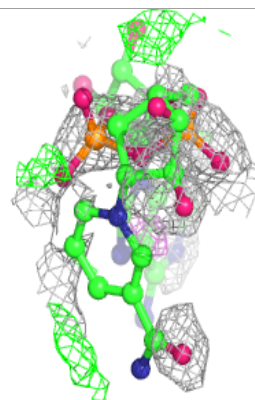
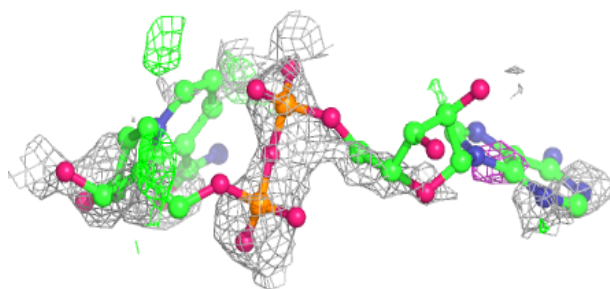
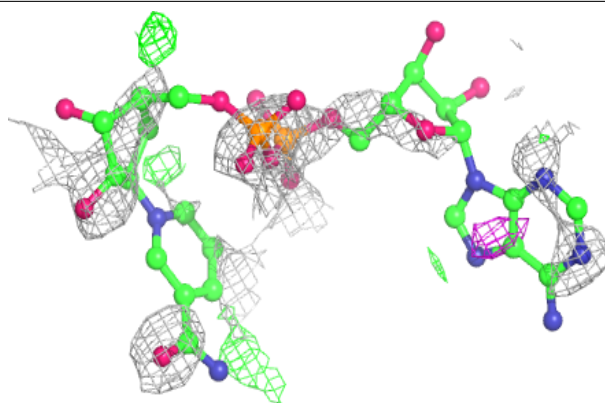
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	CNA	C	403	44/44	0.64	0.49	44,86,122,128	44
5	Y4T	C	402	20/20	0.77	0.35	60,120,147,147	0
4	CNA	A	402	44/44	0.79	0.54	42,114,198,280	44
3	ZN	C	401	1/1	0.98	0.11	52,52,52,52	0
3	ZN	A	401	1/1	0.98	0.07	61,61,61,61	0

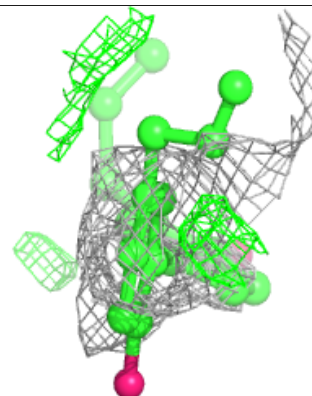
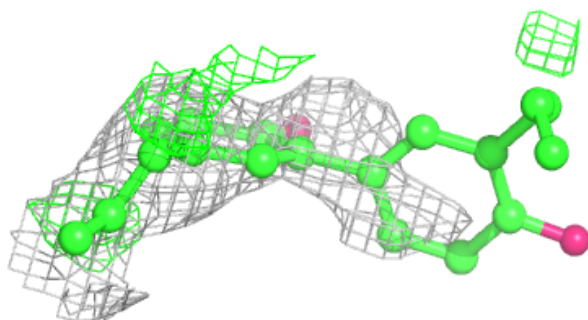
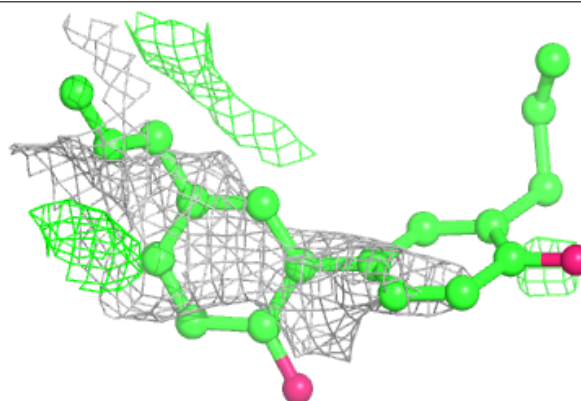
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

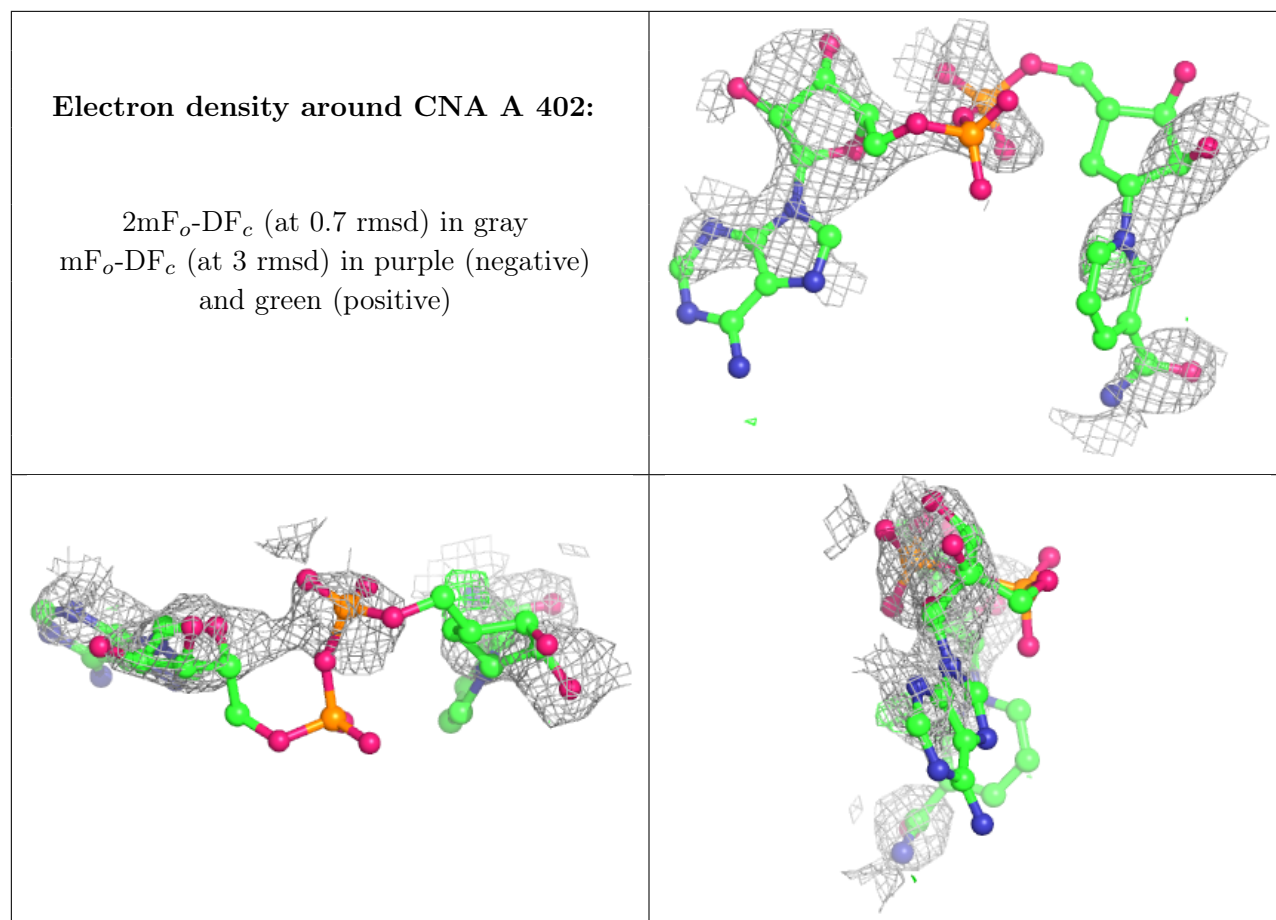
Electron density around CNA C 403:

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

**Electron density around Y4T C 402:**

$2mF_o-DF_c$ (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.