



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2022 – 12:04 PM EDT

PDB ID : 7N4Z
Title : Complex structure of NOS4 with noscapine
Authors : Kim, W.; Zhang, Y.
Deposited on : 2021-06-04
Resolution : 2.21 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 : 2.29
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) : 2.29

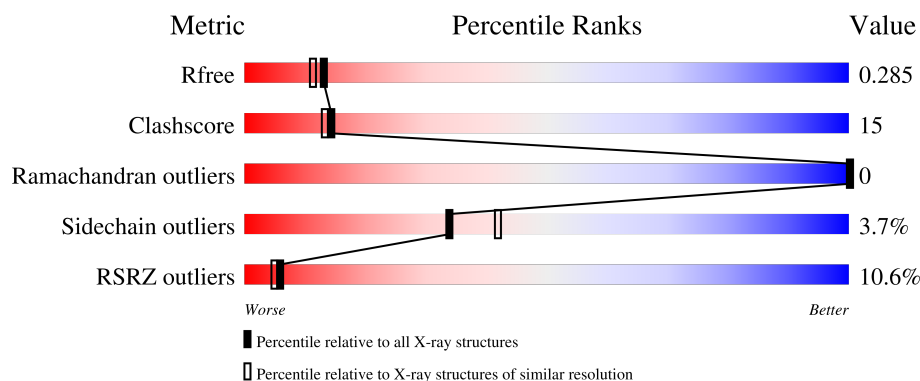
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	193	<div> <div>8%</div> <div> <div>65%</div> <div>26%</div> <div>• 6%</div> </div> </div>
1	B	193	<div> <div>3%</div> <div> <div>70%</div> <div>23%</div> <div>• 6%</div> </div> </div>
1	C	193	<div> <div>7%</div> <div> <div>69%</div> <div>23%</div> <div>• 6%</div> </div> </div>
1	D	193	<div> <div>22%</div> <div> <div>65%</div> <div>22%</div> <div>• 12%</div> </div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5950 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 NOS4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	182	Total	C	N	O	S	1	0	0
			1448	916	259	261	12			
1	C	182	Total	C	N	O	S	2	1	0
			1458	921	261	264	12			
1	B	182	Total	C	N	O	S	0	0	0
			1452	918	260	262	12			
1	D	170	Total	C	N	O	S	2	0	0
			1299	821	233	233	12			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



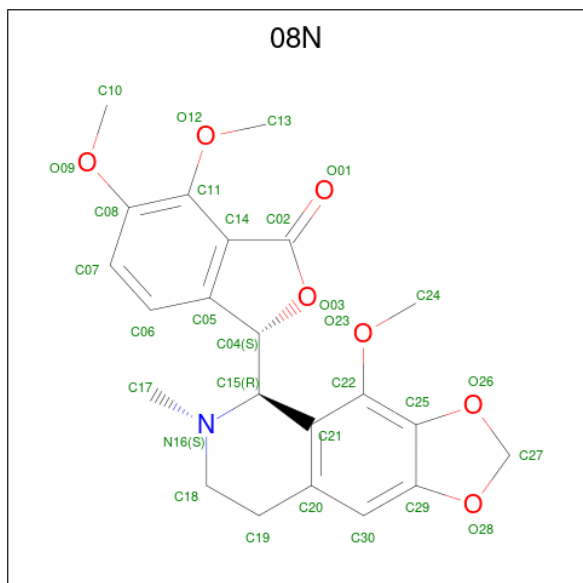
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	5	0
			5	4	1		
2	C	1	Total	O	S	5	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	5	0
			5	4	1		
2	D	1	Total	O	S	5	0
			5	4	1		

- Molecule 3 is noscapine (three-letter code: 08N) (formula: C₂₂H₂₃NO₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			30	22	1	7		
3	C	1	Total	C	N	O	0	0
			30	22	1	7		
3	B	1	Total	C	N	O	0	0
			30	22	1	7		
3	D	1	Total	C	N	O	0	0
			30	22	1	7		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	38	Total	O	0	0
			38	38		
4	C	36	Total	O	0	0
			36	36		
4	B	46	Total	O	0	0
			46	46		

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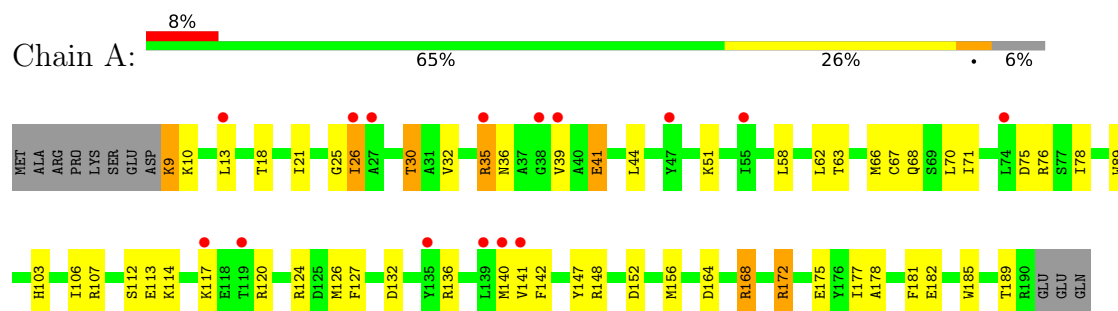
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	33	Total	O	0	0
			33	33		

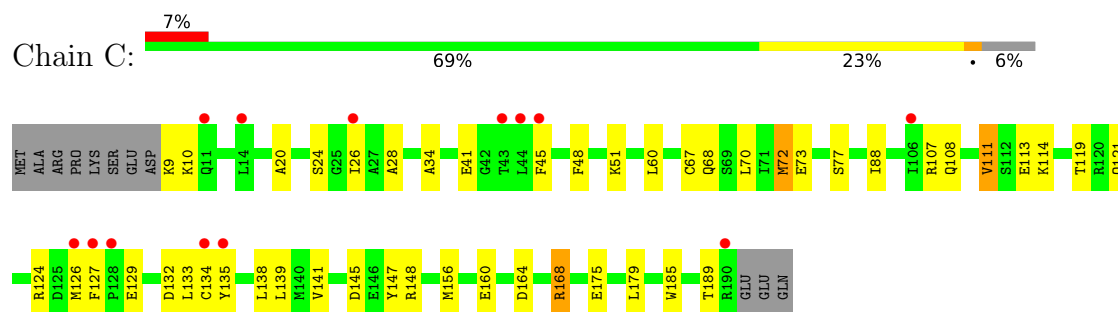
3 Residue-property plots [i](#)

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.

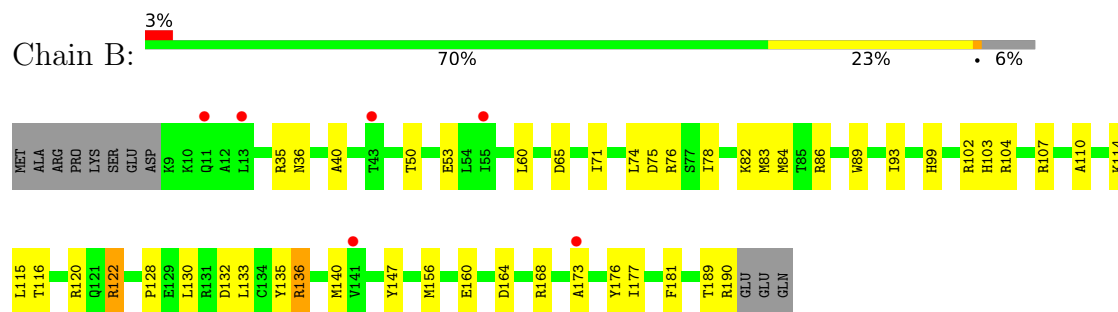
• Molecule 1: NOS4



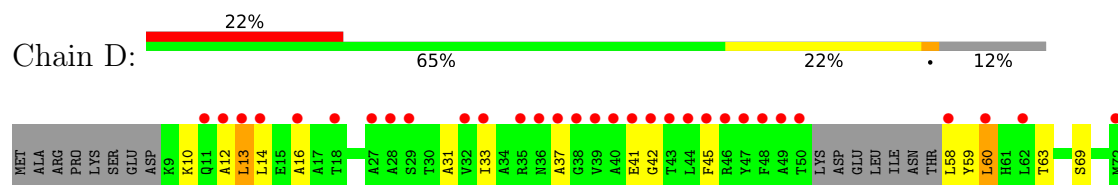
• Molecule 1: NOS4



• Molecule 1: NOS4



• Molecule 1: NOS4





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	41.63Å 54.86Å 92.64Å 74.14° 81.82° 89.96°	Depositor
Resolution (Å)	44.07 – 2.21 44.07 – 2.21	Depositor EDS
% Data completeness (in resolution range)	94.6 (44.07-2.21) 94.6 (44.07-2.21)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.242 , 0.285 0.242 , 0.285	Depositor DCC
R_{free} test set	2005 reflections (5.44%)	wwPDB-VP
Wilson B-factor (Å ²)	37.5	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 59.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.034 for -h,k,k-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5950	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.98% 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: SO4, 08N

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	0.52	1/1475 (0.1%)	0.58	1/1988 (0.1%)
1	B	0.28	0/1479	0.44	0/1993
1	C	0.40	1/1485 (0.1%)	0.51	0/2001
1	D	0.48	0/1323	0.47	0/1784
All	All	0.43	2/5762 (0.0%)	0.50	1/7766 (0.0%)

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	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	73	GLU	CD-OE2	-5.19	1.20	1.25
1	A	177	ILE	C-O	-5.08	1.13	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	ARG	NE-CZ-NH1	6.87	123.73	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	111	VAL	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1448	0	1445	53	0
1	B	1452	0	1451	53	1
1	C	1458	0	1455	31	1
1	D	1299	0	1242	45	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	30	0	0	1	0
3	B	30	0	0	0	0
3	C	30	0	0	0	0
3	D	30	0	0	0	0
4	A	38	0	0	10	0
4	B	46	0	0	19	1
4	C	36	0	0	6	0
4	D	33	0	0	10	1
All	All	5950	0	5593	176	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 15.

All (176) 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:D:14:LEU:HB3	1:D:58:LEU:HD11	1.23	1.13
1:B:40:ALA:HB3	4:B:307:HOH:O	1.52	1.10
1:B:86:ARG:NE	4:B:301:HOH:O	1.86	1.05
1:B:86:ARG:NH2	4:B:301:HOH:O	1.97	0.95
1:D:157:ALA:O	4:D:301:HOH:O	1.86	0.94
1:D:14:LEU:HB3	1:D:58:LEU:CD1	1.99	0.92
1:A:148:ARG:NH2	4:A:302:HOH:O	2.01	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:ASP:N	4:B:302:HOH:O	2.06	0.86
1:C:34:ALA:N	4:C:303:HOH:O	2.07	0.86
1:C:24:SER:HB2	4:C:304:HOH:O	1.74	0.85
1:B:82:LYS:NZ	4:B:304:HOH:O	2.07	0.85
1:B:128:PRO:O	4:B:302:HOH:O	1.97	0.81
1:D:14:LEU:CB	1:D:58:LEU:HD11	2.07	0.81
1:D:59:TYR:CE2	4:D:305:HOH:O	2.34	0.81
1:B:86:ARG:CZ	4:B:301:HOH:O	2.17	0.80
1:C:145:ASP:OD1	4:C:301:HOH:O	2.00	0.80
1:D:60:LEU:HD21	1:D:119:THR:HG23	1.62	0.79
1:B:40:ALA:C	4:B:307:HOH:O	2.21	0.78
1:C:28:ALA:HB2	4:C:304:HOH:O	1.83	0.78
1:B:65:ASP:OD1	4:B:303:HOH:O	2.02	0.77
1:D:14:LEU:CD2	1:D:58:LEU:HD13	2.14	0.77
1:B:40:ALA:CB	4:B:307:HOH:O	2.18	0.76
1:B:50:THR:HG23	1:B:53:GLU:H	1.48	0.76
1:C:160:GLU:OE2	4:C:302:HOH:O	2.04	0.75
1:D:14:LEU:HD22	1:D:58:LEU:CD1	2.16	0.75
1:A:107:ARG:HD2	1:A:156:MET:HB3	1.69	0.75
1:B:99:HIS:HB3	1:B:102:ARG:HD3	1.68	0.74
1:A:114:LYS:HB2	4:A:301:HOH:O	1.90	0.71
1:C:124:ARG:HH21	1:C:148:ARG:HG2	1.56	0.71
1:C:107:ARG:HD3	1:C:156:MET:HB3	1.71	0.71
1:A:189:THR:O	4:A:303:HOH:O	2.09	0.70
1:D:189:THR:O	4:D:304:HOH:O	2.09	0.70
1:D:59:TYR:HE2	4:D:305:HOH:O	1.69	0.70
1:C:20:ALA:O	4:C:304:HOH:O	2.10	0.69
1:A:71:ILE:HG23	4:A:307:HOH:O	1.92	0.69
1:B:93:ILE:HG21	1:B:177:ILE:HD12	1.74	0.69
1:B:114:LYS:NZ	4:B:308:HOH:O	2.25	0.69
1:B:133:LEU:C	4:B:306:HOH:O	2.31	0.68
1:B:132:ASP:O	4:B:306:HOH:O	2.12	0.67
1:A:67:CYS:SG	3:A:202:08N:C10	2.82	0.67
1:B:189:THR:O	4:B:305:HOH:O	2.11	0.67
1:A:71:ILE:N	4:A:307:HOH:O	2.27	0.67
1:D:130:LEU:HA	1:D:133:LEU:HD12	1.76	0.67
1:B:65:ASP:CG	1:B:102:ARG:NH2	2.48	0.66
1:D:14:LEU:CD2	1:D:58:LEU:CD1	2.73	0.66
1:B:65:ASP:CG	1:B:102:ARG:HH21	2.00	0.65
1:B:40:ALA:O	4:B:307:HOH:O	2.14	0.65
1:D:98:ASN:ND2	4:D:302:HOH:O	1.89	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:ASP:OD1	1:B:102:ARG:NH2	2.31	0.64
1:B:40:ALA:CA	4:B:307:HOH:O	2.45	0.64
1:A:182:GLU:OE2	4:A:305:HOH:O	2.15	0.63
1:A:112:SER:OG	4:A:301:HOH:O	1.91	0.63
1:B:173:ALA:HA	1:B:176:TYR:HD2	1.62	0.63
1:C:60:LEU:HG	1:C:119:THR:HG23	1.82	0.62
1:B:135:TYR:N	4:B:306:HOH:O	2.33	0.61
1:A:117:LYS:HA	1:A:120:ARG:HG2	1.82	0.61
1:A:141:VAL:HG21	1:C:179:LEU:HD22	1.82	0.61
1:D:14:LEU:HD23	1:D:58:LEU:HD13	1.81	0.61
1:A:175:GLU:HG3	1:C:147:TYR:OH	2.01	0.60
1:D:33:ILE:HG22	4:D:311:HOH:O	2.01	0.60
1:A:41:GLU:H	1:A:41:GLU:CD	2.06	0.59
1:A:182:GLU:CD	4:A:305:HOH:O	2.40	0.59
1:B:132:ASP:HB3	1:B:136:ARG:HD3	1.85	0.58
1:A:103:HIS:O	1:A:106:ILE:HG22	2.03	0.58
1:A:30:THR:HG23	1:A:51:LYS:HD3	1.84	0.58
1:B:173:ALA:O	1:B:177:ILE:HG12	2.04	0.57
1:A:178:ALA:O	1:A:182:GLU:HG3	2.05	0.57
1:A:124:ARG:HE	1:A:148:ARG:HD3	1.70	0.56
1:B:35:ARG:HD2	1:B:36:ASN:HD22	1.70	0.56
1:B:173:ALA:HA	1:B:176:TYR:CD2	2.39	0.56
1:D:69:SER:O	1:D:73:GLU:HG2	2.06	0.56
1:B:103:HIS:HD2	1:B:104:ARG:HD2	1.71	0.56
1:A:124:ARG:NH2	1:A:152:ASP:OD2	2.38	0.56
1:C:9:LYS:HE3	1:C:10:LYS:H	1.70	0.55
1:C:113:GLU:HG3	1:C:114:LYS:HD2	1.89	0.55
1:D:14:LEU:HD22	1:D:58:LEU:HD12	1.87	0.55
1:D:14:LEU:CB	1:D:58:LEU:CD1	2.75	0.55
1:D:10:LYS:HG3	1:D:13:LEU:HG	1.88	0.54
1:C:107:ARG:O	1:C:111:VAL:HG13	2.07	0.54
1:B:107:ARG:NH2	1:B:160:GLU:OE1	2.29	0.54
1:A:18:THR:CG2	1:A:58:LEU:HD11	2.38	0.54
1:D:16:ALA:HB1	1:D:33:ILE:HB	1.90	0.54
1:D:42:GLY:HA2	1:D:45:PHE:HD2	1.72	0.54
1:D:73:GLU:HG3	1:D:91:SER:OG	2.08	0.54
1:B:147:TYR:CZ	1:D:175:GLU:HG2	2.43	0.53
1:A:18:THR:HG23	1:A:58:LEU:HD11	1.91	0.53
1:D:14:LEU:HD22	1:D:58:LEU:HD13	1.83	0.53
1:A:172:ARG:HH11	1:A:172:ARG:HG2	1.73	0.53
1:C:168:ARG:CD	1:C:168:ARG:N	2.70	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:LEU:HD11	1:A:39:VAL:HG21	1.90	0.53
1:B:65:ASP:OD2	1:B:102:ARG:NH2	2.41	0.53
1:D:59:TYR:O	1:D:63:THR:HG23	2.09	0.52
1:D:12:ALA:HB1	1:D:37:ALA:HB1	1.92	0.52
1:D:133:LEU:HA	1:D:136:ARG:HG2	1.92	0.52
1:A:9:LYS:HD2	1:A:10:LYS:H	1.73	0.51
1:B:99:HIS:CE1	1:B:102:ARG:NH1	2.78	0.51
1:B:99:HIS:CB	1:B:102:ARG:HD3	2.38	0.51
1:D:117:LYS:HG2	1:D:120:ARG:HB2	1.93	0.51
1:D:10:LYS:O	1:D:10:LYS:HG2	2.10	0.51
1:C:68:GLN:O	1:C:72:MET:HB3	2.10	0.51
1:C:67:CYS:HA	1:C:70:LEU:HB2	1.92	0.51
1:B:89:TRP:CD1	1:B:181:PHE:HB2	2.44	0.51
1:A:63:THR:HG23	1:A:106:ILE:HD11	1.92	0.50
1:D:123:ALA:HB3	4:D:305:HOH:O	2.11	0.50
1:A:141:VAL:HG21	1:C:179:LEU:CD2	2.41	0.50
1:B:60:LEU:HD22	1:B:122:ARG:HD2	1.94	0.50
1:C:126:MET:HG2	1:C:127:PHE:CE1	2.47	0.50
1:A:185:TRP:O	1:A:189:THR:OG1	2.26	0.50
1:A:41:GLU:OE2	1:A:41:GLU:N	2.36	0.50
1:B:110:ALA:O	1:B:120:ARG:NH2	2.44	0.50
1:A:120:ARG:HB2	1:A:124:ARG:NH1	2.27	0.49
1:B:164:ASP:O	1:B:168:ARG:HD3	2.13	0.49
1:B:71:ILE:HG23	1:B:130:LEU:HD22	1.94	0.49
1:A:32:VAL:HA	1:A:35:ARG:HD2	1.95	0.49
1:A:62:LEU:HB3	1:A:106:ILE:HD13	1.95	0.49
1:A:141:VAL:O	1:A:147:TYR:HB2	2.13	0.49
1:C:28:ALA:O	1:C:51:LYS:NZ	2.42	0.49
1:A:10:LYS:NZ	4:A:306:HOH:O	2.46	0.48
1:D:86:ARG:NH2	1:D:182:GLU:OE1	2.45	0.48
1:A:89:TRP:CD1	1:A:181:PHE:HB2	2.47	0.48
1:B:116:THR:O	1:B:120:ARG:HG2	2.14	0.48
1:B:103:HIS:CD2	1:B:104:ARG:HD2	2.48	0.48
1:D:60:LEU:O	1:D:63:THR:OG1	2.22	0.47
1:B:93:ILE:HG21	1:B:177:ILE:CD1	2.41	0.47
1:B:115:LEU:HB3	1:B:120:ARG:HD3	1.96	0.47
1:A:32:VAL:HG13	1:A:35:ARG:HD2	1.96	0.47
1:A:44:LEU:C	1:A:44:LEU:HD23	2.34	0.47
1:A:132:ASP:O	1:A:136:ARG:HB2	2.15	0.47
1:C:45:PHE:HA	1:C:48:PHE:O	2.15	0.47
1:A:126:MET:HG3	1:A:127:PHE:HD1	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:VAL:HG12	1:A:36:ASN:ND2	2.31	0.46
1:B:107:ARG:HD3	1:B:156:MET:HB3	1.97	0.46
1:D:31:ALA:HA	1:D:41:GLU:HG3	1.98	0.46
1:D:100:PRO:O	1:D:104:ARG:HG2	2.16	0.46
1:B:99:HIS:CG	1:B:102:ARG:HH11	2.35	0.45
1:C:185:TRP:CE3	1:C:189:THR:HG21	2.52	0.45
1:D:103:HIS:NE2	4:D:303:HOH:O	2.04	0.45
1:C:135:TYR:HA	1:C:138:LEU:HG	1.97	0.45
1:B:99:HIS:CD2	1:B:102:ARG:NH1	2.85	0.45
1:D:59:TYR:HB2	1:D:109:LEU:HD11	1.99	0.45
1:C:26:ILE:HD11	1:C:108:GLN:O	2.16	0.44
1:D:132:ASP:O	1:D:136:ARG:HG2	2.17	0.44
1:C:88:ILE:HD13	1:C:134:CYS:SG	2.58	0.44
1:A:75:ASP:HB3	1:A:78:ILE:HG12	1.98	0.44
1:A:120:ARG:HH21	1:A:124:ARG:HH22	1.65	0.44
1:B:76:ARG:O	1:B:76:ARG:HG2	2.18	0.44
1:D:172:ARG:NE	4:D:306:HOH:O	2.26	0.44
1:C:168:ARG:N	1:C:168:ARG:HD2	2.32	0.44
1:B:74:LEU:HD11	1:B:84:MET:SD	2.58	0.44
1:D:88:ILE:HD13	1:D:134:CYS:SG	2.58	0.43
1:A:13:LEU:HD22	1:A:44:LEU:HD12	2.00	0.43
1:A:126:MET:HG3	1:A:127:PHE:CD1	2.54	0.43
1:C:164:ASP:O	1:C:168:ARG:HD3	2.19	0.43
1:B:136:ARG:N	4:B:306:HOH:O	2.48	0.43
1:A:68:GLN:HA	1:A:71:ILE:HG12	2.00	0.43
1:A:70:LEU:CB	4:A:307:HOH:O	2.67	0.43
1:A:164:ASP:OD1	1:A:168:ARG:HD3	2.18	0.43
1:D:60:LEU:HD21	1:D:119:THR:CG2	2.42	0.43
1:A:9:LYS:HD2	1:A:10:LYS:N	2.33	0.42
1:A:26:ILE:O	1:A:26:ILE:HG13	2.19	0.42
1:A:147:TYR:OH	1:C:175:GLU:HG2	2.19	0.42
1:B:190:ARG:HB2	4:B:319:HOH:O	2.19	0.42
1:A:132:ASP:HB3	1:A:136:ARG:NH2	2.34	0.42
1:D:124:ARG:O	1:D:131:ARG:HB2	2.20	0.42
1:D:122:ARG:HD2	4:D:307:HOH:O	2.19	0.41
1:A:76:ARG:HD2	1:B:140:MET:SD	2.61	0.41
1:A:141:VAL:HG13	1:A:142:PHE:N	2.35	0.41
1:C:108:GLN:O	1:C:111:VAL:HG22	2.20	0.41
1:B:75:ASP:HB3	1:B:78:ILE:HG12	2.03	0.41
1:C:129:GLU:O	1:C:133:LEU:HG	2.20	0.41
1:C:139:LEU:HB3	1:C:141:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:TRP:O	1:B:93:ILE:HG12	2.20	0.41
1:D:99:HIS:HB3	1:D:102:ARG:HG3	2.03	0.40
1:D:132:ASP:HB3	1:D:136:ARG:HD3	2.02	0.40
1:D:10:LYS:O	1:D:13:LEU:HB2	2.21	0.40
1:A:21:ILE:HA	1:A:25:GLY:O	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)
4:B:345:HOH:O	4:D:319:HOH:O[1_545]	1.64	0.56
1:C:41:GLU:OE1	1:B:35:ARG:NH2[1_664]	2.05	0.15

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	180/193 (93%)	180 (100%)	0	0	100	100
1	B	180/193 (93%)	179 (99%)	1 (1%)	0	100	100
1	C	181/193 (94%)	179 (99%)	2 (1%)	0	100	100
1	D	164/193 (85%)	162 (99%)	2 (1%)	0	100	100
All	All	705/772 (91%)	700 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	146/157 (93%)	137 (94%)	9 (6%)	18	19
1	B	147/157 (94%)	144 (98%)	3 (2%)	55	67
1	C	148/157 (94%)	143 (97%)	5 (3%)	37	46
1	D	121/157 (77%)	117 (97%)	4 (3%)	38	47
All	All	562/628 (90%)	541 (96%)	21 (4%)	34	42

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	26	ILE
1	A	30	THR
1	A	35	ARG
1	A	41	GLU
1	A	66	MET
1	A	113	GLU
1	A	140	MET
1	A	168	ARG
1	C	72	MET
1	C	77	SER
1	C	121	GLN
1	C	132	ASP
1	C	168	ARG
1	B	83	MET
1	B	122	ARG
1	B	136	ARG
1	D	13	LEU
1	D	60	LEU
1	D	121	GLN
1	D	131	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	36	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 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$
3	08N	C	202	-	34,34,34	2.18	12 (35%)	51,51,51	1.95	14 (27%)
3	08N	B	202	-	34,34,34	2.15	13 (38%)	51,51,51	2.02	16 (31%)
3	08N	D	202	-	34,34,34	2.31	12 (35%)	51,51,51	2.06	16 (31%)
2	SO4	A	201	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	D	201	-	4,4,4	0.13	0	6,6,6	0.05	0
2	SO4	B	201	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	C	201	-	4,4,4	0.14	0	6,6,6	0.05	0
3	08N	A	202	-	34,34,34	4.44	20 (58%)	51,51,51	2.06	17 (33%)

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
3	08N	B	202	-	-	1/10/41/41	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	08N	D	202	-	-	4/10/41/41	0/5/5/5
3	08N	C	202	-	-	1/10/41/41	0/5/5/5
3	08N	A	202	-	-	4/10/41/41	0/5/5/5

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	202	08N	O03-C04	-12.48	1.30	1.46
3	A	202	08N	O28-C29	-9.49	1.23	1.38
3	A	202	08N	C15-C04	-7.97	1.45	1.55
3	A	202	08N	O26-C25	-7.42	1.27	1.38
3	A	202	08N	O23-C22	-7.11	1.25	1.38
3	D	202	08N	C21-C15	6.18	1.59	1.52
3	C	202	08N	C21-C15	5.97	1.59	1.52
3	A	202	08N	O26-C27	-5.46	1.32	1.43
3	B	202	08N	C21-C15	5.14	1.58	1.52
3	A	202	08N	O28-C27	-4.80	1.34	1.43
3	D	202	08N	C15-C04	4.77	1.61	1.55
3	A	202	08N	C17-N16	-4.73	1.37	1.46
3	A	202	08N	O23-C24	-4.42	1.29	1.42
3	C	202	08N	O03-C04	-4.25	1.41	1.46
3	A	202	08N	C14-C02	-4.20	1.40	1.47
3	D	202	08N	C22-C21	4.19	1.46	1.39
3	B	202	08N	O03-C04	-4.12	1.41	1.46
3	A	202	08N	O12-C11	-4.10	1.31	1.38
3	D	202	08N	O03-C04	-4.09	1.41	1.46
3	A	202	08N	O09-C10	-4.07	1.30	1.42
3	B	202	08N	C15-C04	4.04	1.60	1.55
3	B	202	08N	C22-C21	3.98	1.46	1.39
3	C	202	08N	C15-C04	3.89	1.60	1.55
3	B	202	08N	C05-C04	3.77	1.57	1.51
3	A	202	08N	O12-C13	-3.73	1.31	1.42
3	C	202	08N	C22-C21	3.65	1.45	1.39
3	A	202	08N	O09-C08	-3.65	1.31	1.37
3	D	202	08N	C30-C20	3.56	1.45	1.39
3	C	202	08N	C30-C20	3.51	1.45	1.39
3	A	202	08N	C14-C05	-3.41	1.35	1.39
3	C	202	08N	C05-C04	3.40	1.57	1.51
3	A	202	08N	C25-C22	-3.37	1.32	1.39
3	D	202	08N	C05-C04	3.35	1.56	1.51
3	B	202	08N	C30-C20	3.25	1.45	1.39
3	A	202	08N	C06-C05	-3.25	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	202	08N	C15-N16	3.14	1.52	1.47
3	A	202	08N	C30-C29	-3.09	1.33	1.38
3	A	202	08N	C14-C11	-2.85	1.34	1.40
3	B	202	08N	C15-N16	2.84	1.52	1.47
3	A	202	08N	C19-C20	-2.83	1.46	1.51
3	C	202	08N	C15-N16	2.79	1.52	1.47
3	D	202	08N	C19-C20	2.74	1.55	1.51
3	D	202	08N	C14-C05	2.67	1.42	1.39
3	B	202	08N	C18-C19	2.60	1.56	1.51
3	D	202	08N	C18-C19	2.40	1.56	1.51
3	B	202	08N	C19-C20	2.39	1.55	1.51
3	C	202	08N	C14-C05	2.39	1.42	1.39
3	B	202	08N	C14-C05	2.38	1.42	1.39
3	C	202	08N	C18-C19	2.35	1.56	1.51
3	C	202	08N	C07-C06	2.30	1.42	1.38
3	C	202	08N	C19-C20	2.30	1.55	1.51
3	B	202	08N	C14-C02	2.27	1.51	1.47
3	C	202	08N	O09-C08	2.26	1.40	1.37
3	D	202	08N	C07-C06	2.20	1.42	1.38
3	B	202	08N	C07-C06	2.20	1.42	1.38
3	D	202	08N	O26-C25	2.14	1.41	1.38
3	B	202	08N	O09-C08	2.07	1.40	1.37

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	202	08N	O03-C02-O01	-6.42	115.72	121.19
3	C	202	08N	O03-C02-O01	-6.25	115.86	121.19
3	D	202	08N	O03-C02-O01	-6.17	115.93	121.19
3	A	202	08N	O03-C02-O01	-5.55	116.46	121.19
3	A	202	08N	C17-N16-C18	-5.42	101.67	110.63
3	B	202	08N	C04-C15-N16	-4.63	102.89	109.52
3	B	202	08N	C21-C15-N16	4.42	118.51	115.01
3	D	202	08N	C04-C15-N16	-4.37	103.27	109.52
3	C	202	08N	C04-C15-N16	-4.36	103.28	109.52
3	D	202	08N	C21-C15-N16	4.10	118.26	115.01
3	D	202	08N	O28-C29-C30	4.07	133.30	127.85
3	C	202	08N	C21-C15-N16	3.96	118.15	115.01
3	C	202	08N	O28-C29-C30	3.93	133.11	127.85
3	B	202	08N	O28-C29-C30	3.85	133.00	127.85
3	A	202	08N	O28-C29-C25	-3.36	106.54	109.63
3	D	202	08N	C17-N16-C18	-3.29	105.20	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	202	08N	C27-O28-C29	3.28	109.61	105.34
3	A	202	08N	O09-C08-C11	3.28	120.92	115.16
3	D	202	08N	O28-C29-C25	-3.18	106.70	109.63
3	A	202	08N	O28-C29-C30	3.18	132.10	127.85
3	C	202	08N	C17-N16-C18	-3.17	105.40	110.63
3	D	202	08N	C17-N16-C15	-3.14	108.01	111.87
3	C	202	08N	C17-N16-C15	-3.06	108.11	111.87
3	B	202	08N	C17-N16-C18	-3.05	105.60	110.63
3	D	202	08N	C18-N16-C15	3.00	119.39	113.50
3	B	202	08N	O28-C29-C25	-2.99	106.87	109.63
3	D	202	08N	C18-C19-C20	2.99	116.66	111.35
3	A	202	08N	C21-C15-N16	2.95	117.35	115.01
3	B	202	08N	C17-N16-C15	-2.91	108.30	111.87
3	A	202	08N	C04-C15-N16	-2.90	105.37	109.52
3	A	202	08N	C17-N16-C15	-2.85	108.37	111.87
3	D	202	08N	O28-C27-O26	-2.79	103.62	108.08
3	C	202	08N	O28-C29-C25	-2.74	107.11	109.63
3	D	202	08N	O09-C08-C11	2.74	119.97	115.16
3	D	202	08N	O26-C25-C22	2.71	132.57	128.68
3	B	202	08N	C18-N16-C15	2.70	118.81	113.50
3	B	202	08N	O09-C08-C11	2.68	119.87	115.16
3	C	202	08N	O09-C08-C11	2.68	119.87	115.16
3	B	202	08N	C27-O28-C29	2.66	108.80	105.34
3	A	202	08N	O26-C25-C22	2.65	132.49	128.68
3	B	202	08N	C18-C19-C20	2.64	116.05	111.35
3	D	202	08N	C04-O03-C02	2.60	112.55	111.03
3	C	202	08N	O28-C27-O26	-2.54	104.01	108.08
3	A	202	08N	C18-C19-C20	2.51	115.81	111.35
3	A	202	08N	O03-C02-C14	2.50	110.25	108.26
3	B	202	08N	C04-O03-C02	2.41	112.44	111.03
3	A	202	08N	O03-C04-C15	-2.40	105.47	108.61
3	C	202	08N	C18-N16-C15	2.39	118.20	113.50
3	A	202	08N	C24-O23-C22	2.39	121.33	114.78
3	C	202	08N	O26-C25-C22	2.36	132.08	128.68
3	A	202	08N	C05-C14-C02	-2.30	105.73	108.37
3	C	202	08N	C05-C14-C02	-2.27	105.78	108.37
3	C	202	08N	C18-C19-C20	2.24	115.34	111.35
3	A	202	08N	C18-N16-C15	2.23	117.87	113.50
3	B	202	08N	C05-C14-C02	-2.21	105.85	108.37
3	D	202	08N	C21-C15-C04	2.12	113.56	108.72
3	B	202	08N	O28-C27-O26	-2.12	104.70	108.08
3	B	202	08N	C27-O26-C25	2.11	107.67	105.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	202	08N	O01-C02-C14	2.10	134.99	131.04
3	D	202	08N	C05-C04-C15	2.09	120.04	115.97
3	D	202	08N	C05-C14-C02	-2.09	105.97	108.37
3	B	202	08N	O01-C02-C14	2.07	134.94	131.04
3	A	202	08N	C06-C05-C14	-2.03	117.44	120.47

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	202	08N	C07-C08-O09-C10
3	D	202	08N	C11-C08-O09-C10
3	A	202	08N	C07-C08-O09-C10
3	A	202	08N	C25-C22-O23-C24
3	A	202	08N	C21-C22-O23-C24
3	A	202	08N	C11-C08-O09-C10
3	D	202	08N	C25-C22-O23-C24
3	D	202	08N	C21-C22-O23-C24
3	C	202	08N	C11-C08-O09-C10
3	B	202	08N	C11-C08-O09-C10

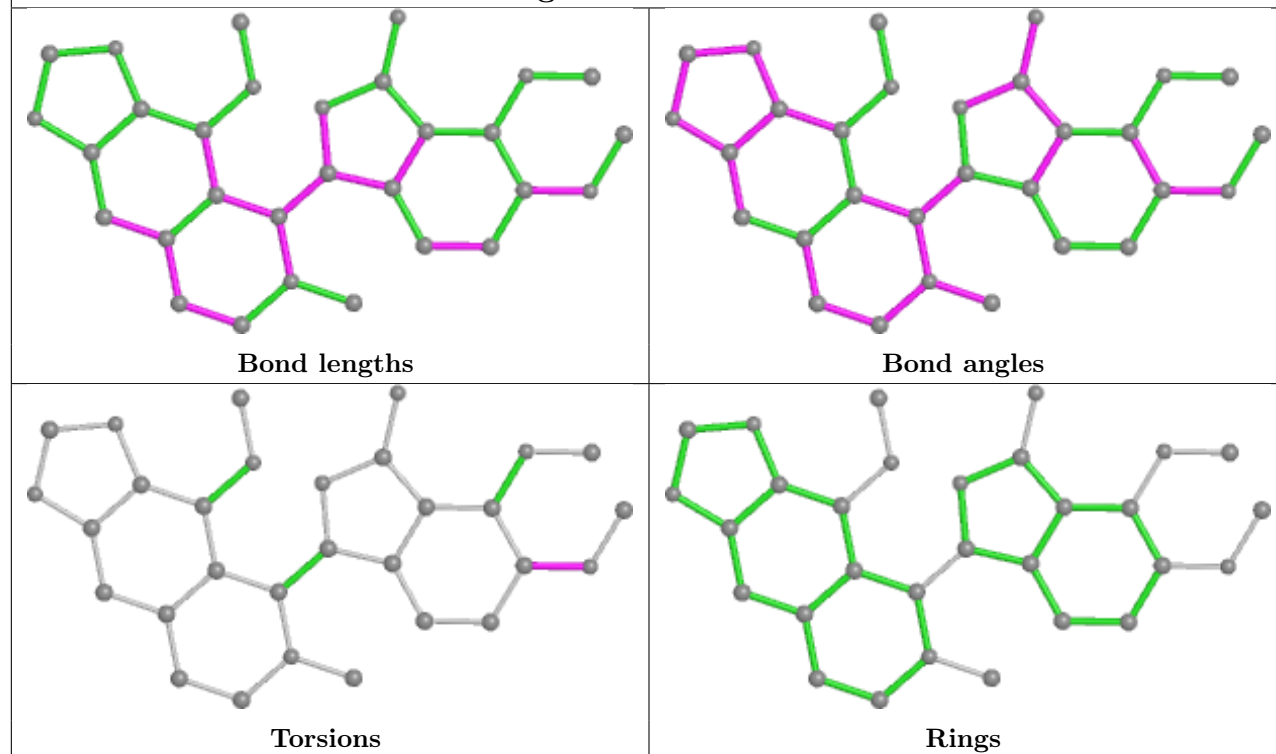
There are no ring outliers.

1 monomer is involved in 1 short contact:

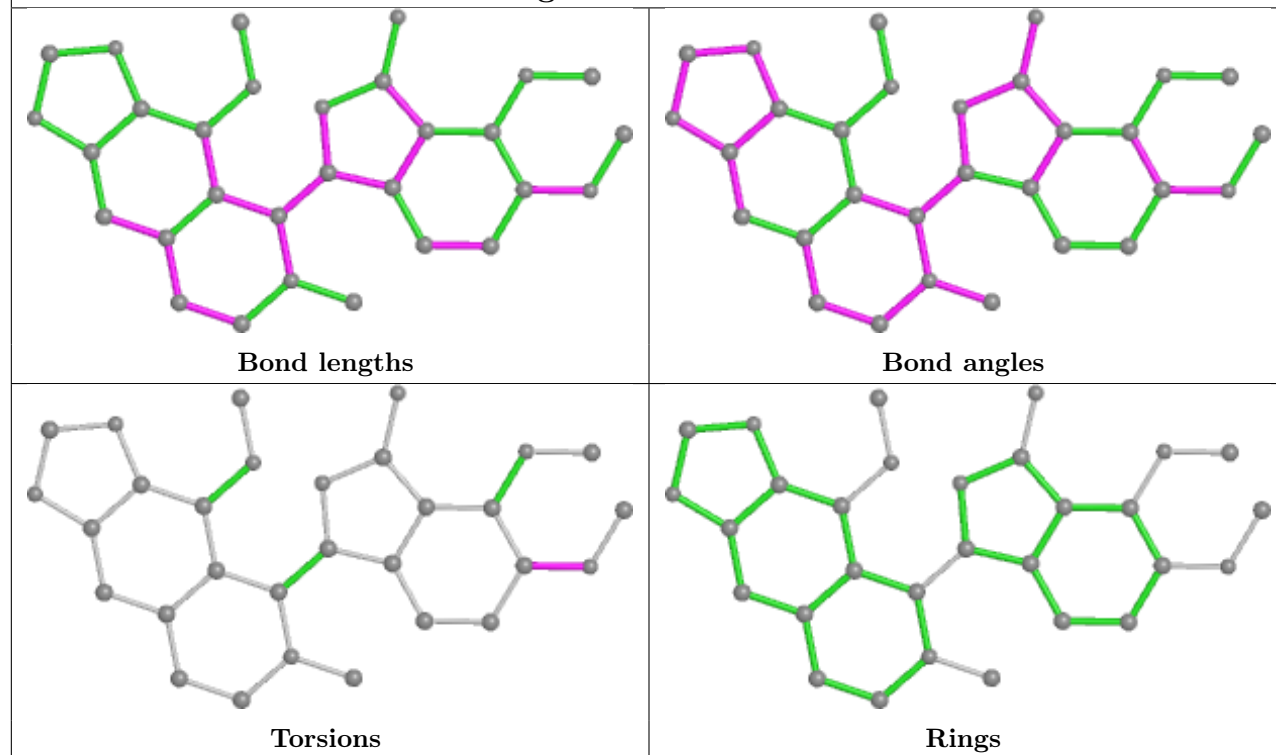
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	202	08N	1	0

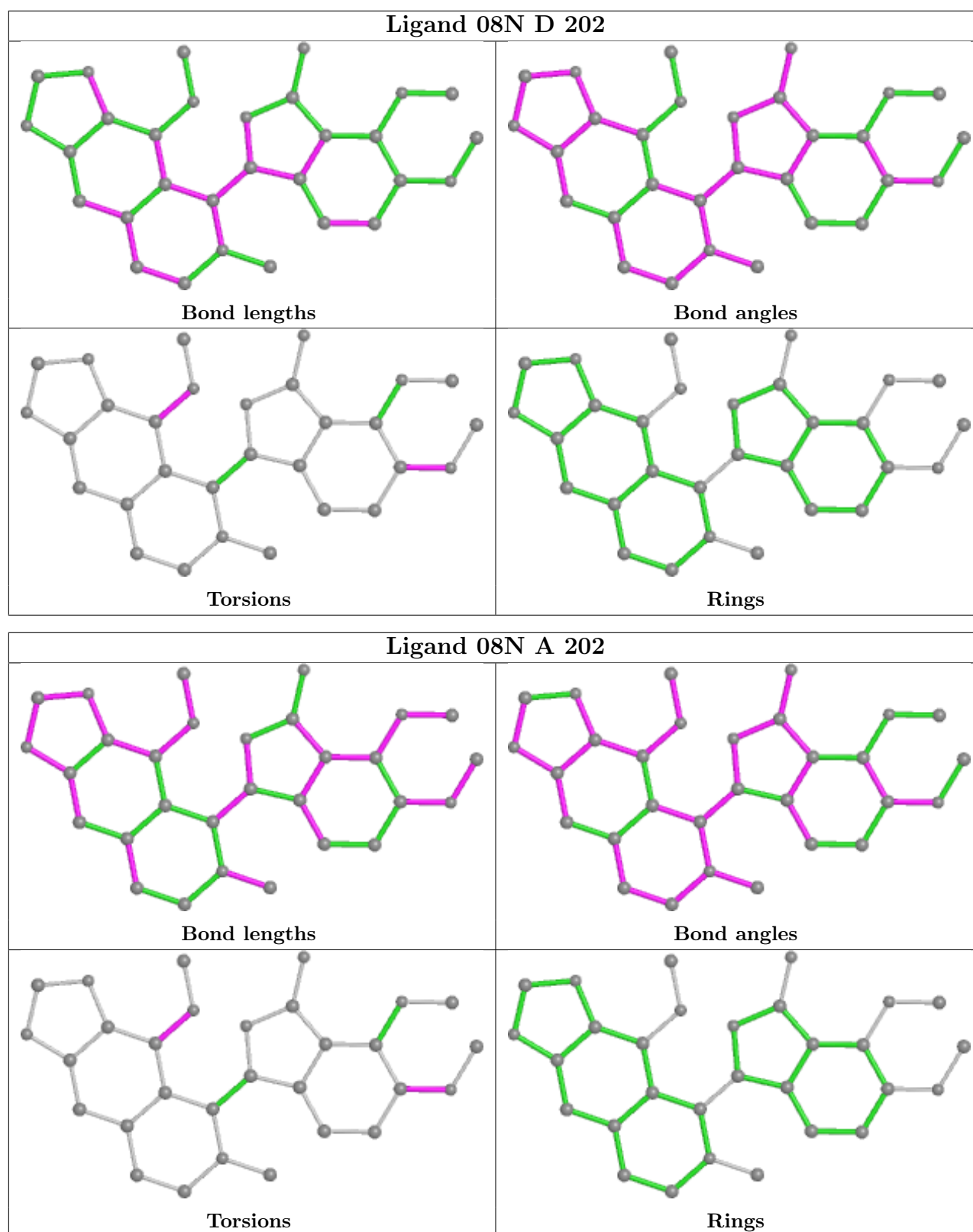
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand 08N C 202



Ligand 08N B 202





5.7 Other polymers ⓘ

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	182/193 (94%)	0.71	15 (8%)	11 10	28, 48, 71, 82	0
1	B	182/193 (94%)	0.46	6 (3%)	46 44	27, 44, 61, 66	0
1	C	182/193 (94%)	0.62	13 (7%)	16 14	28, 51, 71, 77	1 (0%)
1	D	170/193 (88%)	1.16	42 (24%)	0 0	30, 56, 96, 108	1 (0%)
All	All	716/772 (92%)	0.73	76 (10%)	6 5	27, 49, 84, 108	2 (0%)

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	134	CYS	8.8
1	D	45	PHE	6.4
1	D	28	ALA	6.1
1	D	13	LEU	6.0
1	D	39	VAL	5.8
1	D	126	MET	5.7
1	D	27	ALA	5.0
1	D	134	CYS	5.0
1	D	130	LEU	4.7
1	A	47	TYR	4.5
1	C	11	GLN	4.2
1	D	41	GLU	4.2
1	D	14	LEU	4.1
1	D	105	ALA	4.1
1	D	12	ALA	4.0
1	C	135	TYR	4.0
1	D	121	GLN	3.9
1	A	39	VAL	3.9
1	D	42	GLY	3.8
1	D	32	VAL	3.8
1	D	16	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	49	ALA	3.7
1	D	47	TYR	3.6
1	D	33	ILE	3.5
1	D	36	ASN	3.4
1	D	40	ALA	3.4
1	C	14	LEU	3.4
1	D	79	THR	3.4
1	A	38	GLY	3.3
1	D	43	THR	3.3
1	B	55	ILE	3.3
1	A	141	VAL	3.3
1	C	43	THR	3.2
1	D	50	THR	3.2
1	C	44	LEU	3.2
1	D	44	LEU	3.2
1	D	37	ALA	3.1
1	D	35	ARG	3.1
1	A	35	ARG	3.1
1	B	11	GLN	3.0
1	A	26	ILE	2.9
1	A	27	ALA	2.9
1	D	133	LEU	2.9
1	C	26	ILE	2.8
1	C	126	MET	2.8
1	D	62	LEU	2.8
1	B	173	ALA	2.7
1	A	119	THR	2.7
1	A	139	LEU	2.7
1	A	74	LEU	2.7
1	D	108	GLN	2.6
1	A	117	LYS	2.6
1	C	127	PHE	2.5
1	D	127	PHE	2.5
1	D	58	LEU	2.4
1	D	11	GLN	2.4
1	D	60	LEU	2.3
1	D	135	TYR	2.3
1	D	125	ASP	2.2
1	A	140	MET	2.2
1	A	13	LEU	2.2
1	D	29	SER	2.2
1	A	55	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	72	MET	2.2
1	D	18	THR	2.2
1	D	46	ARG	2.2
1	B	13	LEU	2.2
1	C	128	PRO	2.2
1	C	45	PHE	2.1
1	D	38	GLY	2.1
1	A	135	TYR	2.1
1	D	48	PHE	2.1
1	C	106	ILE	2.0
1	B	43	THR	2.0
1	B	141	VAL	2.0
1	C	190	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

LIGAND-RSR INFOmissingINFO

6.5 Other polymers [i](#)

There are no such residues in this entry.