



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 10:21 am BST

PDB ID : 5B7B
Title : Crystal structure of Nucleoprotein-nucleozin complex
Authors : Pang, B.; Zhang, W.Z.; Zhang, H.M.; Hao, Q.
Deposited on : 2016-06-06
Resolution : 3.00 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 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 : 2.11
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) : 2.11

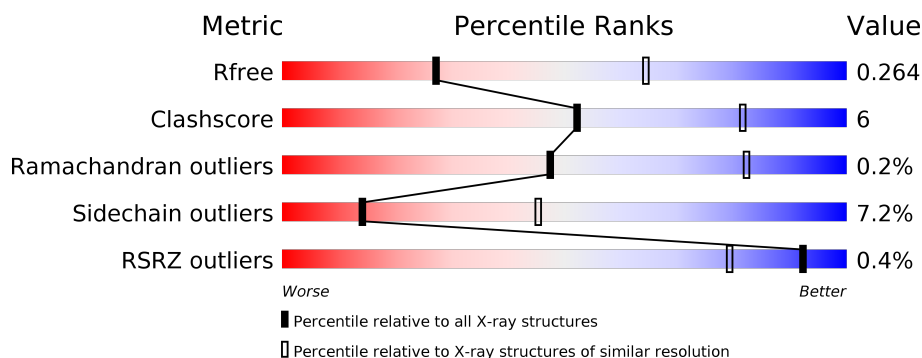
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 on 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.

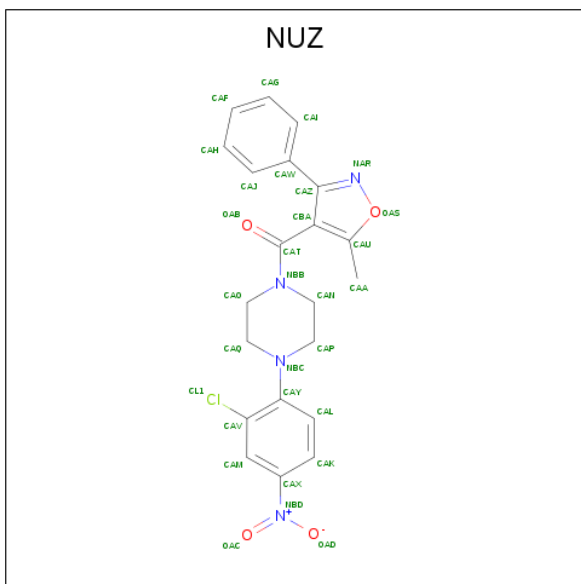
Mol	Chain	Length	Quality of chain
1	A	498	<div> <div>68%</div> <div>16%</div> <div>•</div> <div>15%</div> </div>
1	B	498	<div> <div>68%</div> <div>16%</div> <div>•</div> <div>15%</div> </div>
1	C	498	<div> <div>68%</div> <div>16%</div> <div>•</div> <div>15%</div> </div>
1	D	498	<div> <div>70%</div> <div>13%</div> <div>•</div> <div>16%</div> </div>
1	E	498	<div> <div>69%</div> <div>15%</div> <div>•</div> <div>15%</div> </div>
1	F	498	<div> <div>%</div> <div>71%</div> <div>13%</div> <div>•</div> <div>15%</div> </div>

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 Nucleoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	422	Total 3323	C 2066	N 615	O 616	S 26	0	0	0
1	B	423	Total 3329	C 2069	N 616	O 618	S 26	0	0	0
1	C	424	Total 3326	C 2068	N 611	O 621	S 26	0	0	0
1	D	419	Total 3290	C 2044	N 611	O 610	S 25	0	0	0
1	E	421	Total 3306	C 2057	N 611	O 613	S 25	0	0	0
1	F	424	Total 3320	C 2066	N 613	O 616	S 25	0	0	0

- Molecule 2 is [4-(2-chloro-4-nitrophenyl)piperazin-1-yl](5-methyl-3-phenyl-1,2-oxazol-4-yl)methanone (three-letter code: NUZ) (formula: C₂₁H₁₉ClN₄O₄).

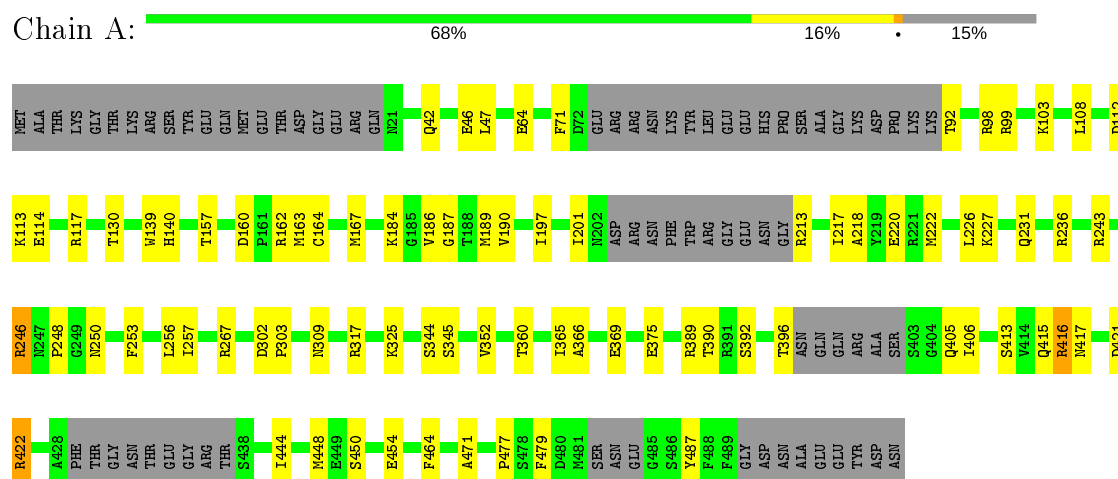


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			30	21	1	4	4		
2	D	1	Total	C	Cl	N	O	0	0
			30	21	1	4	4		

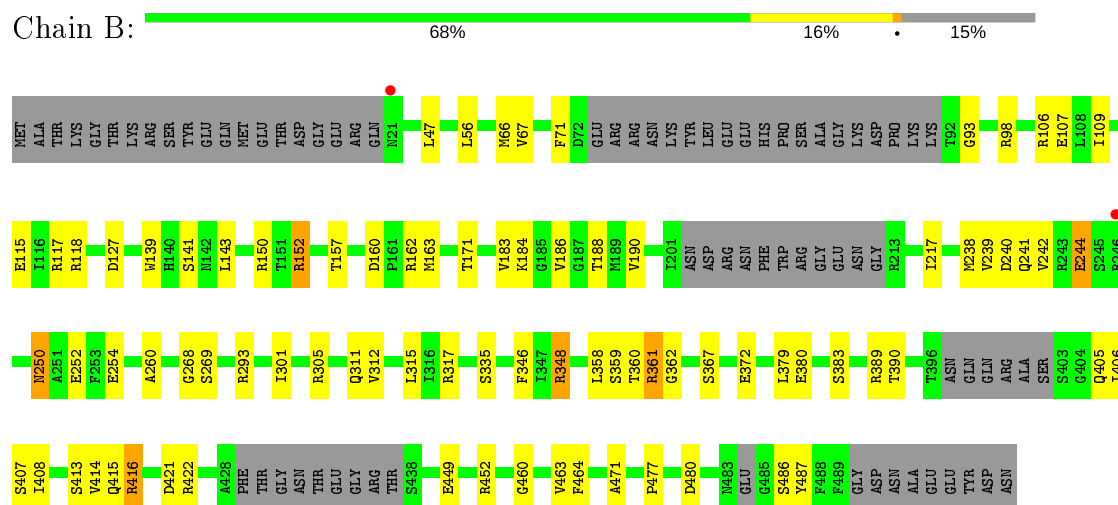
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Nucleoprotein

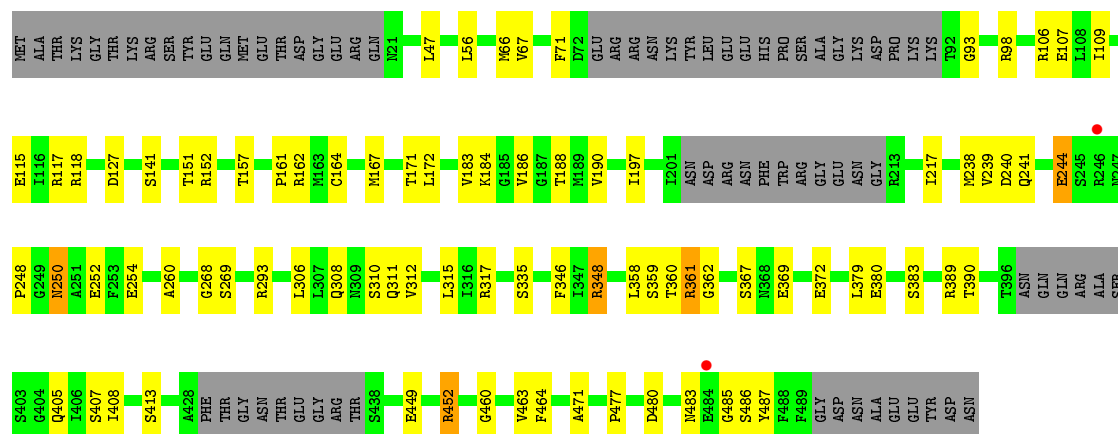


• Molecule 1: Nucleoprotein



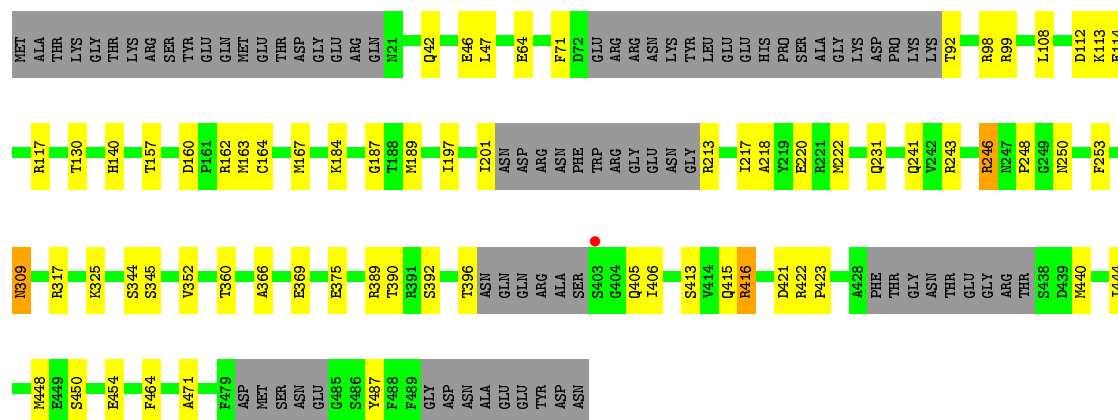
• Molecule 1: Nucleoprotein





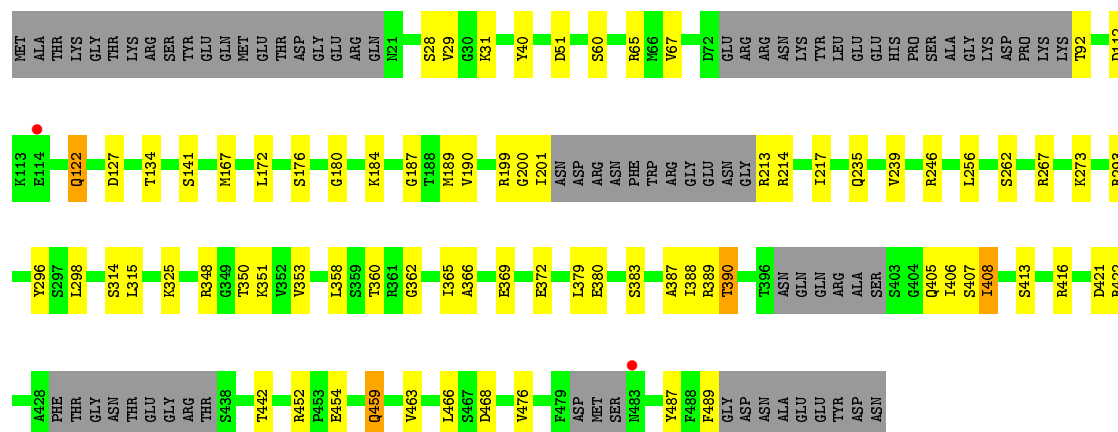
• Molecule 1: Nucleoprotein

Chain D: 70% 13% 16%

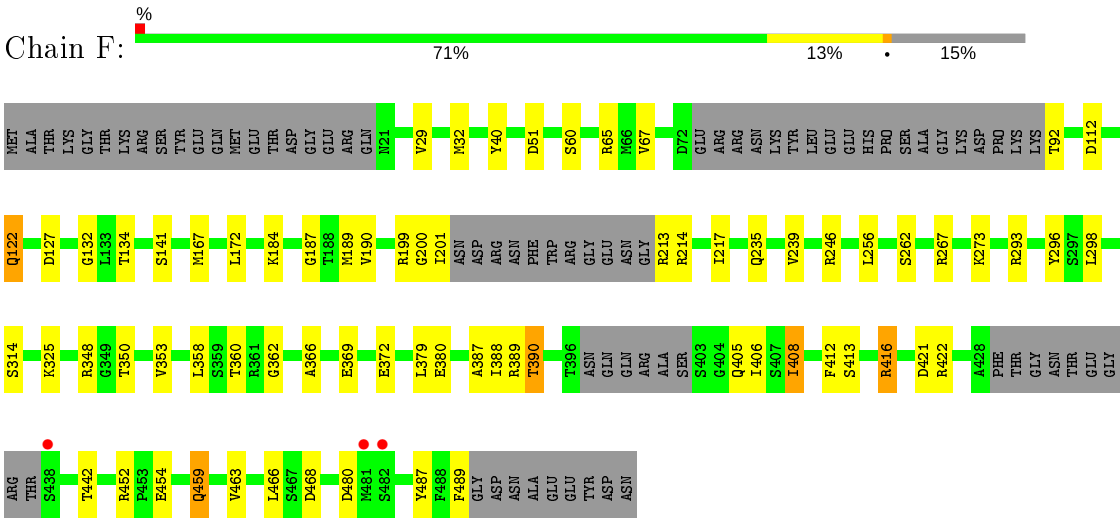


• Molecule 1: Nucleoprotein

Chain E: 69% 15% 15%



• Molecule 1: Nucleoprotein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	129.02Å 121.56Å 195.54Å 90.00° 89.79° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 40.54 – 3.00	Depositor EDS
% Data completeness (in resolution range)	92.0 (50.00-3.00) 92.0 (40.54-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, R_{free}	0.200 , 0.262 0.201 , 0.264	Depositor DCC
R_{free} test set	2824 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	71.5	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.417 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	19954	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NUZ

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	0.50	0/3375	0.73	0/4536
1	B	0.52	0/3381	0.76	0/4544
1	C	0.52	0/3379	0.74	1/4545 (0.0%)
1	D	0.50	0/3341	0.73	0/4491
1	E	0.50	0/3358	0.72	0/4515
1	F	0.49	0/3373	0.71	0/4538
All	All	0.50	0/20207	0.73	1/27169 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	172	LEU	CA-CB-CG	5.20	127.26	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3323	0	3321	50	0
1	B	3329	0	3326	44	0
1	C	3326	0	3311	43	0
1	D	3290	0	3286	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3306	0	3297	40	0
1	F	3320	0	3301	33	0
2	A	30	0	19	4	0
2	D	30	0	19	3	0
All	All	19954	0	19880	220	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 6.

All (220) 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)
2:A:501:NUZ:H9	2:A:501:NUZ:H5	1.31	1.10
1:D:416:ARG:HG2	1:D:416:ARG:HH11	1.22	1.03
1:A:416:ARG:HH11	1:A:416:ARG:HG2	1.21	1.01
2:A:501:NUZ:CAO	2:A:501:NUZ:H5	1.95	0.96
1:D:416:ARG:CG	1:D:416:ARG:HH11	1.81	0.91
1:A:416:ARG:CG	1:A:416:ARG:HH11	1.85	0.88
1:D:487:TYR:HB3	1:E:405:GLN:HG3	1.59	0.83
1:B:162:ARG:HB3	1:D:406:ILE:HG12	1.61	0.82
1:A:487:TYR:HB3	1:F:405:GLN:HG3	1.61	0.82
1:D:416:ARG:HG2	1:D:416:ARG:NH1	1.93	0.81
1:F:360:THR:HG22	1:F:362:GLY:H	1.44	0.81
1:E:360:THR:HG22	1:E:362:GLY:H	1.47	0.79
1:C:308:GLN:HE22	2:D:501:NUZ:H13	1.51	0.75
1:B:460:GLY:H	1:D:415:GLN:HE21	1.34	0.72
1:F:412:PHE:O	1:F:416:ARG:NH2	2.21	0.72
1:A:416:ARG:HG2	1:A:416:ARG:NH1	1.94	0.72
2:A:501:NUZ:H9	2:A:501:NUZ:CAJ	2.17	0.71
1:B:405:GLN:HG3	1:E:487:TYR:HB3	1.72	0.71
1:A:47:LEU:O	1:A:98:ARG:NH2	2.22	0.70
1:C:483:ASN:HD22	1:C:485:GLY:H	1.39	0.70
1:B:244:GLU:CD	1:B:244:GLU:H	1.94	0.69
1:A:415:GLN:HE21	1:C:460:GLY:H	1.40	0.69
1:D:184:LYS:HD2	1:D:189:MET:HE2	1.74	0.69
1:C:244:GLU:H	1:C:244:GLU:CD	1.95	0.68
1:A:406:ILE:HG12	1:C:162:ARG:HB3	1.74	0.68
1:C:405:GLN:HG3	1:F:487:TYR:HB3	1.74	0.68
1:D:325:LYS:HD3	1:D:360:THR:HG21	1.76	0.68
1:A:184:LYS:HD2	1:A:189:MET:HE2	1.76	0.66
1:A:325:LYS:HD3	1:A:360:THR:HG21	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:47:LEU:O	1:D:98:ARG:NH2	2.28	0.66
1:A:114:GLU:HG2	1:A:117:ARG:HH22	1.61	0.65
1:B:162:ARG:HB3	1:D:406:ILE:CG1	2.27	0.65
1:C:348:ARG:NH2	1:C:380:GLU:O	2.30	0.65
1:C:360:THR:HG22	1:C:362:GLY:H	1.62	0.65
1:A:325:LYS:HD3	1:A:360:THR:CG2	2.28	0.64
1:B:47:LEU:O	1:B:98:ARG:NH2	2.32	0.63
1:D:114:GLU:HG2	1:D:117:ARG:HH22	1.62	0.63
1:B:360:THR:HG22	1:B:362:GLY:H	1.64	0.62
1:A:405:GLN:HG3	1:C:487:TYR:HB3	1.81	0.62
1:F:406:ILE:HG23	1:F:421:ASP:HB3	1.80	0.62
1:D:42:GLN:O	1:D:46:GLU:HG2	1.99	0.61
1:B:66:MET:SD	1:B:93:GLY:HA2	2.41	0.61
1:D:325:LYS:HD3	1:D:360:THR:CG2	2.30	0.61
1:E:406:ILE:HG23	1:E:421:ASP:HB3	1.81	0.61
1:D:366:ALA:HB3	1:D:369:GLU:HG3	1.83	0.60
1:A:42:GLN:O	1:A:46:GLU:HG2	2.00	0.60
1:A:406:ILE:HG23	1:A:421:ASP:HB3	1.82	0.60
1:A:366:ALA:HB3	1:A:369:GLU:HG3	1.84	0.60
1:A:390:THR:HG23	1:F:413:SER:HB2	1.84	0.59
1:B:487:TYR:HB3	1:D:405:GLN:HG3	1.85	0.58
1:A:167:MET:HE1	1:A:187:GLY:HA3	1.85	0.57
1:C:47:LEU:O	1:C:98:ARG:NH2	2.38	0.57
1:B:348:ARG:NH2	1:B:380:GLU:O	2.38	0.57
1:C:66:MET:SD	1:C:93:GLY:HA2	2.46	0.56
1:D:464:PHE:CZ	1:D:471:ALA:HB1	2.40	0.56
1:D:406:ILE:HG23	1:D:421:ASP:HB3	1.88	0.56
1:D:160:ASP:HB3	1:D:163:MET:HG3	1.87	0.56
1:A:464:PHE:CZ	1:A:471:ALA:HB1	2.42	0.55
1:A:406:ILE:CG1	1:C:162:ARG:HB3	2.37	0.55
1:B:390:THR:HG23	1:D:413:SER:HB2	1.89	0.55
1:D:167:MET:HE1	1:D:187:GLY:HA3	1.88	0.55
1:B:115:GLU:HG3	1:B:118:ARG:HH12	1.71	0.55
1:F:213:ARG:HG3	1:F:214:ARG:H	1.72	0.54
1:D:487:TYR:HD1	1:E:408:ILE:HD12	1.72	0.54
1:E:459:GLN:H	1:E:459:GLN:HE21	1.56	0.54
1:F:353:VAL:HG23	1:F:358:LEU:HD12	1.89	0.54
1:E:167:MET:HE2	1:E:187:GLY:HA3	1.90	0.54
1:B:346:PHE:CE2	1:B:477:PRO:HB3	2.43	0.53
1:F:459:GLN:HE21	1:F:459:GLN:H	1.57	0.53
1:C:115:GLU:HG3	1:C:118:ARG:HH12	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:213:ARG:HG3	1:E:214:ARG:H	1.73	0.52
1:A:218:ALA:O	1:A:222:MET:HG3	2.08	0.52
1:B:186:VAL:HG21	1:B:268:GLY:HA3	1.91	0.52
1:F:184:LYS:HD2	1:F:189:MET:CE	2.40	0.52
1:E:348:ARG:NH2	1:E:380:GLU:O	2.42	0.52
1:A:160:ASP:HB3	1:A:163:MET:HG3	1.91	0.51
1:C:346:PHE:CE2	1:C:477:PRO:HB3	2.44	0.51
1:A:477:PRO:HG2	1:A:479:PHE:CZ	2.46	0.51
1:A:464:PHE:CE2	1:A:471:ALA:HB1	2.46	0.51
1:E:184:LYS:HD2	1:E:189:MET:CE	2.41	0.51
2:A:501:NUZ:H10	2:A:501:NUZ:H5	1.89	0.51
1:A:405:GLN:CG	1:C:487:TYR:HB3	2.41	0.51
1:C:186:VAL:HG21	1:C:268:GLY:HA3	1.92	0.50
1:E:353:VAL:HG23	1:E:358:LEU:HD12	1.92	0.50
2:D:501:NUZ:H14	2:D:501:NUZ:H5	1.94	0.50
1:B:115:GLU:HG3	1:B:118:ARG:NH1	2.27	0.50
1:C:464:PHE:CZ	1:C:471:ALA:HB1	2.47	0.50
1:E:141:SER:HB2	1:E:172:LEU:HD13	1.92	0.50
1:B:464:PHE:CZ	1:B:471:ALA:HB1	2.48	0.49
1:D:92:THR:HB	1:D:113:LYS:HE2	1.94	0.49
1:A:413:SER:HB2	1:C:390:THR:HG23	1.95	0.49
1:A:92:THR:HB	1:A:113:LYS:HE2	1.94	0.49
1:C:115:GLU:HG3	1:C:118:ARG:NH1	2.28	0.49
1:C:413:SER:HB2	1:F:390:THR:HG23	1.95	0.49
1:C:312:VAL:HG12	1:C:379:LEU:HD12	1.94	0.49
1:D:444:ILE:O	1:D:448:MET:HG3	2.13	0.49
1:F:141:SER:HB2	1:F:172:LEU:HD13	1.94	0.48
1:E:366:ALA:HB3	1:E:369:GLU:HG3	1.95	0.48
1:D:487:TYR:HB3	1:E:405:GLN:CG	2.37	0.48
1:B:250:ASN:O	1:B:254:GLU:HG2	2.14	0.48
1:C:360:THR:HG22	1:C:362:GLY:N	2.29	0.48
1:F:29:VAL:HG12	1:F:296:TYR:HB3	1.96	0.48
1:F:366:ALA:HB3	1:F:369:GLU:HG3	1.96	0.48
1:C:93:GLY:HA3	1:C:109:ILE:O	2.14	0.47
1:B:162:ARG:HD2	1:D:406:ILE:HD11	1.95	0.47
1:D:317:ARG:HD3	1:D:369:GLU:OE1	2.13	0.47
1:A:406:ILE:HD11	1:C:162:ARG:HD2	1.96	0.47
1:C:317:ARG:CZ	1:C:361:ARG:HB2	2.44	0.47
1:A:197:ILE:HG12	1:A:248:PRO:HB2	1.96	0.47
1:B:407:SER:OG	1:E:267:ARG:NH1	2.48	0.47
1:A:416:ARG:CG	1:A:416:ARG:NH1	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:314:SER:HB3	1:E:379:LEU:HD21	1.96	0.47
1:A:422:ARG:HD2	1:C:452:ARG:HH12	1.80	0.46
1:A:64:GLU:OE1	1:A:140:HIS:HE1	1.98	0.46
1:B:312:VAL:HG12	1:B:379:LEU:HD12	1.96	0.46
1:B:414:VAL:O	1:B:416:ARG:HG3	2.15	0.46
1:C:346:PHE:HE2	1:C:463:VAL:HG21	1.80	0.46
1:A:317:ARG:HD3	1:A:369:GLU:OE1	2.15	0.46
1:A:487:TYR:HB3	1:F:405:GLN:CG	2.41	0.46
1:A:253:PHE:O	1:A:257:ILE:HG12	2.15	0.46
1:E:40:TYR:HE1	1:E:60:SER:HA	1.81	0.46
1:B:56:LEU:HD11	1:B:315:LEU:HG	1.98	0.46
1:C:56:LEU:HD11	1:C:315:LEU:HG	1.98	0.46
1:D:390:THR:HG23	1:E:413:SER:HB2	1.96	0.46
1:F:167:MET:CE	1:F:187:GLY:HA3	2.46	0.46
1:C:405:GLN:HG2	1:F:489:PHE:HB2	1.97	0.46
1:B:317:ARG:CZ	1:B:361:ARG:HB2	2.46	0.46
1:C:317:ARG:NH1	1:C:369:GLU:OE2	2.44	0.46
1:A:444:ILE:O	1:A:448:MET:HG3	2.16	0.45
1:B:71:PHE:CZ	1:B:117:ARG:HG2	2.52	0.45
1:C:250:ASN:O	1:C:254:GLU:HG2	2.16	0.45
1:E:29:VAL:HG12	1:E:296:TYR:HB3	1.99	0.45
1:D:64:GLU:OE1	1:D:140:HIS:HE1	1.99	0.45
1:F:348:ARG:NH2	1:F:380:GLU:O	2.48	0.45
1:B:346:PHE:HE2	1:B:463:VAL:HG21	1.81	0.45
1:F:314:SER:HB3	1:F:379:LEU:HD21	1.98	0.45
1:D:309:ASN:HB3	2:D:501:NUZ:H10	1.98	0.45
1:B:360:THR:HG22	1:B:362:GLY:N	2.32	0.45
1:B:422:ARG:HH12	1:E:452:ARG:CZ	2.29	0.45
1:C:317:ARG:NH2	1:C:361:ARG:HB2	2.32	0.45
1:E:167:MET:CE	1:E:187:GLY:HA3	2.46	0.45
1:E:273:LYS:HB3	1:E:298:LEU:HD23	1.99	0.45
1:D:197:ILE:HG12	1:D:248:PRO:HB2	1.98	0.44
1:F:235:GLN:O	1:F:239:VAL:HG23	2.17	0.44
1:A:302:ASP:HB2	1:A:303:PRO:HD3	1.98	0.44
1:C:71:PHE:CZ	1:C:117:ARG:HG2	2.53	0.44
1:D:162:ARG:HB3	1:E:406:ILE:HG12	1.99	0.44
1:F:387:ALA:HB2	1:F:463:VAL:HG12	1.99	0.44
1:B:390:THR:CG2	1:D:413:SER:HB2	2.48	0.44
1:B:487:TYR:HB3	1:D:405:GLN:CG	2.48	0.44
1:D:218:ALA:O	1:D:222:MET:HG3	2.16	0.44
1:F:325:LYS:HD2	1:F:360:THR:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ARG:HB3	1:F:406:ILE:HG12	2.00	0.44
1:A:220:GLU:HG2	1:A:243:ARG:HG3	1.99	0.44
1:C:197:ILE:HG12	1:C:248:PRO:HB2	1.99	0.44
1:D:241:GLN:HE22	1:D:440:MET:HG3	1.82	0.44
1:A:267:ARG:HD3	1:F:408:ILE:O	2.17	0.44
1:B:242:VAL:HG13	1:B:252:GLU:HB3	2.00	0.44
1:D:345:SER:HA	1:D:352:VAL:HG23	2.00	0.44
1:A:345:SER:HA	1:A:352:VAL:HG23	2.00	0.43
1:B:184:LYS:HG2	1:B:188:THR:HG21	2.00	0.43
1:B:317:ARG:NH2	1:B:361:ARG:HB2	2.34	0.43
1:C:184:LYS:HG2	1:C:188:THR:HG21	2.00	0.43
1:D:220:GLU:HG2	1:D:243:ARG:HG3	2.00	0.43
1:E:325:LYS:HD2	1:E:360:THR:HG23	2.00	0.43
1:F:32:MET:HG3	1:F:132:GLY:HA2	2.00	0.43
1:D:421:ASP:OD1	1:D:423:PRO:HD2	2.19	0.43
1:C:151:THR:HG23	1:C:161:PRO:HB3	2.01	0.43
1:E:176:SER:HB2	1:E:180:GLY:HA3	2.01	0.43
1:D:487:TYR:CD1	1:E:408:ILE:HD12	2.52	0.43
1:F:40:TYR:HE1	1:F:60:SER:HA	1.84	0.43
1:C:190:VAL:HG11	1:C:260:ALA:HB2	2.01	0.43
1:C:239:VAL:C	1:C:241:GLN:H	2.22	0.42
1:E:28:SER:O	1:E:31:LYS:HB3	2.19	0.42
1:A:71:PHE:CE2	1:A:117:ARG:HG2	2.53	0.42
1:F:190:VAL:HG13	1:F:256:LEU:HB3	2.00	0.42
1:A:416:ARG:HD2	1:A:417:ASN:O	2.20	0.42
1:B:93:GLY:HA3	1:B:109:ILE:O	2.20	0.42
1:B:406:ILE:HG23	1:B:421:ASP:HB3	2.01	0.42
1:B:160:ASP:HB3	1:B:163:MET:HG3	2.02	0.42
1:B:239:VAL:C	1:B:241:GLN:H	2.24	0.42
1:B:301:ILE:HD13	1:B:305:ARG:NH2	2.35	0.42
1:D:71:PHE:CE2	1:D:117:ARG:HG2	2.55	0.42
1:E:235:GLN:O	1:E:239:VAL:HG23	2.20	0.42
1:A:103:LYS:HD3	1:E:351:LYS:HB3	2.01	0.41
1:B:346:PHE:CZ	1:B:477:PRO:HB3	2.54	0.41
1:F:167:MET:HE2	1:F:187:GLY:HA3	2.02	0.41
1:D:344:SER:HB3	1:D:352:VAL:HG21	2.01	0.41
1:E:190:VAL:HG13	1:E:256:LEU:HB3	2.02	0.41
1:F:122:GLN:HE21	1:F:122:GLN:HB3	1.61	0.41
1:A:164:CYS:SG	1:F:405:GLN:HB3	2.60	0.41
1:B:139:TRP:CH2	1:B:143:LEU:HD13	2.56	0.41
1:B:190:VAL:HG11	1:B:260:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:GLN:HB3	1:E:476:VAL:HG13	2.02	0.41
1:A:190:VAL:HG13	1:A:256:LEU:HB3	2.01	0.41
1:B:413:SER:HB2	1:E:390:THR:HG23	2.03	0.41
1:A:186:VAL:HG13	1:A:226:LEU:HD11	2.01	0.41
1:E:122:GLN:HB3	1:E:122:GLN:HE21	1.61	0.41
1:C:407:SER:OG	1:F:267:ARG:NH1	2.54	0.41
1:F:273:LYS:HB3	1:F:298:LEU:HD23	2.03	0.41
1:B:150:ARG:HH11	1:B:152:ARG:NH2	2.19	0.41
1:A:246:ARG:H	1:A:246:ARG:HG2	1.68	0.41
1:B:405:GLN:HG2	1:E:489:PHE:HB2	2.02	0.41
1:A:344:SER:HB3	1:A:352:VAL:HG21	2.02	0.41
1:F:200:GLY:O	1:F:201:ILE:HG13	2.21	0.41
1:C:317:ARG:HD3	1:C:369:GLU:OE1	2.21	0.40
1:C:346:PHE:CZ	1:C:477:PRO:HB3	2.55	0.40
1:D:167:MET:HE1	1:D:187:GLY:CA	2.50	0.40
1:E:200:GLY:O	1:E:201:ILE:HG13	2.20	0.40
1:A:250:ASN:O	1:A:253:PHE:HB3	2.22	0.40
1:C:164:CYS:HA	1:C:167:MET:HG2	2.04	0.40
1:C:248:PRO:HB3	1:C:252:GLU:HG2	2.03	0.40
1:E:315:LEU:HD12	1:E:365:ILE:HD12	2.04	0.40
1:E:387:ALA:HB2	1:E:463:VAL:HG12	2.02	0.40
1:A:227:LYS:HG2	1:A:236:ARG:HG2	2.02	0.40
1:D:246:ARG:HG2	1:D:246:ARG:H	1.70	0.40
1:D:250:ASN:O	1:D:253:PHE:HB3	2.22	0.40
1:E:348:ARG:HA	1:E:383:SER:CB	2.51	0.40
1:D:164:CYS:SG	1:E:405:GLN:HB3	2.61	0.40
1:E:405:GLN:NE2	1:E:407:SER:O	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	410/498 (82%)	392 (96%)	18 (4%)	0	100	100
1	B	411/498 (82%)	390 (95%)	20 (5%)	1 (0%)	47	82
1	C	414/498 (83%)	394 (95%)	19 (5%)	1 (0%)	47	82
1	D	407/498 (82%)	388 (95%)	19 (5%)	0	100	100
1	E	409/498 (82%)	389 (95%)	19 (5%)	1 (0%)	47	82
1	F	414/498 (83%)	390 (94%)	22 (5%)	2 (0%)	29	68
All	All	2465/2988 (82%)	2343 (95%)	117 (5%)	5 (0%)	47	82

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	468	ASP
1	F	468	ASP
1	B	240	ASP
1	F	480	ASP
1	C	240	ASP

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	357/422 (85%)	336 (94%)	21 (6%)	19	54
1	B	358/422 (85%)	327 (91%)	31 (9%)	10	37
1	C	357/422 (85%)	325 (91%)	32 (9%)	9	35
1	D	352/422 (83%)	333 (95%)	19 (5%)	22	57
1	E	354/422 (84%)	329 (93%)	25 (7%)	14	46
1	F	353/422 (84%)	327 (93%)	26 (7%)	13	44
All	All	2131/2532 (84%)	1977 (93%)	154 (7%)	14	45

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	ARG
1	A	108	LEU
1	A	112	ASP
1	A	130	THR
1	A	139	TRP
1	A	157	THR
1	A	201	ILE
1	A	213	ARG
1	A	217	ILE
1	A	231	GLN
1	A	246	ARG
1	A	309	ASN
1	A	365	ILE
1	A	375	GLU
1	A	389	ARG
1	A	392	SER
1	A	396	THR
1	A	416	ARG
1	A	422	ARG
1	A	450	SER
1	A	454	GLU
1	B	67	VAL
1	B	106	ARG
1	B	107	GLU
1	B	127	ASP
1	B	141	SER
1	B	152	ARG
1	B	157	THR
1	B	171	THR
1	B	183	VAL
1	B	217	ILE
1	B	238	MET
1	B	244	GLU
1	B	250	ASN
1	B	269	SER
1	B	293	ARG
1	B	311	GLN
1	B	335	SER
1	B	348	ARG
1	B	358	LEU
1	B	359	SER
1	B	361	ARG
1	B	367	SER

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Mol	Chain	Res	Type
1	B	372	GLU
1	B	383	SER
1	B	389	ARG
1	B	408	ILE
1	B	416	ARG
1	B	449	GLU
1	B	452	ARG
1	B	480	ASP
1	B	486	SER
1	C	67	VAL
1	C	106	ARG
1	C	107	GLU
1	C	127	ASP
1	C	141	SER
1	C	152	ARG
1	C	157	THR
1	C	171	THR
1	C	183	VAL
1	C	217	ILE
1	C	238	MET
1	C	244	GLU
1	C	250	ASN
1	C	269	SER
1	C	293	ARG
1	C	306	LEU
1	C	310	SER
1	C	311	GLN
1	C	335	SER
1	C	348	ARG
1	C	358	LEU
1	C	359	SER
1	C	361	ARG
1	C	367	SER
1	C	372	GLU
1	C	383	SER
1	C	389	ARG
1	C	408	ILE
1	C	449	GLU
1	C	452	ARG
1	C	480	ASP
1	C	486	SER
1	D	99	ARG

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Mol	Chain	Res	Type
1	D	108	LEU
1	D	112	ASP
1	D	130	THR
1	D	157	THR
1	D	201	ILE
1	D	213	ARG
1	D	217	ILE
1	D	231	GLN
1	D	246	ARG
1	D	309	ASN
1	D	375	GLU
1	D	389	ARG
1	D	392	SER
1	D	396	THR
1	D	416	ARG
1	D	422	ARG
1	D	450	SER
1	D	454	GLU
1	E	51	ASP
1	E	65	ARG
1	E	67	VAL
1	E	92	THR
1	E	112	ASP
1	E	122	GLN
1	E	127	ASP
1	E	134	THR
1	E	199	ARG
1	E	217	ILE
1	E	246	ARG
1	E	262	SER
1	E	293	ARG
1	E	350	THR
1	E	372	GLU
1	E	388	ILE
1	E	389	ARG
1	E	390	THR
1	E	408	ILE
1	E	416	ARG
1	E	422	ARG
1	E	442	THR
1	E	454	GLU
1	E	459	GLN

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Mol	Chain	Res	Type
1	E	466	LEU
1	F	51	ASP
1	F	65	ARG
1	F	67	VAL
1	F	92	THR
1	F	112	ASP
1	F	122	GLN
1	F	127	ASP
1	F	134	THR
1	F	199	ARG
1	F	217	ILE
1	F	246	ARG
1	F	262	SER
1	F	293	ARG
1	F	350	THR
1	F	372	GLU
1	F	388	ILE
1	F	389	ARG
1	F	390	THR
1	F	408	ILE
1	F	416	ARG
1	F	422	ARG
1	F	442	THR
1	F	452	ARG
1	F	454	GLU
1	F	459	GLN
1	F	466	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	HIS
1	A	241	GLN
1	A	415	GLN
1	B	483	ASN
1	C	483	ASN
1	D	140	HIS
1	D	241	GLN
1	D	415	GLN
1	E	122	GLN
1	E	459	GLN
1	F	122	GLN

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Mol	Chain	Res	Type
1	F	459	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 carbohydrates 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	NUZ	D	501	-	29,33,33	2.60	7 (24%)	35,47,47	2.56	13 (37%)
2	NUZ	A	501	-	29,33,33	2.76	8 (27%)	35,47,47	3.32	10 (28%)

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	NUZ	D	501	-	-	10/14/30/30	0/4/4/4
2	NUZ	A	501	-	-	11/14/30/30	0/4/4/4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	NUZ	OAC-NBD	10.38	1.40	1.22
2	D	501	NUZ	OAC-NBD	10.02	1.39	1.22
2	D	501	NUZ	CAW-CAZ	-6.06	1.42	1.49
2	A	501	NUZ	CAW-CAZ	-5.65	1.42	1.49
2	A	501	NUZ	CBA-CAZ	4.54	1.46	1.41
2	D	501	NUZ	CBA-CAZ	3.65	1.45	1.41
2	D	501	NUZ	CAV-CL1	3.29	1.81	1.73
2	A	501	NUZ	CAV-CL1	3.05	1.80	1.73
2	A	501	NUZ	CAY-CAV	2.92	1.43	1.39
2	A	501	NUZ	CBA-CAT	2.91	1.55	1.51
2	A	501	NUZ	CAZ-NAR	2.76	1.38	1.33
2	A	501	NUZ	CAA-CAU	2.38	1.51	1.48
2	D	501	NUZ	CAZ-NAR	2.36	1.37	1.33
2	D	501	NUZ	CAA-CAU	2.35	1.51	1.48
2	D	501	NUZ	CBA-CAT	2.15	1.54	1.51

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	NUZ	CBA-CAT-NBB	13.34	133.07	117.87
2	D	501	NUZ	CBA-CAT-NBB	8.92	128.03	117.87
2	A	501	NUZ	CAY-CAV-CL1	6.64	127.17	120.22
2	D	501	NUZ	CAO-CAQ-NBC	-5.57	99.89	110.70
2	A	501	NUZ	CAZ-CBA-CAT	5.56	137.92	127.08
2	A	501	NUZ	OAB-CAT-NBB	-4.97	114.13	122.34
2	D	501	NUZ	CAZ-CBA-CAT	4.76	136.35	127.08
2	A	501	NUZ	CAL-CAY-NBC	-4.49	115.14	122.30
2	D	501	NUZ	OAB-CAT-NBB	-4.43	115.02	122.34
2	A	501	NUZ	CAP-NBC-CAY	4.39	126.68	116.27
2	A	501	NUZ	CAM-CAV-CL1	-3.45	112.92	118.49
2	A	501	NUZ	OAB-CAT-CBA	-3.22	112.80	119.43
2	D	501	NUZ	CAL-CAY-NBC	-3.19	117.21	122.30
2	D	501	NUZ	CAP-NBC-CAY	3.16	123.77	116.27
2	D	501	NUZ	CAM-CAX-NBD	3.03	121.42	118.75
2	A	501	NUZ	CAJ-CAW-CAZ	3.00	125.36	120.61
2	D	501	NUZ	CAJ-CAW-CAZ	2.78	125.01	120.61
2	D	501	NUZ	CAN-NBB-CAO	2.47	117.38	112.62
2	D	501	NUZ	CAN-CAP-NBC	-2.43	105.98	110.70
2	A	501	NUZ	CAP-NBC-CAQ	2.33	116.66	111.52
2	D	501	NUZ	CAP-NBC-CAQ	2.14	116.23	111.52
2	D	501	NUZ	CAI-CAW-CAZ	-2.12	117.24	120.61
2	D	501	NUZ	CAM-CAV-CAY	-2.11	119.02	120.74

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	501	NUZ	CAI-CAW-CAZ-CBA
2	D	501	NUZ	CAJ-CAW-CAZ-CBA
2	D	501	NUZ	CBA-CAT-NBB-CAO
2	D	501	NUZ	CBA-CAT-NBB-CAN
2	D	501	NUZ	OAB-CAT-NBB-CAN
2	D	501	NUZ	CAV-CAY-NBC-CAP
2	D	501	NUZ	CAM-CAX-NBD-OAC
2	D	501	NUZ	CAK-CAX-NBD-OAC
2	A	501	NUZ	CAI-CAW-CAZ-CBA
2	A	501	NUZ	CAJ-CAW-CAZ-CBA
2	A	501	NUZ	CBA-CAT-NBB-CAN
2	A	501	NUZ	OAB-CAT-NBB-CAO
2	A	501	NUZ	CAV-CAY-NBC-CAP
2	A	501	NUZ	CAM-CAX-NBD-OAC
2	A	501	NUZ	CAK-CAX-NBD-OAC
2	D	501	NUZ	OAB-CAT-NBB-CAO
2	A	501	NUZ	OAB-CAT-NBB-CAN
2	A	501	NUZ	CBA-CAT-NBB-CAO
2	A	501	NUZ	CAV-CAY-NBC-CAQ
2	D	501	NUZ	CAL-CAY-NBC-CAP
2	A	501	NUZ	CAL-CAY-NBC-CAQ

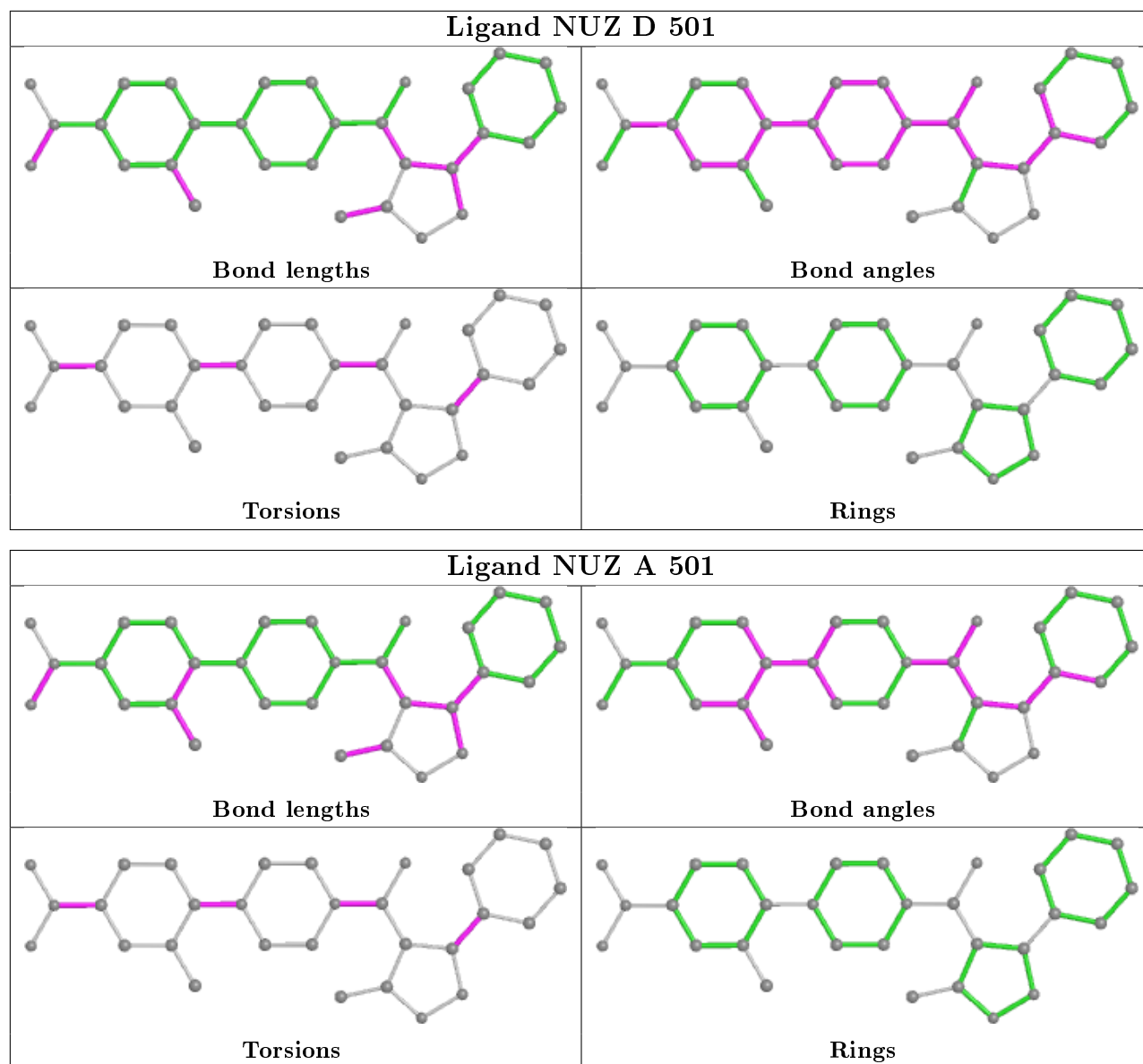
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	NUZ	3	0
2	A	501	NUZ	4	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 ⓘ

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	422/498 (84%)	-0.29	0 100 100	43, 69, 102, 149	0
1	B	423/498 (84%)	-0.31	2 (0%) 91 75	41, 67, 109, 151	0
1	C	424/498 (85%)	-0.34	2 (0%) 91 75	44, 67, 110, 144	0
1	D	419/498 (84%)	-0.34	1 (0%) 95 87	45, 68, 101, 135	0
1	E	421/498 (84%)	-0.29	2 (0%) 91 75	48, 79, 113, 174	0
1	F	424/498 (85%)	-0.21	3 (0%) 87 69	47, 78, 115, 184	0
All	All	2533/2988 (84%)	-0.30	10 (0%) 92 79	41, 71, 111, 184	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	482	SER	5.5
1	F	481	MET	3.6
1	F	438	SER	3.2
1	E	483	ASN	2.9
1	B	21	ASN	2.8
1	C	484	GLU	2.8
1	B	246	ARG	2.5
1	D	403	SER	2.5
1	C	246	ARG	2.1
1	E	114	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

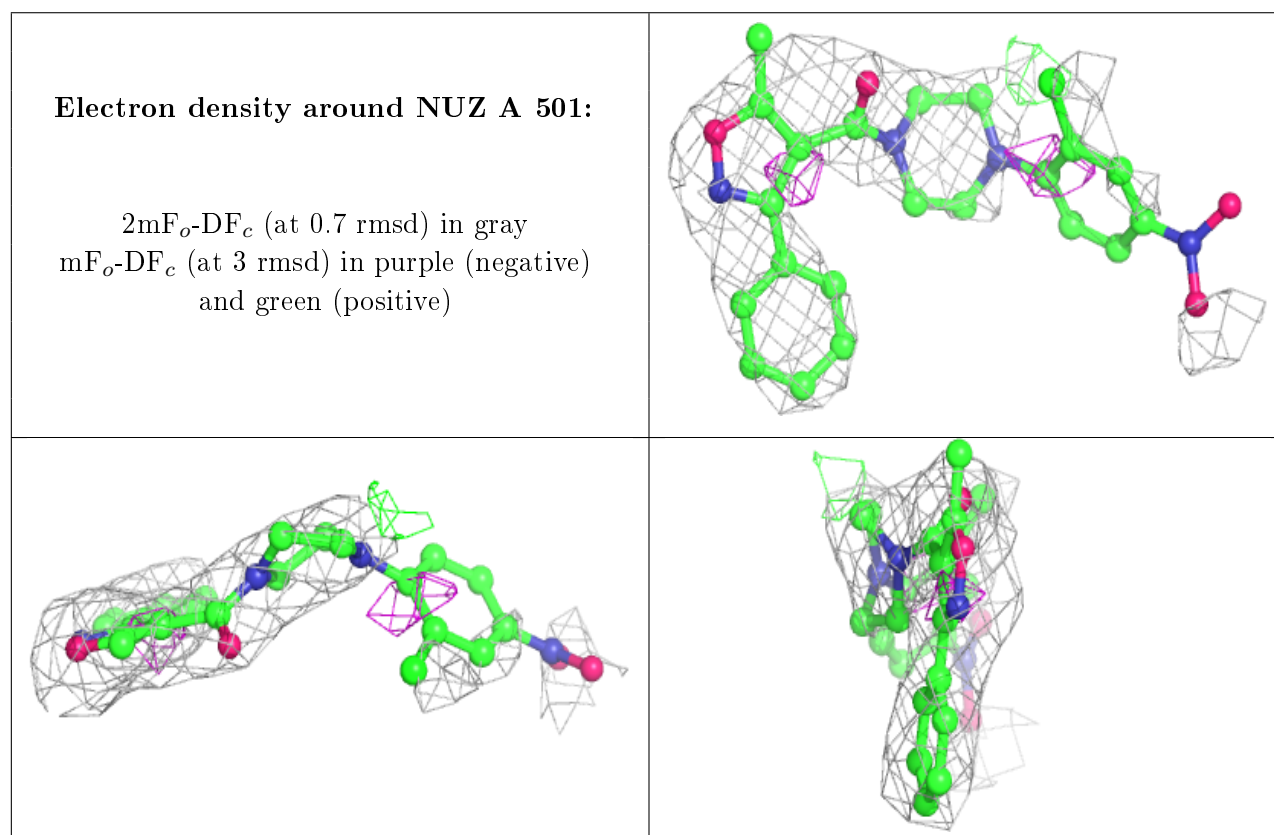
There are no carbohydrates in this entry.

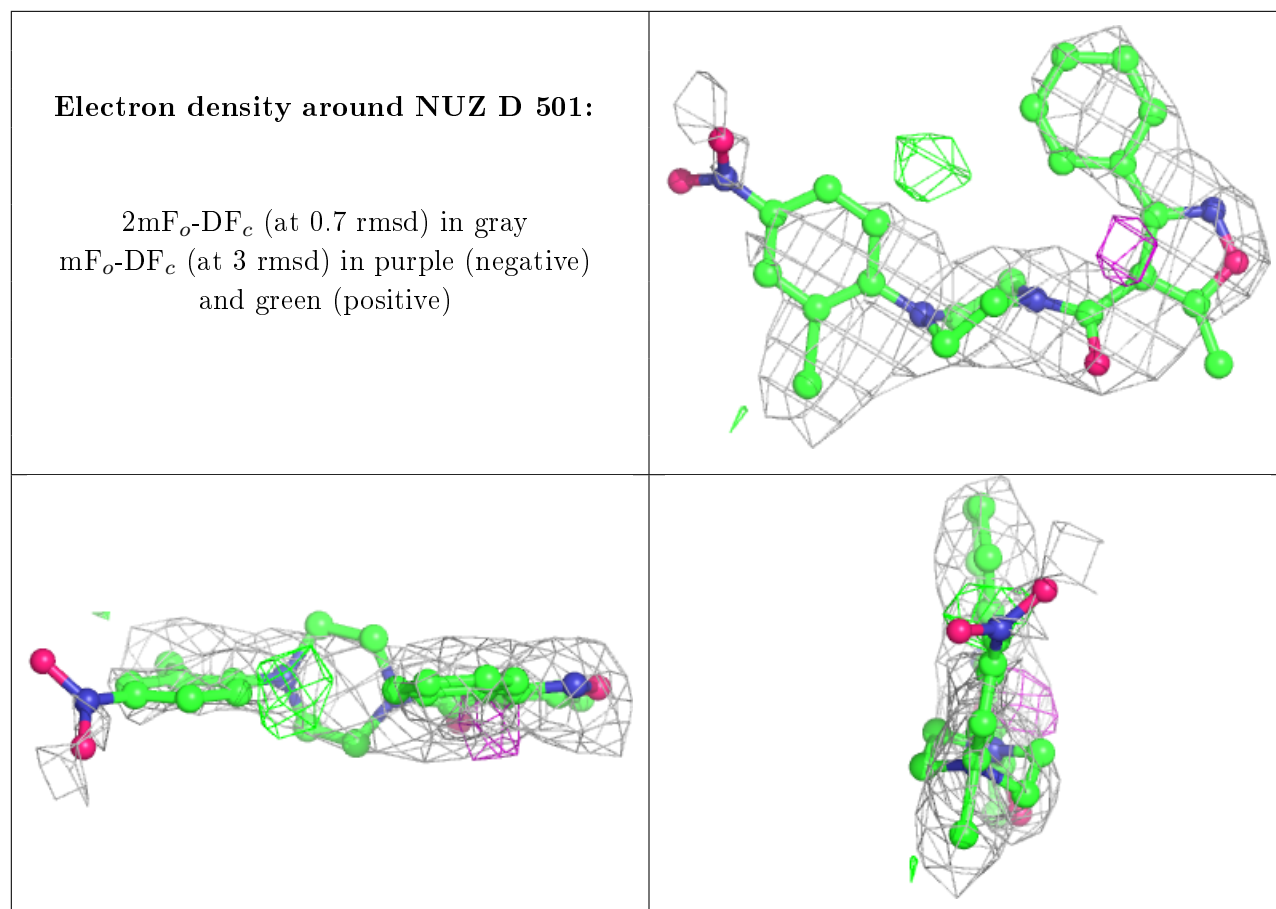
6.4 Ligands [i](#)

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
2	NUZ	A	501	30/30	0.78	0.38	79,109,169,171	0
2	NUZ	D	501	30/30	0.81	0.41	87,109,148,150	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.





6.5 Other polymers ⓘ

There are no such residues in this entry.