



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:51 AM UTC

PDB ID : 8J6H / pdb_00008j6h
Title : Structure and allosteric regulation of the inosine 5'-monophosphate-specific phosphatase ISN1 from *Saccharomyces cerevisiae*
Authors : Byun, S.J.; Rhee, S.
Deposited on : 2023-04-25
Resolution : 2.44 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

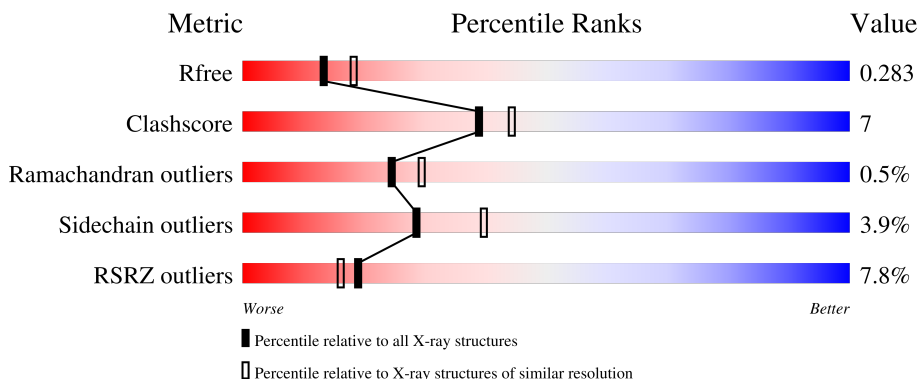
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.44 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	455	7% 70% 17% • 12%
1	B	455	7% 74% 13% • 11%
1	C	455	8% 71% 18% 11%
1	D	455	5% 71% 17% • 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13149 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 IMP-specific 5'-nucleotidase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	402	Total	C	N	O	S	Se	0	0	0
			3241	2061	563	610	4	3			
1	B	403	Total	C	N	O	S	Se	0	0	0
			3242	2061	561	612	4	4			
1	C	403	Total	C	N	O	S	Se	0	0	0
			3252	2070	564	610	4	4			
1	D	407	Total	C	N	O	S	Se	0	0	0
			3294	2092	579	616	4	3			

There are 32 discrepancies between the modelled and reference sequences:

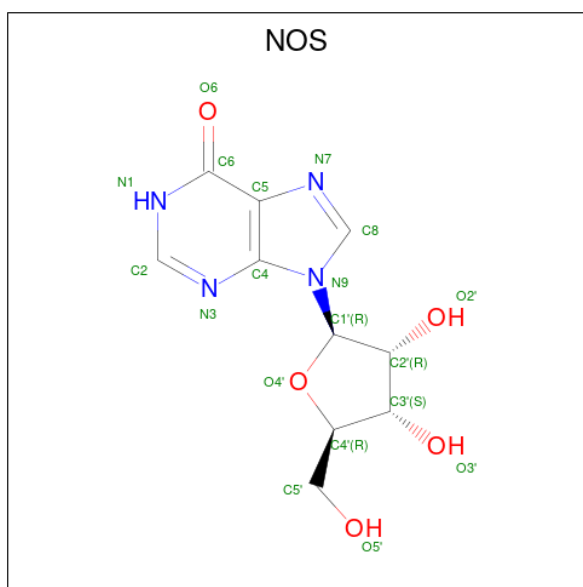
Chain	Residue	Modelled	Actual	Comment	Reference
A	451	HIS	-	expression tag	UNP Q99312
A	452	HIS	-	expression tag	UNP Q99312
A	453	HIS	-	expression tag	UNP Q99312
A	454	HIS	-	expression tag	UNP Q99312
A	455	HIS	-	expression tag	UNP Q99312
A	456	HIS	-	expression tag	UNP Q99312
A	457	HIS	-	expression tag	UNP Q99312
A	458	HIS	-	expression tag	UNP Q99312
B	451	HIS	-	expression tag	UNP Q99312
B	452	HIS	-	expression tag	UNP Q99312
B	453	HIS	-	expression tag	UNP Q99312
B	454	HIS	-	expression tag	UNP Q99312
B	455	HIS	-	expression tag	UNP Q99312
B	456	HIS	-	expression tag	UNP Q99312
B	457	HIS	-	expression tag	UNP Q99312
B	458	HIS	-	expression tag	UNP Q99312
C	451	HIS	-	expression tag	UNP Q99312
C	452	HIS	-	expression tag	UNP Q99312
C	453	HIS	-	expression tag	UNP Q99312
C	454	HIS	-	expression tag	UNP Q99312
C	455	HIS	-	expression tag	UNP Q99312

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Chain	Residue	Modelled	Actual	Comment	Reference
C	456	HIS	-	expression tag	UNP Q99312
C	457	HIS	-	expression tag	UNP Q99312
C	458	HIS	-	expression tag	UNP Q99312
D	451	HIS	-	expression tag	UNP Q99312
D	452	HIS	-	expression tag	UNP Q99312
D	453	HIS	-	expression tag	UNP Q99312
D	454	HIS	-	expression tag	UNP Q99312
D	455	HIS	-	expression tag	UNP Q99312
D	456	HIS	-	expression tag	UNP Q99312
D	457	HIS	-	expression tag	UNP Q99312
D	458	HIS	-	expression tag	UNP Q99312

- Molecule 2 is INOSINE (CCD ID: NOS) (formula: $C_{10}H_{12}N_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			19	10	4	5		
2	B	1	Total	C	N	O	0	0
			19	10	4	5		
2	C	1	Total	C	N	O	0	0
			19	10	4	5		
2	D	1	Total	C	N	O	0	0
			19	10	4	5		

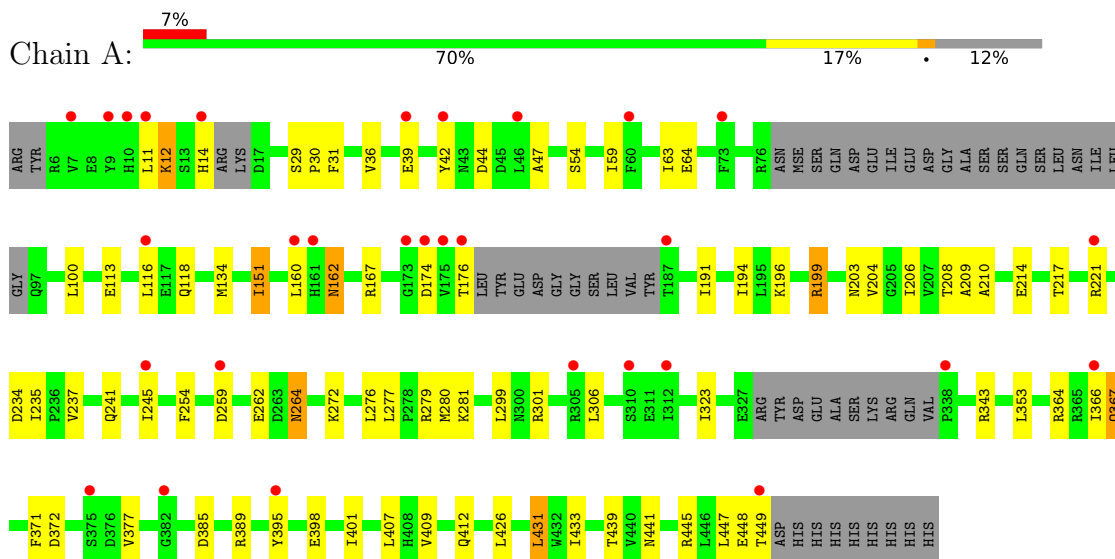
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	12	Total 12	O 12	0	0
3	B	8	Total 8	O 8	0	0
3	C	6	Total 6	O 6	0	0
3	D	18	Total 18	O 18	0	0

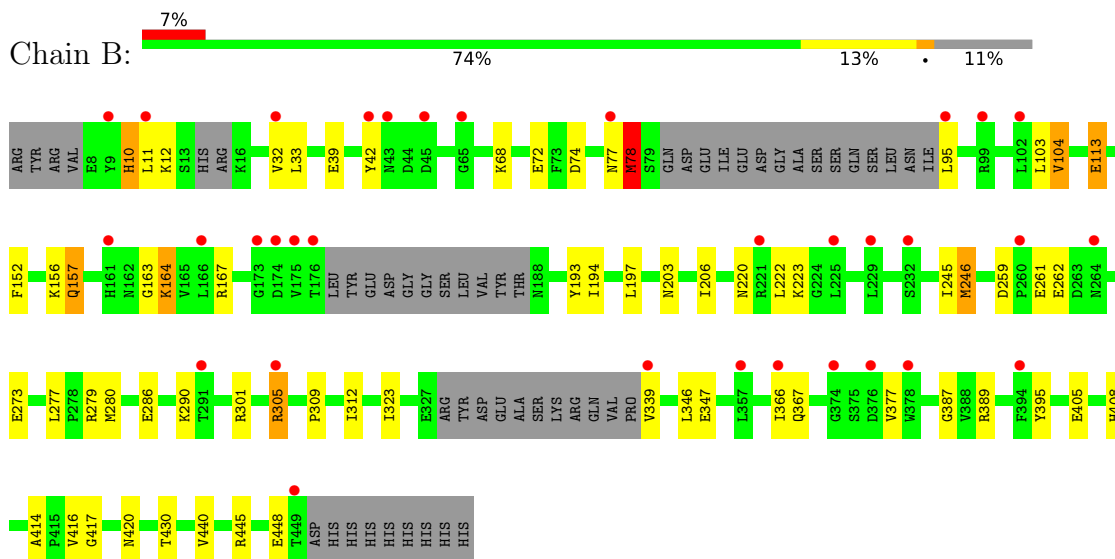
3 Residue-property plots [i](#)

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.

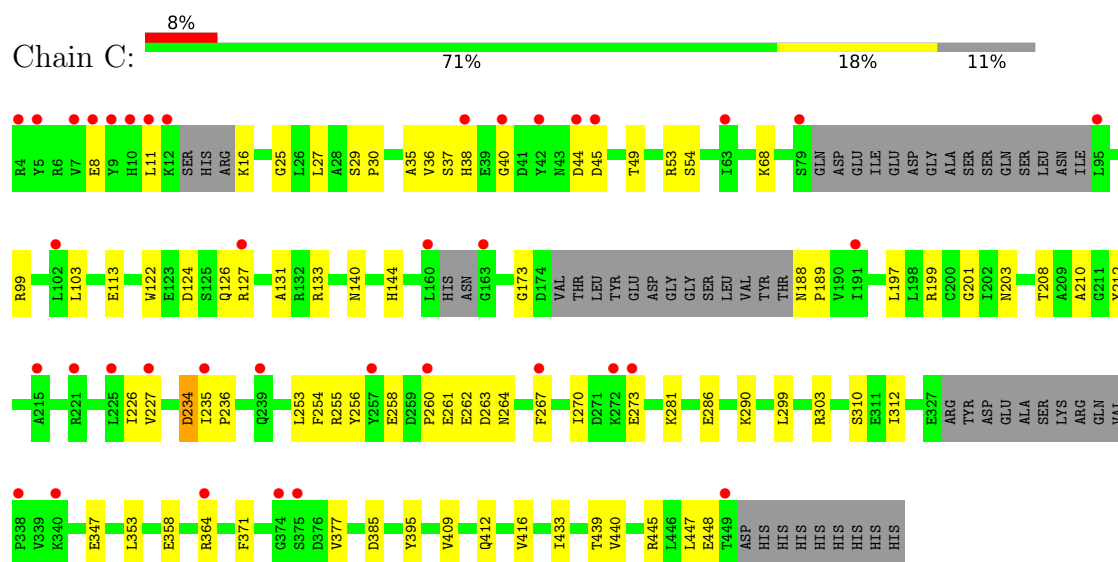
• Molecule 1: IMP-specific 5'-nucleotidase 1



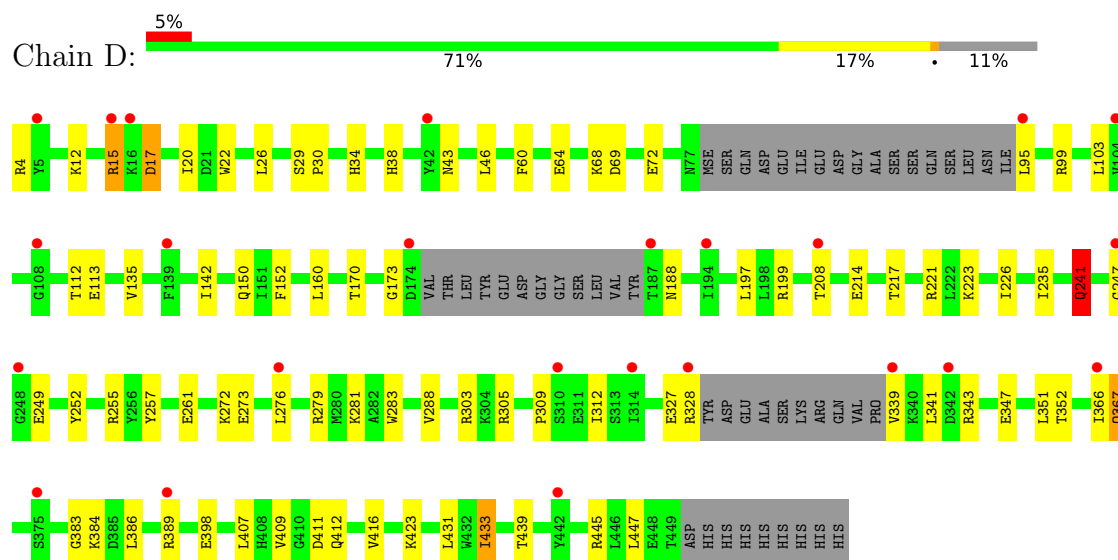
• Molecule 1: IMP-specific 5'-nucleotidase 1



• Molecule 1: IMP-specific 5'-nucleotidase 1



• Molecule 1: IMP-specific 5'-nucleotidase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	147.39Å 165.06Å 82.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.09 – 2.44 47.09 – 2.44	Depositor EDS
% Data completeness (in resolution range)	98.8 (47.09-2.44) 98.8 (47.09-2.44)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.236 , 0.279 0.243 , 0.283	Depositor DCC
R_{free} test set	2000 reflections (2.64%)	wwPDB-VP
Wilson B-factor (Å ²)	55.7	Xtriage
Anisotropy	0.452	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 51.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13149	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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: NOS

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	0.31	0/3305	0.75	1/4467 (0.0%)
1	B	0.30	0/3303	0.75	4/4460 (0.1%)
1	C	0.29	0/3313	0.74	0/4470
1	D	0.31	0/3359	0.75	0/4537
All	All	0.30	0/13280	0.74	5/17934 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	104	VAL	CA-C-N	5.38	124.71	118.85
1	B	104	VAL	C-N-CA	5.38	124.71	118.85
1	A	191	ILE	CB-CA-C	-5.15	108.81	113.70
1	B	259	ASP	CA-C-N	5.02	124.62	119.05
1	B	259	ASP	C-N-CA	5.02	124.62	119.05

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	3241	0	3201	55	2
1	B	3242	0	3204	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3252	0	3221	46	2
1	D	3294	0	3259	53	0
2	A	19	0	12	0	0
2	B	19	0	12	0	0
2	C	19	0	12	0	0
2	D	19	0	12	1	0
3	A	12	0	0	0	0
3	B	8	0	0	0	0
3	C	6	0	0	0	0
3	D	18	0	0	0	0
All	All	13149	0	12933	178	2

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 7.

All (178) 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:B:261:GLU:HG2	1:B:262:GLU:HG3	1.60	0.82
1:B:279:ARG:HH12	1:B:389:ARG:HH22	1.24	0.80
1:A:264:ASN:HD22	1:A:264:ASN:N	1.85	0.74
1:A:276:LEU:O	1:A:281:LYS:NZ	2.21	0.73
1:A:42:TYR:HE1	1:B:305:ARG:HH21	1.36	0.73
1:C:260:PRO:HA	1:C:263:ASP:HA	1.72	0.72
1:A:12:LYS:H	1:A:14:HIS:CE1	2.08	0.71
1:C:303:ARG:NH2	1:C:312:ILE:O	2.23	0.71
1:A:206:ILE:HB	1:A:245:ILE:HG22	1.72	0.69
1:A:208:THR:HG22	1:A:210:ALA:H	1.57	0.68
1:D:241:GLN:OE1	1:D:257:TYR:HA	1.92	0.68
1:C:35:ALA:O	1:C:37:SER:N	2.27	0.66
1:D:288:VAL:HG23	1:D:366:ILE:HD13	1.76	0.65
1:A:113:GLU:OE1	1:A:113:GLU:N	2.26	0.64
1:A:151:ILE:HD11	1:A:431:LEU:HD21	1.80	0.64
1:C:303:ARG:HH22	1:C:310:SER:HA	1.63	0.63
1:C:273:GLU:OE1	1:C:281:LYS:NZ	2.31	0.62
1:B:417:GLY:O	1:B:420:ASN:ND2	2.30	0.62
1:A:364:ARG:HH22	1:D:95:LEU:HB2	1.65	0.60
1:D:272:LYS:N	1:D:272:LYS:HD3	2.17	0.60
1:D:303:ARG:NH2	1:D:312:ILE:O	2.34	0.60
1:B:157:GLN:HG3	1:B:163:GLY:HA3	1.84	0.59
1:B:366:ILE:HG22	1:B:367:GLN:H	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:ARG:HH22	1:D:17:ASP:HA	1.68	0.58
1:B:74:ASP:O	1:B:78:MSE:HG2	2.02	0.58
1:D:173:GLY:HA3	1:D:208:THR:HG22	1.85	0.58
1:C:262:GLU:HB2	1:C:264:ASN:HB2	1.85	0.58
1:D:309:PRO:HB2	1:D:328:ARG:HH22	1.68	0.57
1:C:286:GLU:HG2	1:C:290:LYS:HD2	1.86	0.57
1:A:199:ARG:NH1	1:A:234:ASP:OD2	2.38	0.56
1:B:309:PRO:HG2	1:B:312:ILE:HG12	1.88	0.56
1:D:150:GLN:NE2	2:D:501:NOS:O3'	2.39	0.55
1:A:398:GLU:OE1	1:A:398:GLU:N	2.35	0.55
1:A:214:GLU:OE2	1:A:217:THR:OG1	2.19	0.54
1:C:253:LEU:HG	1:C:270:ILE:HD13	1.89	0.54
1:B:279:ARG:HH12	1:B:389:ARG:NH2	2.00	0.54
1:A:272:LYS:N	1:A:272:LYS:HD3	2.22	0.54
1:A:44:ASP:OD1	1:A:47:ALA:HB3	2.07	0.54
1:D:214:GLU:OE2	1:D:217:THR:OG1	2.20	0.54
1:B:32:VAL:HG11	1:D:22:TRP:HE1	1.72	0.54
1:D:199:ARG:HB2	1:D:235:ILE:HG12	1.89	0.54
1:C:258:GLU:C	1:C:260:PRO:HD3	2.33	0.54
1:D:68:LYS:O	1:D:72:GLU:HG3	2.08	0.54
1:C:385:ASP:N	1:C:385:ASP:OD1	2.41	0.53
1:A:245:ILE:HG13	1:A:254:PHE:HB2	1.89	0.53
1:B:246:MSE:HE3	1:B:387:GLY:HA2	1.89	0.53
1:D:398:GLU:OE1	1:D:398:GLU:N	2.41	0.53
1:C:49:THR:OG1	1:C:133:ARG:NH2	2.42	0.52
1:A:12:LYS:H	1:A:14:HIS:HE1	1.53	0.52
1:B:323:ILE:HG22	1:B:377:VAL:HB	1.91	0.52
1:D:312:ILE:HG21	1:D:341:LEU:HD21	1.91	0.52
1:A:366:ILE:HG22	1:A:367:GLN:O	2.10	0.51
1:C:261:GLU:OE1	1:C:261:GLU:N	2.35	0.51
1:C:53:ARG:NH1	1:C:124:ASP:OD2	2.44	0.51
1:C:226:ILE:HG23	1:C:256:TYR:HE1	1.76	0.50
1:A:441:ASN:O	1:A:445:ARG:HG3	2.11	0.50
1:D:367:GLN:OE1	1:D:386:LEU:HD11	2.10	0.50
1:D:197:LEU:HD23	1:D:447:LEU:HD21	1.92	0.50
1:B:68:LYS:O	1:B:72:GLU:HG3	2.12	0.50
1:C:199:ARG:HB2	1:C:235:ILE:HD12	1.94	0.50
1:C:260:PRO:HA	1:C:263:ASP:CA	2.41	0.50
1:A:343:ARG:NH2	1:A:372:ASP:OD1	2.45	0.50
1:B:286:GLU:HG2	1:B:290:LYS:HD2	1.94	0.50
1:A:196:LYS:HG2	1:A:447:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:309:PRO:CB	1:D:328:ARG:HH22	2.26	0.49
1:C:412:GLN:HB3	1:C:416:VAL:HG21	1.94	0.49
1:D:412:GLN:HB3	1:D:416:VAL:HG21	1.95	0.49
1:A:343:ARG:NH1	1:A:372:ASP:O	2.46	0.49
1:B:10:HIS:CE1	1:B:12:LYS:O	2.66	0.48
1:A:364:ARG:NH2	1:D:95:LEU:HB2	2.29	0.48
1:B:152:PHE:O	1:B:156:LYS:HG2	2.14	0.48
1:A:237:VAL:O	1:A:241:GLN:HG3	2.13	0.47
1:B:346:LEU:HD22	1:B:377:VAL:HG23	1.95	0.47
1:B:12:LYS:HB2	1:B:12:LYS:HE2	1.68	0.47
1:C:189:PRO:HB2	1:C:440:VAL:HG21	1.96	0.47
1:C:347:GLU:HB3	1:D:135:VAL:HG21	1.97	0.47
1:B:220:ASN:O	1:B:223:LYS:HE2	2.14	0.47
1:C:38:HIS:CE1	1:D:352:THR:HA	2.50	0.47
1:C:234:ASP:N	1:C:234:ASP:OD1	2.47	0.47
1:D:407:LEU:HD11	1:D:431:LEU:HG	1.96	0.47
1:A:389:ARG:NH1	1:A:426:LEU:O	2.48	0.47
1:B:113:GLU:H	1:B:113:GLU:HG2	1.50	0.47
1:D:247:GLY:N	1:D:252:TYR:O	2.48	0.46
1:B:10:HIS:HD2	1:B:347:GLU:OE2	1.98	0.46
1:A:64:GLU:HG2	1:A:116:LEU:HD13	1.97	0.46
1:D:22:TRP:O	1:D:26:LEU:HG	2.16	0.46
1:A:29:SER:HB2	1:A:30:PRO:HD3	1.97	0.46
1:C:38:HIS:HE1	1:D:352:THR:HA	1.81	0.45
1:C:255:ARG:HB2	1:C:270:ILE:HD11	1.98	0.45
1:A:39:GLU:HG3	1:A:134:MSE:SE	2.65	0.45
1:C:261:GLU:H	1:C:261:GLU:CD	2.21	0.45
1:A:299:LEU:HD21	1:A:353:LEU:HD11	1.99	0.45
1:B:167:ARG:HD3	1:B:405:GLU:CD	2.42	0.45
1:A:174:ASP:HA	1:A:209:ALA:H	1.81	0.45
1:A:167:ARG:NH1	1:A:401:ILE:HA	2.32	0.45
1:D:384:LYS:HB2	1:D:384:LYS:HE3	1.75	0.45
1:A:160:LEU:O	1:A:162:ASN:N	2.46	0.44
1:D:12:LYS:HG2	1:D:351:LEU:HD11	1.99	0.44
1:A:176:THR:O	1:A:221:ARG:NH1	2.41	0.44
1:C:131:ALA:O	1:D:305:ARG:HD3	2.17	0.44
1:C:140:ASN:O	1:C:144:HIS:ND1	2.50	0.44
1:A:199:ARG:HB2	1:A:235:ILE:HG12	2.00	0.44
1:C:210:ALA:HB1	1:C:212:TYR:CD2	2.53	0.44
1:D:99:ARG:O	1:D:103:LEU:HG	2.18	0.44
1:C:409:VAL:HG11	1:C:439:THR:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:LEU:HB2	1:A:280:MSE:HG3	2.00	0.44
1:A:301:ARG:H	1:A:301:ARG:HG2	1.62	0.44
1:D:34:HIS:O	1:D:38:HIS:ND1	2.51	0.44
1:B:408:HIS:HB3	1:B:430:THR:HG22	2.00	0.44
1:D:261:GLU:N	1:D:261:GLU:OE1	2.50	0.44
1:A:194:ILE:HG23	1:A:204:VAL:HG11	1.99	0.43
1:C:199:ARG:HB2	1:C:235:ILE:CD1	2.48	0.43
1:A:234:ASP:N	1:A:234:ASP:OD1	2.43	0.43
1:D:249:GLU:HB3	1:D:383:GLY:C	2.43	0.43
1:B:222:LEU:HD12	1:B:245:ILE:HD11	2.00	0.43
1:C:299:LEU:HD21	1:C:353:LEU:HD11	2.01	0.43
1:A:272:LYS:HD3	1:A:272:LYS:H	1.82	0.43
1:D:276:LEU:HD23	1:D:276:LEU:HA	1.90	0.43
1:A:272:LYS:H	1:A:272:LYS:CD	2.32	0.43
1:C:358:GLU:O	1:C:364:ARG:HD3	2.18	0.43
1:D:29:SER:HB2	1:D:30:PRO:HD3	2.00	0.43
1:D:273:GLU:OE1	1:D:281:LYS:NZ	2.44	0.43
1:D:309:PRO:HG2	1:D:312:ILE:HG12	2.00	0.43
1:D:398:GLU:H	1:D:398:GLU:CD	2.24	0.43
1:A:174:ASP:HB2	1:A:412:GLN:HE22	1.83	0.43
1:C:25:GLY:HA3	1:D:4:ARG:HD2	2.00	0.43
1:D:241:GLN:O	1:D:255:ARG:NE	2.46	0.43
1:D:411:ASP:HB3	1:D:433:ILE:HD11	2.01	0.43
1:A:203:ASN:HB3	1:A:395:TYR:CZ	2.53	0.43
1:C:29:SER:HB2	1:C:30:PRO:HD3	2.00	0.43
1:C:197:LEU:HG	1:C:447:LEU:HD11	2.01	0.43
1:C:197:LEU:HD23	1:C:447:LEU:HD21	2.01	0.42
1:A:214:GLU:N	1:A:214:GLU:OE1	2.52	0.42
1:D:217:THR:HG22	1:D:221:ARG:HD3	2.01	0.42
1:A:259:ASP:OD2	1:A:262:GLU:HG2	2.19	0.42
1:C:203:ASN:HB3	1:C:395:TYR:CZ	2.54	0.42
1:B:203:ASN:HB3	1:B:395:TYR:CZ	2.54	0.42
1:D:279:ARG:HE	1:D:279:ARG:HB2	1.73	0.42
1:C:8:GLU:OE1	1:C:8:GLU:N	2.50	0.42
1:D:20:ILE:HG23	1:D:142:ILE:HB	2.00	0.42
1:D:60:PHE:O	1:D:64:GLU:HG3	2.19	0.42
1:D:283:TRP:CG	1:D:366:ILE:HG12	2.54	0.42
1:A:276:LEU:HD23	1:A:276:LEU:HA	1.90	0.42
1:A:385:ASP:OD1	1:A:385:ASP:N	2.53	0.42
1:B:77:ASN:O	1:B:78:MSE:HG2	2.20	0.42
1:C:173:GLY:HA3	1:C:208:THR:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:ASN:HA	1:C:189:PRO:HD3	1.79	0.42
1:D:409:VAL:HG11	1:D:439:THR:HG23	2.02	0.42
1:A:174:ASP:HA	1:A:208:THR:HA	2.02	0.41
1:A:409:VAL:HG11	1:A:439:THR:HG23	2.03	0.41
1:B:103:LEU:HD23	1:C:11:LEU:HD21	2.03	0.41
1:C:254:PHE:HB3	1:C:267:PHE:HB3	2.01	0.41
1:D:69:ASP:OD2	1:D:99:ARG:NH1	2.53	0.41
1:A:31:PHE:O	1:A:36:VAL:HG23	2.19	0.41
1:D:214:GLU:OE1	1:D:214:GLU:N	2.54	0.41
1:A:301:ARG:HD3	1:B:42:TYR:CE1	2.55	0.41
1:B:10:HIS:CE1	1:B:12:LYS:C	2.99	0.41
1:A:100:LEU:HD12	1:A:100:LEU:HA	1.92	0.41
1:A:371:PHE:O	1:A:377:VAL:HA	2.20	0.41
1:B:194:ILE:HA	1:B:197:LEU:HD12	2.02	0.41
1:B:445:ARG:O	1:B:448:GLU:HG2	2.20	0.41
1:C:235:ILE:HG22	1:C:236:PRO:O	2.21	0.41
1:D:152:PHE:HE1	1:D:445:ARG:HD3	1.85	0.41
1:A:366:ILE:HG22	1:A:367:GLN:N	2.36	0.41
1:B:193:TYR:CE2	1:B:440:VAL:HG13	2.56	0.41
1:C:199:ARG:C	1:C:201:GLY:H	2.29	0.41
1:D:17:ASP:OD1	1:D:20:ILE:HG13	2.21	0.41
1:A:42:TYR:HE1	1:B:305:ARG:NH2	2.10	0.41
1:B:277:LEU:HB2	1:B:280:MSE:HG3	2.02	0.41
1:D:223:LYS:HA	1:D:226:ILE:HG12	2.03	0.41
1:A:59:ILE:O	1:A:63:ILE:HG13	2.22	0.40
1:A:407:LEU:HD11	1:A:431:LEU:HD13	2.02	0.40
1:C:99:ARG:O	1:C:103:LEU:HG	2.22	0.40
1:C:122:TRP:O	1:C:126:GLN:HG2	2.21	0.40
1:C:371:PHE:O	1:C:377:VAL:HA	2.21	0.40
1:D:445:ARG:CZ	1:D:445:ARG:HB2	2.50	0.40
1:B:414:ALA:O	1:B:416:VAL:N	2.53	0.40
1:B:301:ARG:O	1:B:305:ARG:HG3	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:GLN:NE2	1:C:44:ASP:OD1[2_545]	2.04	0.16
1:A:54:SER:OG	1:C:54:SER:OG[2_545]	2.19	0.01

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	392/455 (86%)	379 (97%)	12 (3%)	1 (0%)	36	44
1	B	393/455 (86%)	381 (97%)	10 (2%)	2 (0%)	24	29
1	C	391/455 (86%)	373 (95%)	16 (4%)	2 (0%)	24	29
1	D	399/455 (88%)	385 (96%)	11 (3%)	3 (1%)	16	18
All	All	1575/1820 (86%)	1518 (96%)	49 (3%)	8 (0%)	24	29

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	78	MSE
1	C	36	VAL
1	D	241	GLN
1	C	40	GLY
1	D	17	ASP
1	D	43	ASN
1	A	162	ASN
1	B	164	LYS

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	356/399 (89%)	343 (96%)	13 (4%)	30	41
1	B	356/399 (89%)	341 (96%)	15 (4%)	26	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	356/399 (89%)	345 (97%)	11 (3%)	35	47
1	D	360/399 (90%)	344 (96%)	16 (4%)	25	35
All	All	1428/1596 (90%)	1373 (96%)	55 (4%)	28	40

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	12	LYS
1	A	151	ILE
1	A	199	ARG
1	A	264	ASN
1	A	279	ARG
1	A	306	LEU
1	A	323	ILE
1	A	367	GLN
1	A	431	LEU
1	A	433	ILE
1	A	448	GLU
1	A	449	THR
1	B	10	HIS
1	B	11	LEU
1	B	33	LEU
1	B	39	GLU
1	B	78	MSE
1	B	95	LEU
1	B	104	VAL
1	B	113	GLU
1	B	157	GLN
1	B	164	LYS
1	B	206	ILE
1	B	246	MSE
1	B	273	GLU
1	B	305	ARG
1	B	339	VAL
1	C	16	LYS
1	C	27	LEU
1	C	45	ASP
1	C	68	LYS
1	C	113	GLU
1	C	127	ARG

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Mol	Chain	Res	Type
1	C	227	VAL
1	C	234	ASP
1	C	433	ILE
1	C	445	ARG
1	C	448	GLU
1	D	15	ARG
1	D	46	LEU
1	D	112	THR
1	D	113	GLU
1	D	160	LEU
1	D	170	THR
1	D	188	ASN
1	D	241	GLN
1	D	327	GLU
1	D	339	VAL
1	D	343	ARG
1	D	347	GLU
1	D	367	GLN
1	D	389	ARG
1	D	423	LYS
1	D	433	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	264	ASN
1	B	10	HIS
1	B	153	HIS
1	B	230	HIS
1	B	355	ASN
1	C	10	HIS
1	C	34	HIS
1	C	77	ASN
1	C	140	ASN
1	C	150	GLN
1	D	126	GLN
1	D	150	GLN
1	D	157	GLN
1	D	402	GLN
1	D	437	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	NOS	A	501	-	21,21,21	2.81	3 (14%)	31,31,31	2.83	11 (35%)
2	NOS	D	501	-	21,21,21	2.80	3 (14%)	31,31,31	2.90	11 (35%)
2	NOS	B	501	-	21,21,21	2.81	3 (14%)	31,31,31	2.86	11 (35%)
2	NOS	C	501	-	21,21,21	2.80	3 (14%)	31,31,31	2.88	11 (35%)

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	NOS	A	501	-	-	2/6/22/22	0/3/3/3
2	NOS	D	501	-	-	2/6/22/22	0/3/3/3
2	NOS	B	501	-	-	1/6/22/22	0/3/3/3
2	NOS	C	501	-	-	2/6/22/22	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NOS	O6-C6	11.55	1.45	1.23
2	A	501	NOS	O6-C6	11.53	1.45	1.23
2	D	501	NOS	O6-C6	11.52	1.45	1.23
2	C	501	NOS	O6-C6	11.52	1.45	1.23
2	A	501	NOS	C2-N3	4.09	1.37	1.30
2	B	501	NOS	C2-N3	4.05	1.37	1.30
2	C	501	NOS	C2-N3	4.01	1.37	1.30
2	D	501	NOS	C2-N3	4.00	1.37	1.30
2	A	501	NOS	C4-N3	2.58	1.41	1.35
2	D	501	NOS	C4-N3	2.56	1.41	1.35
2	C	501	NOS	C4-N3	2.55	1.41	1.35
2	B	501	NOS	C4-N3	2.53	1.41	1.35

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	NOS	C5-C6-N1	6.78	120.52	110.78
2	C	501	NOS	C5-C6-N1	6.72	120.45	110.78
2	B	501	NOS	C5-C6-N1	6.66	120.36	110.78
2	A	501	NOS	C5-C6-N1	6.66	120.35	110.78
2	B	501	NOS	C5-C4-N3	-6.21	118.12	127.27
2	C	501	NOS	C5-C4-N3	-6.21	118.14	127.27
2	D	501	NOS	C5-C4-N3	-6.18	118.18	127.27
2	A	501	NOS	C5-C4-N3	-6.17	118.18	127.27
2	D	501	NOS	C1'-N9-C8	5.68	142.87	126.73
2	D	501	NOS	C1'-N9-C4	-5.68	109.72	126.49
2	C	501	NOS	C1'-N9-C8	5.63	142.73	126.73
2	B	501	NOS	C1'-N9-C8	5.58	142.59	126.73
2	C	501	NOS	C1'-N9-C4	-5.57	110.04	126.49
2	B	501	NOS	C1'-N9-C4	-5.52	110.18	126.49
2	D	501	NOS	C2-N3-C4	5.46	121.14	111.53
2	A	501	NOS	C1'-N9-C8	5.44	142.20	126.73
2	C	501	NOS	C2-N3-C4	5.41	121.05	111.53
2	A	501	NOS	C1'-N9-C4	-5.38	110.59	126.49
2	B	501	NOS	C2-N3-C4	5.37	120.97	111.53
2	A	501	NOS	C2-N3-C4	5.30	120.86	111.53
2	D	501	NOS	N1-C2-N3	-4.91	119.85	125.50
2	C	501	NOS	N1-C2-N3	-4.79	119.99	125.50
2	B	501	NOS	N1-C2-N3	-4.71	120.08	125.50
2	A	501	NOS	N1-C2-N3	-4.67	120.12	125.50
2	B	501	NOS	C2-N1-C6	-3.99	119.62	125.09
2	C	501	NOS	C2-N1-C6	-3.98	119.63	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	NOS	C2-N1-C6	-3.98	119.64	125.09
2	D	501	NOS	C2-N1-C6	-3.96	119.66	125.09
2	B	501	NOS	O6-C6-N1	-3.54	113.98	120.75
2	C	501	NOS	O6-C6-N1	-3.53	113.99	120.75
2	D	501	NOS	O6-C6-N1	-3.48	114.10	120.75
2	A	501	NOS	O6-C6-N1	-3.44	114.17	120.75
2	D	501	NOS	N9-C4-N3	3.32	134.45	126.90
2	C	501	NOS	N9-C4-N3	3.29	134.40	126.90
2	A	501	NOS	N9-C4-N3	3.28	134.38	126.90
2	B	501	NOS	N9-C4-N3	3.28	134.38	126.90
2	D	501	NOS	N9-C8-N7	-2.51	108.74	113.40
2	B	501	NOS	N9-C8-N7	-2.47	108.83	113.40
2	C	501	NOS	N9-C8-N7	-2.44	108.87	113.40
2	A	501	NOS	N9-C8-N7	-2.41	108.93	113.40
2	B	501	NOS	C8-N7-C5	2.10	108.00	104.26
2	D	501	NOS	C8-N7-C5	2.05	107.91	104.26
2	A	501	NOS	C8-N7-C5	2.05	107.91	104.26
2	C	501	NOS	C8-N7-C5	2.05	107.91	104.26

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NOS	C3'-C4'-C5'-O5'
2	C	501	NOS	O4'-C4'-C5'-O5'
2	A	501	NOS	O4'-C4'-C5'-O5'
2	C	501	NOS	C3'-C4'-C5'-O5'
2	D	501	NOS	O4'-C4'-C5'-O5'
2	D	501	NOS	C3'-C4'-C5'-O5'
2	B	501	NOS	O4'-C4'-C5'-O5'

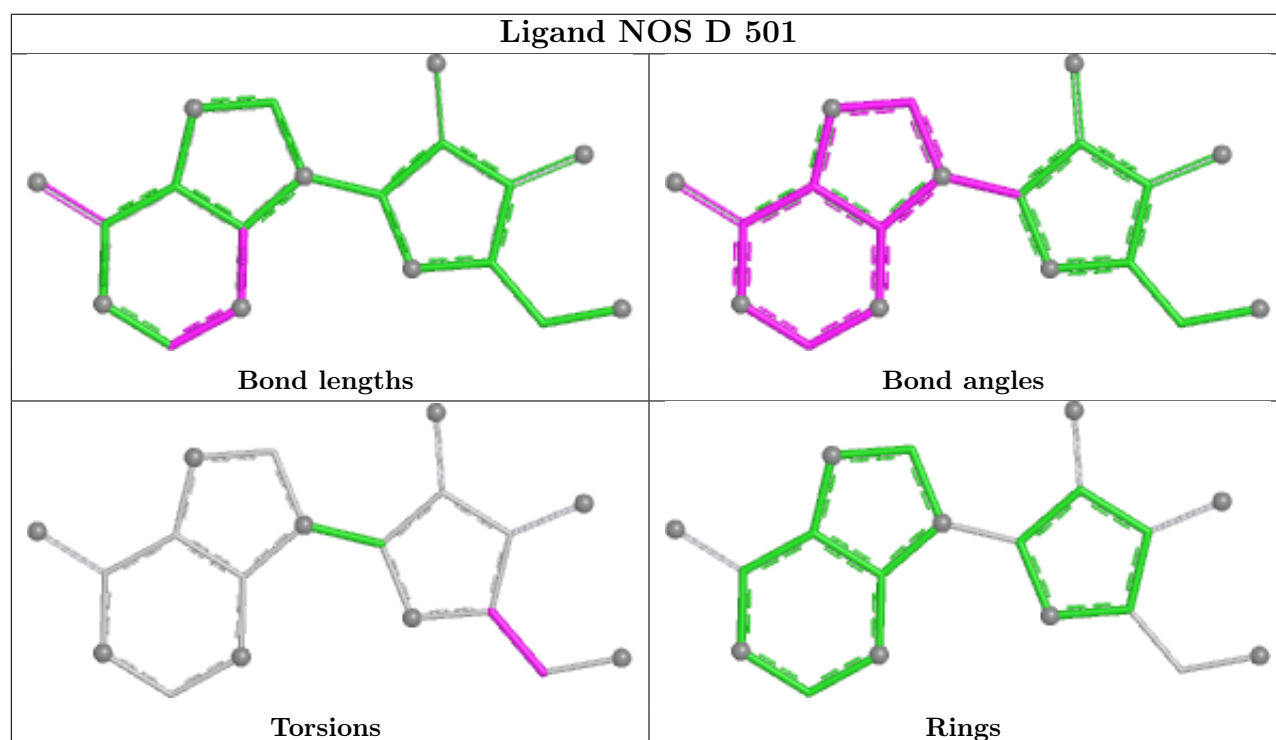
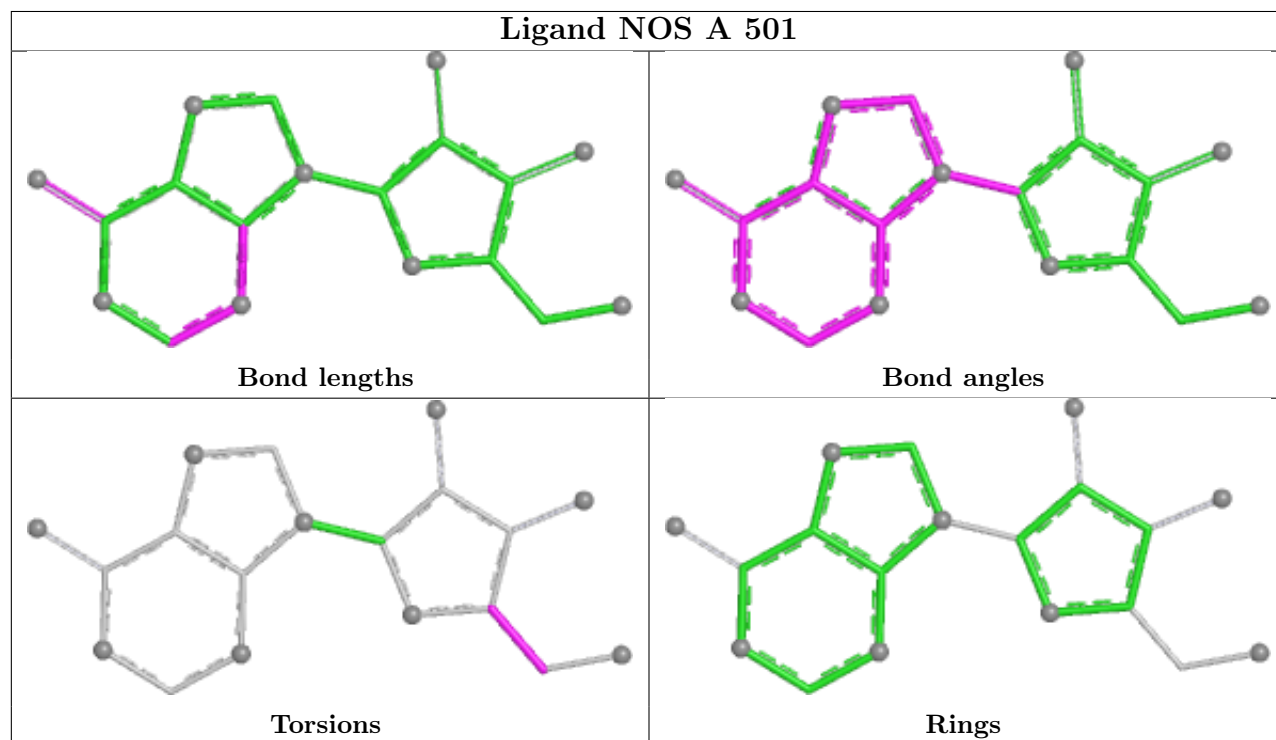
There are no ring outliers.

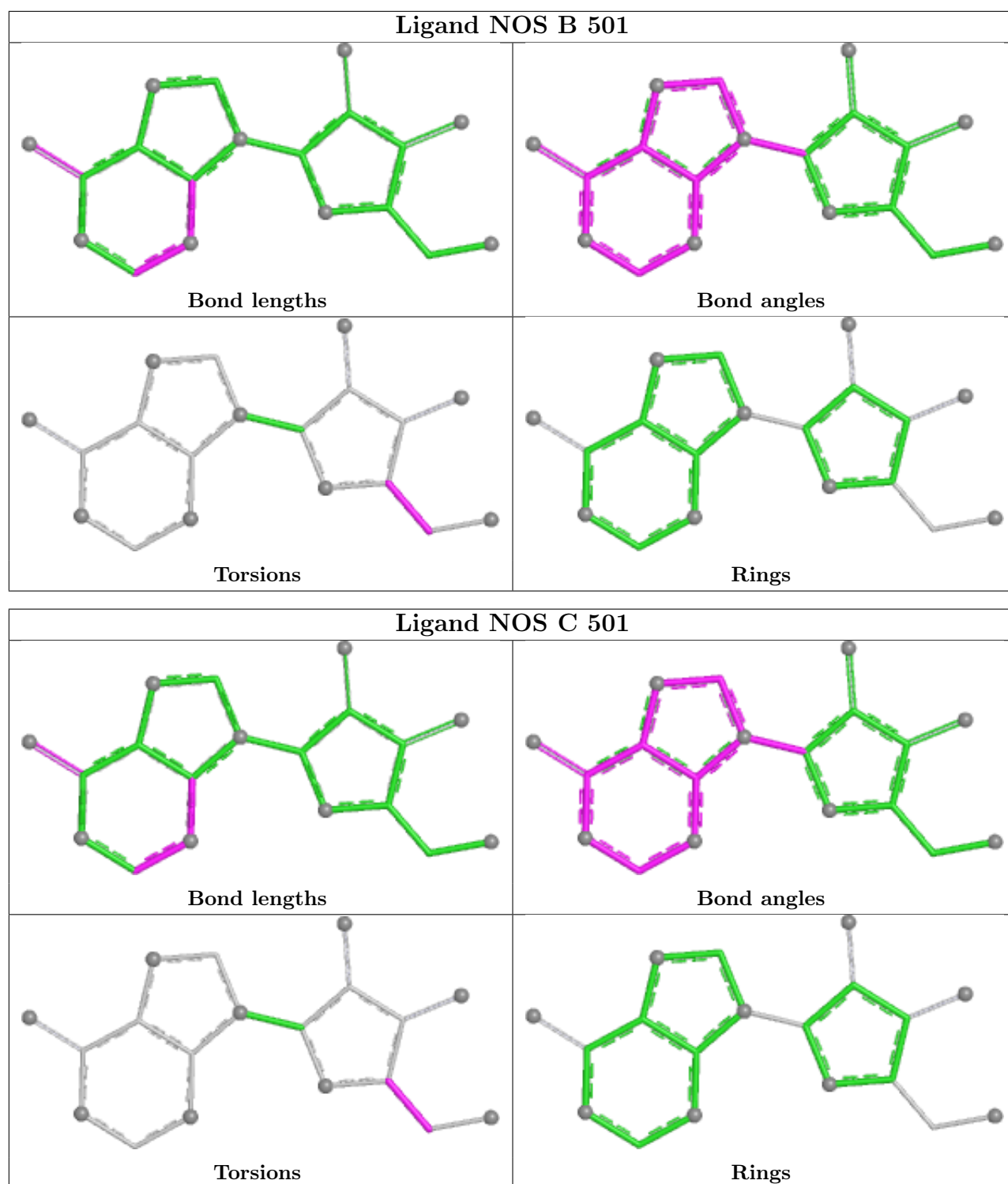
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	NOS	1	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 ⓘ

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	399/455 (87%)	0.73	30 (7%)	20	17	43, 58, 91, 110	0
1	B	399/455 (87%)	0.81	33 (8%)	17	14	46, 66, 95, 118	0
1	C	399/455 (87%)	0.82	38 (9%)	14	11	45, 63, 96, 115	0
1	D	404/455 (88%)	0.75	24 (5%)	28	25	44, 64, 88, 109	0
All	All	1601/1820 (87%)	0.78	125 (7%)	19	16	43, 63, 93, 118	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	176	THR	4.3
1	B	95	LEU	4.2
1	A	176	THR	4.1
1	C	267	PHE	4.0
1	C	95	LEU	4.0
1	B	9	TYR	4.0
1	D	339	VAL	4.0
1	A	175	VAL	3.9
1	C	38	HIS	3.9
1	D	366	ILE	3.9
1	A	11	LEU	3.9
1	C	163	GLY	3.9
1	D	95	LEU	3.8
1	C	45	ASP	3.7
1	A	338	PRO	3.7
1	A	174	ASP	3.5
1	B	175	VAL	3.5
1	C	338	PRO	3.5
1	C	364	ARG	3.4
1	A	449	THR	3.4
1	B	11	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	12	LYS	3.2
1	C	40	GLY	3.2
1	B	173	GLY	3.1
1	D	328	ARG	3.1
1	C	340	LYS	3.1
1	A	116	LEU	3.1
1	C	11	LEU	3.1
1	D	42	TYR	3.1
1	B	339	VAL	3.1
1	D	208	THR	3.0
1	A	160	LEU	3.0
1	B	449	THR	3.0
1	A	382	GLY	3.0
1	B	374	GLY	2.9
1	D	314	ILE	2.9
1	A	14	HIS	2.9
1	A	187	THR	2.8
1	B	174	ASP	2.8
1	A	10	HIS	2.8
1	A	42	TYR	2.8
1	C	5	TYR	2.8
1	A	9	TYR	2.7
1	A	7	VAL	2.7
1	A	375	SER	2.7
1	C	42	TYR	2.7
1	D	16	LYS	2.7
1	A	245	ILE	2.7
1	D	139	PHE	2.6
1	C	221	ARG	2.6
1	C	375	SER	2.6
1	C	7	VAL	2.5
1	D	104	VAL	2.5
1	C	215	ALA	2.5
1	B	45	ASP	2.5
1	A	161	HIS	2.5
1	B	264	ASN	2.5
1	B	99	ARG	2.5
1	B	225	LEU	2.5
1	C	10	HIS	2.5
1	B	65	GLY	2.4
1	B	357	LEU	2.4
1	B	161	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	305	ARG	2.4
1	C	374	GLY	2.4
1	C	239	GLN	2.4
1	C	8	GLU	2.4
1	C	44	ASP	2.4
1	C	235	ILE	2.4
1	B	229	LEU	2.4
1	C	160	LEU	2.4
1	D	442	TYR	2.4
1	A	173	GLY	2.4
1	A	305	ARG	2.4
1	C	225	LEU	2.4
1	B	221	ARG	2.3
1	C	260	PRO	2.3
1	B	232	SER	2.3
1	C	257	TYR	2.3
1	A	259	ASP	2.3
1	C	272	LYS	2.3
1	A	39	GLU	2.3
1	D	310	SER	2.3
1	A	366	ILE	2.3
1	A	46	LEU	2.2
1	A	310	SER	2.2
1	B	43	ASN	2.2
1	C	9	TYR	2.2
1	D	248	GLY	2.2
1	C	79	SER	2.2
1	B	291	THR	2.2
1	C	102	LEU	2.2
1	B	378	TRP	2.2
1	B	77	ASN	2.2
1	A	395	TYR	2.2
1	B	42	TYR	2.2
1	B	166	LEU	2.2
1	D	247	GLY	2.2
1	B	376	ASP	2.2
1	B	32	VAL	2.1
1	A	60	PHE	2.1
1	B	394	PHE	2.1
1	C	227	VAL	2.1
1	B	366	ILE	2.1
1	D	194	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	273	GLU	2.1
1	D	276	LEU	2.1
1	C	449	THR	2.1
1	D	187	THR	2.1
1	A	221	ARG	2.1
1	C	191	ILE	2.1
1	D	174	ASP	2.1
1	B	260	PRO	2.1
1	D	108	GLY	2.1
1	A	312	ILE	2.1
1	D	5	TYR	2.1
1	B	102	LEU	2.0
1	D	342	ASP	2.0
1	A	73	PHE	2.0
1	C	4	ARG	2.0
1	C	127	ARG	2.0
1	D	15	ARG	2.0
1	D	389	ARG	2.0
1	C	63	ILE	2.0
1	D	375	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [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.

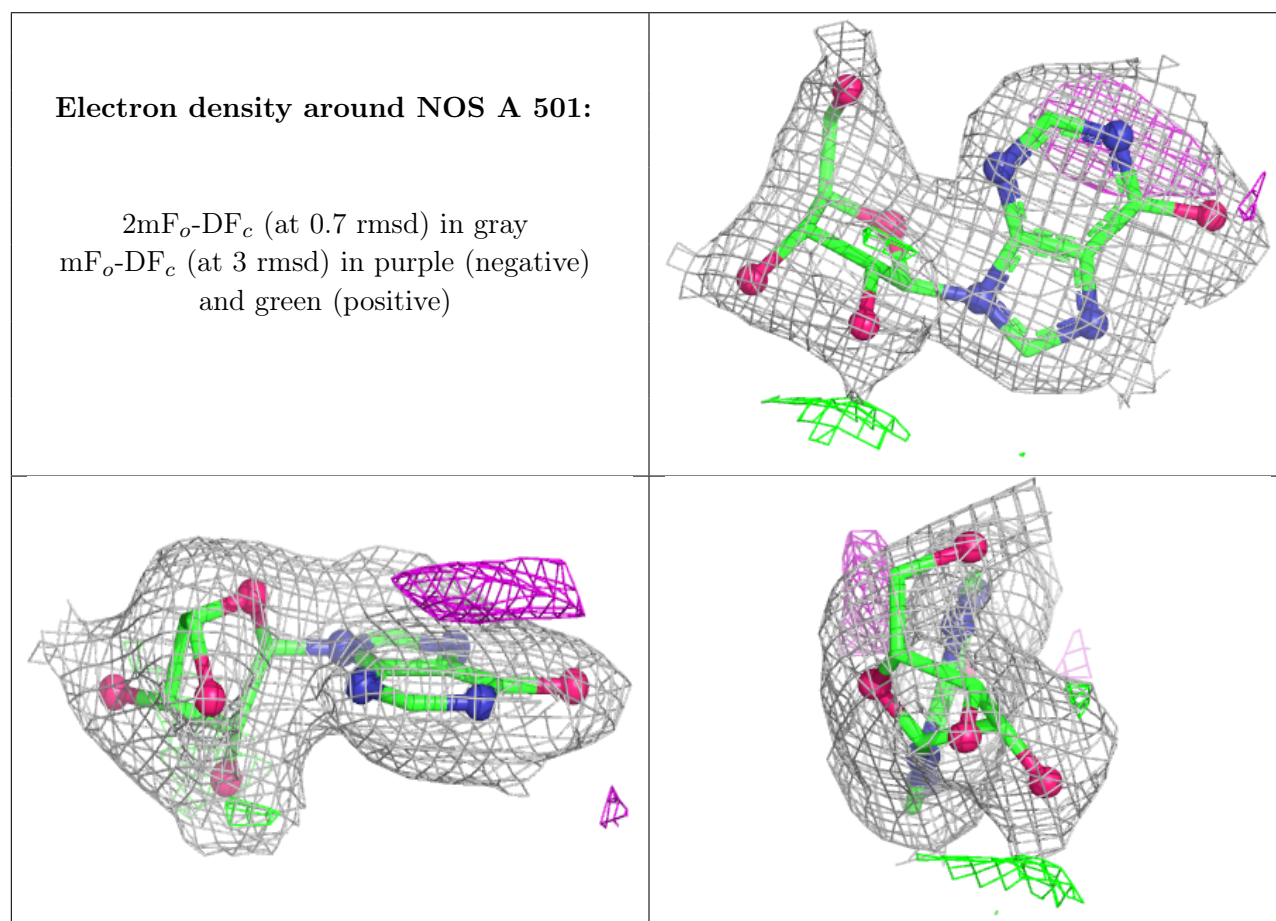
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NOS	A	501	19/19	0.90	0.11	41,48,55,56	0
2	NOS	D	501	19/19	0.90	0.11	47,54,59,60	0
2	NOS	C	501	19/19	0.92	0.09	42,49,54,64	0

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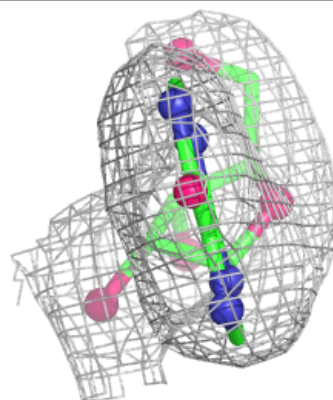
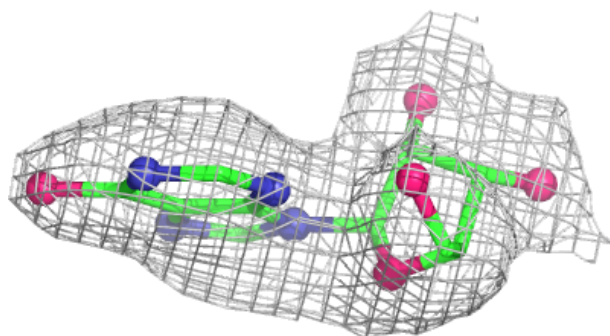
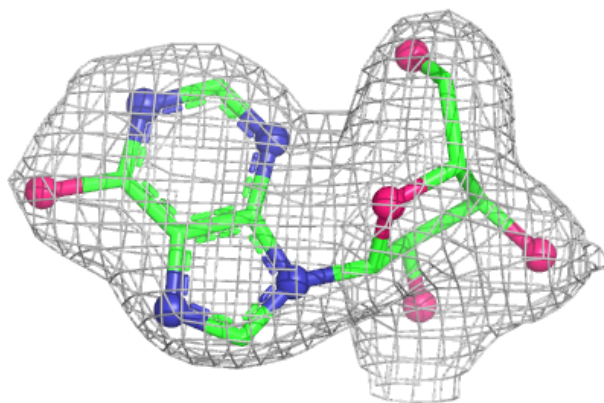
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NOS	B	501	19/19	0.94	0.09	40,52,57,59	0

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.

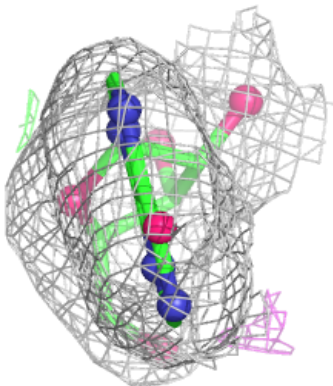
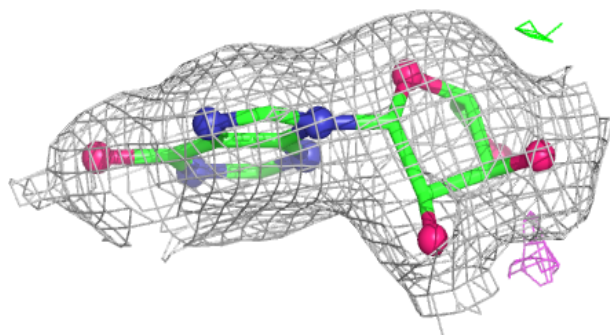
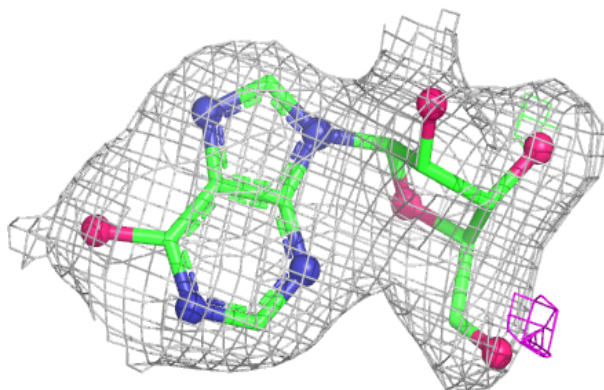


Electron density around NOS D 501:

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

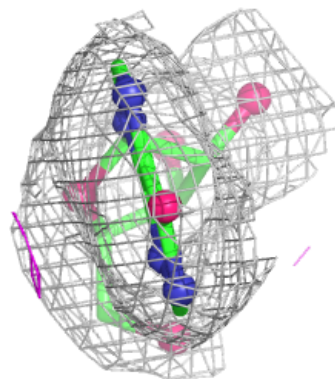
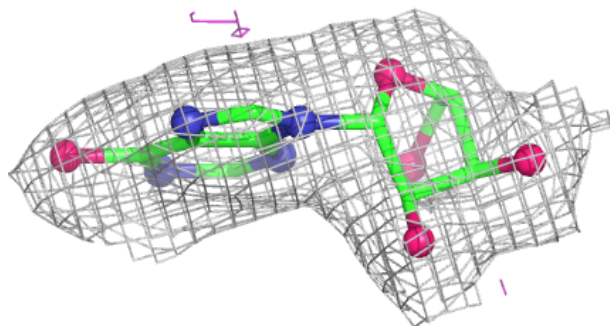
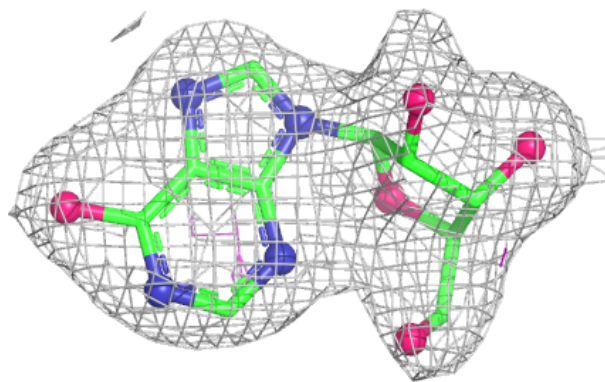
**Electron density around NOS C 501:**

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



Electron density around NOS B 501:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.