



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 04:15 AM BST

PDB ID : 6OYH
Title : Crystal structure of MraY bound to carbacaprazamycin
Authors : Mashalidis, E.H.; Lee, S.Y.
Deposited on : 2019-05-14
Resolution : 2.95 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 : 2.13.1
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) : 2.13.1

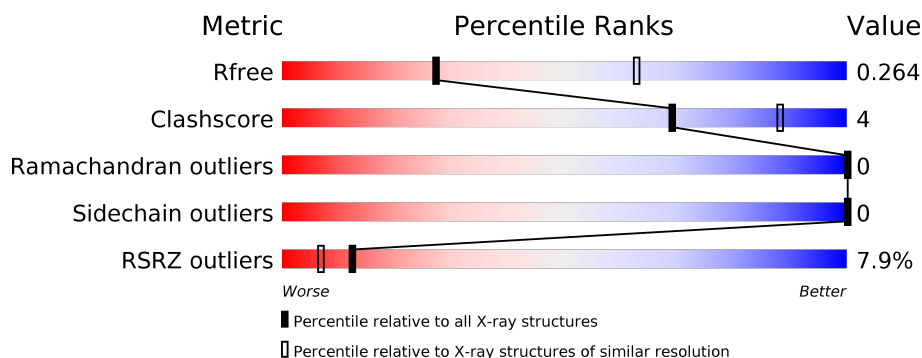
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	E	137	<div> <div>6%</div> <div>85%</div> <div>5%</div> <div>9%</div> </div>
1	F	137	<div> <div>2%</div> <div>81%</div> <div>10%</div> <div>9%</div> </div>
1	G	137	<div> <div>5%</div> <div>85%</div> <div>6%</div> <div>9%</div> </div>
1	H	137	<div> <div>6%</div> <div>92%</div> <div>8%</div> </div>
2	A	365	<div> <div>4%</div> <div>79%</div> <div>10%</div> <div>11%</div> </div>
2	B	365	<div> <div>9%</div> <div>85%</div> <div>5%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
2	C	365	<div><div></div><div>8%</div><div>79%</div><div>10%</div><div>10%</div></div>
2	D	365	<div><div></div><div>11%</div><div>84%</div><div>8%</div><div>8%</div></div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 27565 atoms, of which 13714 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 MraYAA nanobody.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	E	124	Total	C	H	N	O	S	0	0	0
			1800	580	872	160	184	4			
1	G	125	Total	C	H	N	O	S	0	0	0
			1760	573	847	157	179	4			
1	F	125	Total	C	H	N	O	S	0	0	0
			1812	584	878	160	186	4			
1	H	126	Total	C	H	N	O	S	0	0	0
			1794	580	864	162	184	4			

- Molecule 2 is a protein called Phospho-N-acetylmuramoyl-pentapeptide-transferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	A	326	Total	C	H	N	O	S	0	0	0
			5046	1682	2558	379	419	8			
2	C	328	Total	C	H	N	O	S	0	0	0
			4949	1656	2487	379	419	8			
2	B	330	Total	C	H	N	O	S	0	0	0
			4998	1678	2511	380	422	7			
2	D	337	Total	C	H	N	O	S	0	0	0
			4902	1656	2433	379	426	8			

There are 24 discrepancies between the modelled and reference sequences:

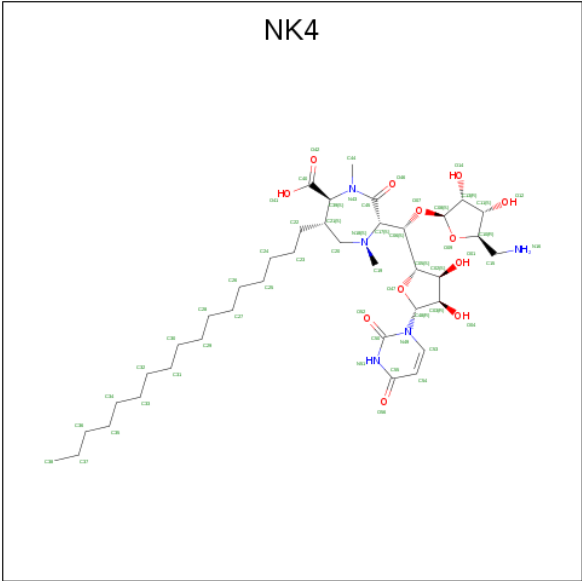
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP O66465
A	-4	PRO	-	expression tag	UNP O66465
A	-3	ALA	-	expression tag	UNP O66465
A	-2	VAL	-	expression tag	UNP O66465
A	-1	PRO	-	expression tag	UNP O66465
A	0	ARG	-	expression tag	UNP O66465
C	-5	GLY	-	expression tag	UNP O66465
C	-4	PRO	-	expression tag	UNP O66465

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	ALA	-	expression tag	UNP O66465
C	-2	VAL	-	expression tag	UNP O66465
C	-1	PRO	-	expression tag	UNP O66465
C	0	ARG	-	expression tag	UNP O66465
B	-5	GLY	-	expression tag	UNP O66465
B	-4	PRO	-	expression tag	UNP O66465
B	-3	ALA	-	expression tag	UNP O66465
B	-2	VAL	-	expression tag	UNP O66465
B	-1	PRO	-	expression tag	UNP O66465
B	0	ARG	-	expression tag	UNP O66465
D	-5	GLY	-	expression tag	UNP O66465
D	-4	PRO	-	expression tag	UNP O66465
D	-3	ALA	-	expression tag	UNP O66465
D	-2	VAL	-	expression tag	UNP O66465
D	-1	PRO	-	expression tag	UNP O66465
D	0	ARG	-	expression tag	UNP O66465

- Molecule 3 is (5S)-5'-O-(5-amino-5-deoxy-beta-D-ribofuranosyl)-5'-C-[(2S,5S,6S)-5-carb oxy-6-heptadecyl-1,4-dimethyl-3-oxo-1,4-diazepan-2-yl]uridine (three-letter code: NK4) (formula: C₃₉H₆₇N₅O₁₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			122	39	66	5	12		
3	C	1	Total	C	H	N	O	0	0
			122	39	66	5	12		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total 122	C 39	H 66	N 5	O 12	0	0
3	D	1	Total 122	C 39	H 66	N 5	O 12	0	0

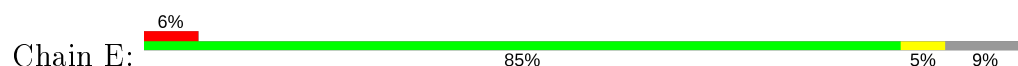
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	2	Total 2	O 2	0	0
4	A	5	Total 5	O 5	0	0
4	C	6	Total 6	O 6	0	0
4	B	1	Total 1	O 1	0	0
4	D	2	Total 2	O 2	0	0

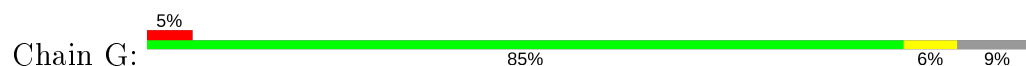
3 Residue-property plots [i](#)

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.

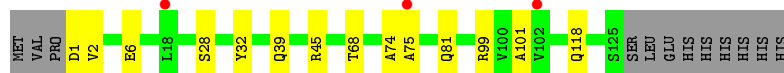
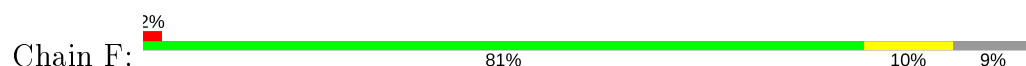
- Molecule 1: MraYAA nanobody



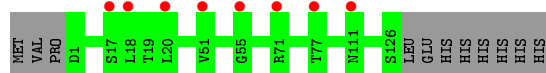
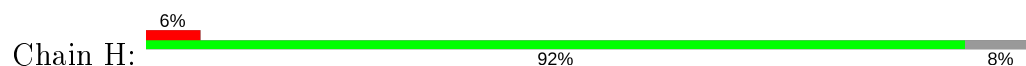
- Molecule 1: MraYAA nanobody



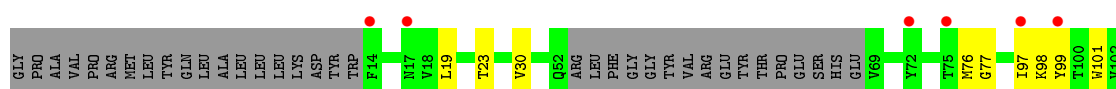
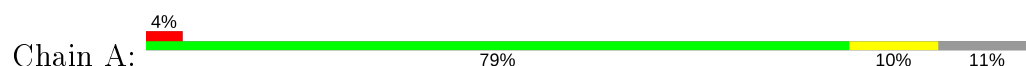
- Molecule 1: MraYAA nanobody

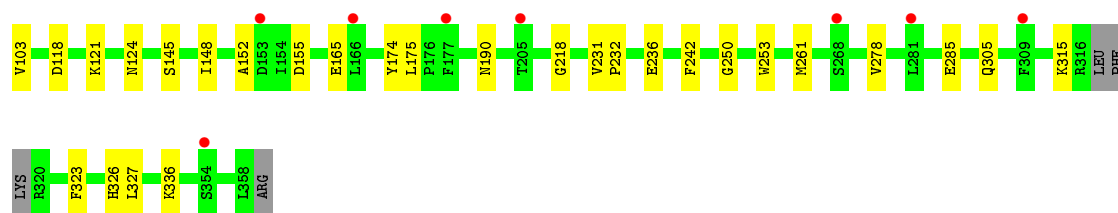


- Molecule 1: MraYAA nanobody

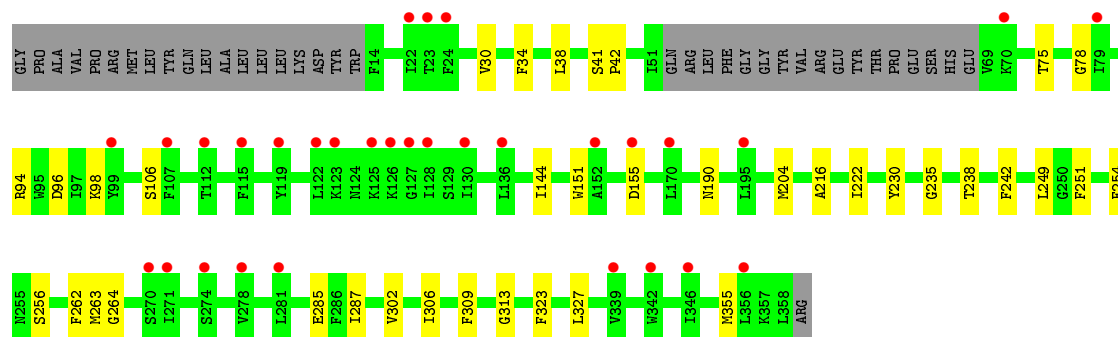
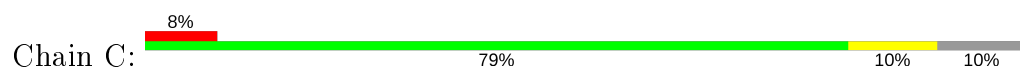


- Molecule 2: Phospho-N-acetylmuramoyl-pentapeptide-transferase

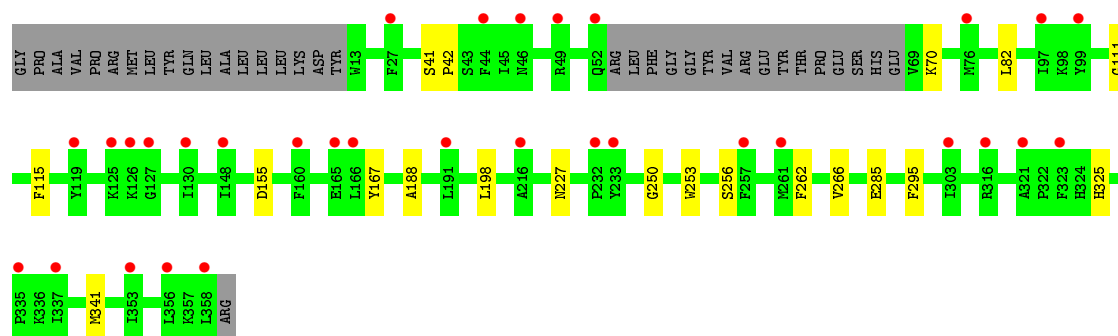
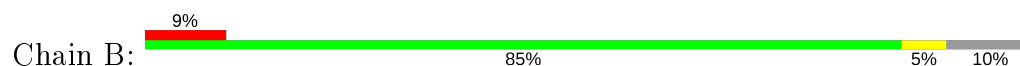




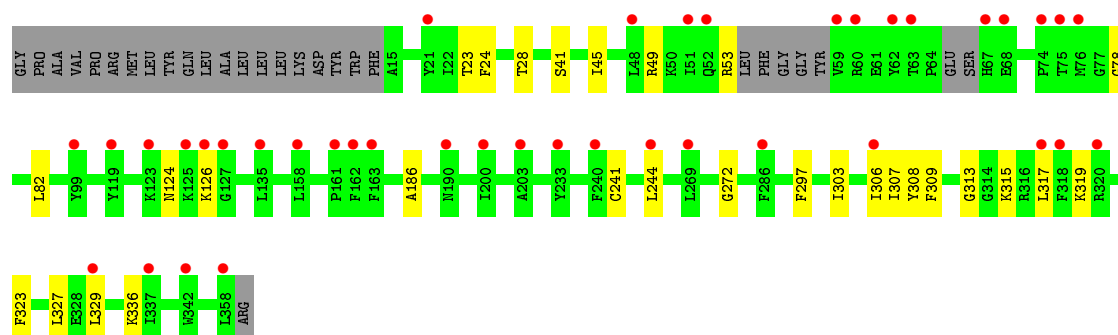
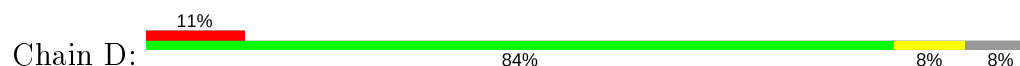
• Molecule 2: Phospho-N-acetylmuramoyl-pentapeptide-transferase



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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.89 Å 129.58 Å 129.43 Å 90.00° 109.33° 90.00°	Depositor
Resolution (Å)	43.94 – 2.95 88.88 – 2.95	Depositor EDS
% Data completeness (in resolution range)	98.7 (43.94-2.95) 90.2 (88.88-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.93 (at 2.96 Å)	Xtriage
Refinement program	PHENIX (1.12 _2829)	Depositor
R, R_{free}	0.248 , 0.268 0.248 , 0.264	Depositor DCC
R_{free} test set	2632 reflections (4.32%)	wwPDB-VP
Wilson B-factor (Å ²)	65.2	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	27565	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NK4

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	E	0.32	0/946	0.50	0/1285
1	F	0.32	0/952	0.50	0/1294
1	G	0.31	0/931	0.50	0/1267
1	H	0.30	0/948	0.49	0/1291
2	A	0.31	0/2550	0.45	0/3480
2	B	0.28	0/2550	0.42	0/3492
2	C	0.38	0/2522	0.48	0/3447
2	D	0.32	0/2527	0.47	0/3463
All	All	0.32	0/13926	0.47	0/19019

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	928	872	872	4	0
1	F	934	878	880	11	0
1	G	913	847	849	9	0
1	H	930	864	866	0	0
2	A	2488	2558	2559	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2487	2511	2511	14	0
2	C	2462	2487	2486	28	0
2	D	2469	2433	2435	22	0
3	A	56	66	0	1	0
3	B	56	66	0	1	0
3	C	56	66	0	3	0
3	D	56	66	0	0	0
4	A	5	0	0	0	0
4	B	1	0	0	0	0
4	C	6	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
All	All	13851	13714	13458	102	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 4.

All (102) 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:D:308:TYR:CD1	2:D:317:LEU:HD21	2.14	0.82
2:B:285:GLU:OE1	2:B:285:GLU:N	2.24	0.70
2:A:305:GLN:OE1	2:A:315:LYS:CB	2.41	0.69
2:C:256:SER:O	2:D:336:LYS:NZ	2.25	0.68
2:A:165:GLU:OE1	2:A:165:GLU:N	2.31	0.63
2:D:308:TYR:CG	2:D:317:LEU:HG	2.34	0.63
2:A:19:LEU:O	2:A:23:THR:HG22	1.98	0.63
2:D:309:PHE:O	2:D:313:GLY:O	2.19	0.61
2:C:251:PHE:CZ	2:C:263:MET:HB2	2.37	0.60
1:E:101:ALA:O	2:A:155:ASP:N	2.35	0.60
2:A:190:ASN:OD1	3:A:401:NK4:N16	2.36	0.58
2:A:305:GLN:CD	2:A:315:LYS:CB	2.72	0.58
2:D:309:PHE:HA	2:D:315:LYS:O	2.03	0.58
2:C:264:GLY:N	3:C:401:NK4:O12	2.37	0.57
2:A:174:TYR:OH	2:A:285:GLU:OE2	2.24	0.56
2:A:145:SER:HB3	2:A:175:LEU:HD23	1.89	0.55
2:A:305:GLN:HA	2:A:315:LYS:CB	2.37	0.55
2:D:308:TYR:CD1	2:D:317:LEU:CD2	2.89	0.55
2:C:285:GLU:OE1	2:C:285:GLU:N	2.31	0.54
2:D:241:CYS:O	2:D:244:LEU:HB3	2.10	0.52
1:F:99:ARG:NH2	2:B:227:ASN:OD1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:75:THR:OG1	3:C:401:NK4:O14	2.21	0.52
2:D:23:THR:OG1	2:D:28:THR:OG1	2.29	0.50
2:C:98:LYS:HB2	2:C:151:TRP:CH2	2.46	0.50
1:F:39:GLN:OE1	1:F:45:ARG:HG3	2.12	0.50
2:B:188:ALA:HB1	2:B:295:PHE:HB3	1.94	0.49
2:D:303:ILE:O	2:D:306:ILE:HG22	2.12	0.49
2:D:78:GLY:O	2:D:82:LEU:HD13	2.13	0.49
2:C:41:SER:HB2	2:C:254:PHE:CE2	2.48	0.48
2:D:308:TYR:CD2	2:D:317:LEU:HG	2.47	0.48
1:G:32:TYR:CE1	1:G:99:ARG:HG3	2.48	0.48
1:F:28:SER:HB3	2:B:167:TYR:OH	2.12	0.48
1:G:32:TYR:CD1	1:G:99:ARG:HG3	2.48	0.48
2:D:49:ARG:O	2:D:53:ARG:O	2.32	0.48
1:E:53:ARG:NH1	1:E:100:VAL:O	2.45	0.48
2:A:98:LYS:HA	2:A:101:TRP:HD1	1.79	0.48
1:F:101:ALA:O	2:B:155:ASP:HB2	2.13	0.48
2:B:115:PHE:CA	2:B:266:VAL:HG22	2.44	0.47
2:C:34:PHE:CE2	2:C:38:LEU:HD11	2.49	0.47
1:E:6:GLU:OE1	1:E:119:GLY:N	2.47	0.47
2:C:34:PHE:CZ	2:C:38:LEU:HD11	2.49	0.47
2:A:323:PHE:CE1	2:A:326:HIS:HD2	2.32	0.47
2:D:297:PHE:HE2	2:D:323:PHE:CG	2.33	0.47
2:B:70:LYS:HG2	2:B:262:PHE:HZ	1.80	0.47
1:G:101:ALA:O	2:C:155:ASP:N	2.46	0.46
2:C:94:ARG:NH1	2:C:96:ASP:OD2	2.48	0.46
1:G:67:PHE:CE1	1:G:82:MET:HB2	2.50	0.46
2:D:41:SER:O	2:D:45:ILE:HG12	2.16	0.46
2:D:306:ILE:HG23	2:D:307:ILE:N	2.31	0.46
2:D:124:ASN:ND2	2:D:126:LYS:O	2.47	0.46
2:C:235:GLY:O	2:C:238:THR:HB	2.15	0.46
2:B:115:PHE:N	2:B:266:VAL:HG22	2.31	0.45
2:A:323:PHE:CZ	2:A:327:LEU:HD11	2.50	0.45
1:G:101:ALA:O	2:C:155:ASP:HB2	2.16	0.45
2:B:250:GLY:O	2:B:253:TRP:HB3	2.17	0.45
2:C:309:PHE:O	2:C:313:GLY:O	2.34	0.45
2:C:323:PHE:CE2	2:C:327:LEU:CD1	3.00	0.45
1:G:53:ARG:NH1	1:G:100:VAL:O	2.48	0.45
2:A:19:LEU:HD23	2:A:19:LEU:HA	1.89	0.44
2:B:325:HIS:NE2	3:B:401:NK4:O42	2.45	0.44
2:C:323:PHE:CE2	2:C:327:LEU:HD11	2.52	0.44
2:C:106:SER:HA	2:C:144:ILE:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:77:GLY:HA3	2:A:261:MET:HE2	2.00	0.44
2:A:97:ILE:HG13	2:A:236:GLU:HG3	2.00	0.44
2:D:308:TYR:CE1	2:D:317:LEU:HD21	2.51	0.44
2:C:78:GLY:N	2:C:263:MET:O	2.35	0.43
2:D:297:PHE:HE2	2:D:323:PHE:CD2	2.37	0.43
2:C:190:ASN:OD1	3:C:401:NK4:N16	2.52	0.43
1:F:1:ASP:OD1	1:F:2:VAL:N	2.51	0.43
2:B:82:LEU:HD21	2:B:111:GLY:HA3	2.00	0.43
2:C:302:VAL:O	2:C:306:ILE:HG22	2.18	0.43
2:A:148:ILE:O	2:A:152:ALA:O	2.36	0.43
1:F:74:ALA:O	1:F:75:ALA:HB3	2.18	0.43
2:C:287:ILE:HA	2:C:355:MET:CE	2.49	0.43
2:D:24:PHE:O	2:D:28:THR:OG1	2.37	0.43
1:F:32:TYR:CE2	1:F:99:ARG:HG3	2.54	0.42
2:D:323:PHE:CE2	2:D:327:LEU:HD11	2.53	0.42
2:A:76:MET:SD	2:A:118:ASP:HB3	2.58	0.42
2:C:75:THR:HA	2:C:262:PHE:HB2	2.01	0.42
1:F:28:SER:OG	1:F:28:SER:O	2.36	0.42
2:A:99:TYR:HE2	2:A:232:PRO:O	2.01	0.42
2:D:186:ALA:HA	2:D:272:GLY:HA3	2.00	0.42
1:E:24:THR:HG21	1:E:32:TYR:HE1	1.85	0.41
2:A:30:VAL:HG23	2:A:242:PHE:HB3	2.02	0.41
2:A:250:GLY:O	2:A:253:TRP:HB3	2.21	0.41
2:A:121:LYS:HA	2:A:124:ASN:O	2.20	0.41
1:G:100:VAL:HG12	2:C:230:TYR:CD2	2.54	0.41
1:G:100:VAL:HG12	2:C:230:TYR:HD2	1.85	0.41
2:C:216:ALA:HA	2:C:222:ILE:HG21	2.02	0.41
1:F:118:GLN:OE1	1:F:118:GLN:N	2.43	0.41
2:C:30:VAL:HG23	2:C:242:PHE:HB3	2.01	0.41
2:A:218:GLY:HA2	2:A:231:VAL:O	2.20	0.41
2:A:103:VAL:HG21	2:A:278:VAL:HG23	2.03	0.41
1:G:98:PHE:CE1	1:G:100:VAL:CG1	3.04	0.41
1:F:68:THR:OG1	1:F:81:GLN:HG2	2.21	0.41
2:B:41:SER:N	2:B:42:PRO:CD	2.84	0.41
1:F:6:GLU:OE1	1:F:6:GLU:N	2.53	0.41
2:A:336:LYS:NZ	2:B:256:SER:O	2.53	0.41
2:B:198:LEU:HD11	2:B:341:MET:HG3	2.03	0.40
2:C:38:LEU:O	2:C:42:PRO:HD3	2.21	0.40
2:D:319:LYS:CB	2:D:329:LEU:HD12	2.52	0.40
2:C:204:MET:HE1	2:C:249:LEU:HD23	2.04	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	E	122/137 (89%)	122 (100%)	0	0	100	100
1	F	123/137 (90%)	119 (97%)	4 (3%)	0	100	100
1	G	123/137 (90%)	119 (97%)	4 (3%)	0	100	100
1	H	124/137 (90%)	123 (99%)	1 (1%)	0	100	100
2	A	320/365 (88%)	301 (94%)	19 (6%)	0	100	100
2	B	326/365 (89%)	307 (94%)	19 (6%)	0	100	100
2	C	324/365 (89%)	311 (96%)	13 (4%)	0	100	100
2	D	331/365 (91%)	315 (95%)	16 (5%)	0	100	100
All	All	1793/2008 (89%)	1717 (96%)	76 (4%)	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	E	93/110 (84%)	93 (100%)	0	100	100
1	F	94/110 (86%)	94 (100%)	0	100	100
1	G	88/110 (80%)	88 (100%)	0	100	100
1	H	92/110 (84%)	92 (100%)	0	100	100
2	A	259/309 (84%)	259 (100%)	0	100	100
2	B	253/309 (82%)	253 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	250/309 (81%)	250 (100%)	0	100	100
2	D	243/309 (79%)	243 (100%)	0	100	100
All	All	1372/1676 (82%)	1372 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
2	A	326	HIS

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 ⓘ

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
3	NK4	A	401	-	45,59,59	3.86	7 (15%)	47,81,81	1.66	7 (14%)
3	NK4	B	401	-	45,59,59	3.94	7 (15%)	47,81,81	1.56	9 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NK4	C	401	-	45,59,59	3.93	7 (15%)	47,81,81	1.32	5 (10%)
3	NK4	D	401	-	45,59,59	3.97	7 (15%)	47,81,81	1.41	6 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NK4	A	401	-	-	12/29/95/95	0/3/4/4
3	NK4	B	401	-	-	10/29/95/95	0/3/4/4
3	NK4	C	401	-	-	10/29/95/95	0/3/4/4
3	NK4	D	401	-	-	13/29/95/95	0/3/4/4

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	401	NK4	C45-N43	-23.11	1.11	1.35
3	C	401	NK4	C45-N43	-23.03	1.11	1.35
3	B	401	NK4	C45-N43	-23.02	1.11	1.35
3	A	401	NK4	C45-N43	-22.24	1.12	1.35
3	A	401	NK4	C53-N49	-8.51	1.25	1.35
3	B	401	NK4	C53-N49	-8.43	1.25	1.35
3	D	401	NK4	C53-N49	-8.27	1.25	1.35
3	C	401	NK4	C53-N49	-8.23	1.25	1.35
3	A	401	NK4	C50-N51	-6.08	1.26	1.38
3	D	401	NK4	C50-N51	-6.07	1.26	1.38
3	B	401	NK4	C50-N51	-6.01	1.26	1.38
3	C	401	NK4	C50-N51	-5.90	1.26	1.38
3	D	401	NK4	C55-N51	-4.44	1.25	1.33
3	A	401	NK4	C55-N51	-4.21	1.25	1.33
3	C	401	NK4	C08-C13	-3.97	1.47	1.52
3	D	401	NK4	C08-C13	-3.96	1.47	1.52
3	C	401	NK4	C55-N51	-3.92	1.26	1.33
3	B	401	NK4	C55-N51	-3.91	1.26	1.33
3	A	401	NK4	C08-C13	-3.81	1.48	1.52
3	B	401	NK4	C08-C13	-3.37	1.48	1.52
3	D	401	NK4	C03-C48	-3.30	1.48	1.53
3	C	401	NK4	C03-C48	-2.93	1.49	1.53
3	A	401	NK4	C03-C48	-2.84	1.49	1.53
3	B	401	NK4	C03-C48	-2.77	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	NK4	O47-C48	2.63	1.44	1.41
3	D	401	NK4	O47-C48	2.62	1.44	1.41
3	C	401	NK4	O47-C48	2.40	1.44	1.41
3	B	401	NK4	O47-C48	2.32	1.44	1.41

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	NK4	C44-N43-C45	-4.98	112.48	118.60
3	D	401	NK4	C44-N43-C45	-4.93	112.54	118.60
3	A	401	NK4	O46-C45-C17	-4.40	115.41	121.41
3	A	401	NK4	O46-C45-N43	-4.36	116.83	121.66
3	C	401	NK4	C44-N43-C45	-3.95	113.74	118.60
3	B	401	NK4	O46-C45-C17	-3.91	116.07	121.41
3	B	401	NK4	C44-N43-C45	-3.74	114.00	118.60
3	B	401	NK4	O46-C45-N43	-3.66	117.60	121.66
3	D	401	NK4	O46-C45-N43	-3.58	117.68	121.66
3	C	401	NK4	O46-C45-N43	-3.28	118.02	121.66
3	D	401	NK4	O46-C45-C17	-3.20	117.04	121.41
3	A	401	NK4	C02-C03-C48	3.05	105.56	100.98
3	B	401	NK4	C02-C05-C06	-3.00	111.07	115.74
3	A	401	NK4	C02-C05-C06	-2.94	111.17	115.74
3	B	401	NK4	C08-C13-C11	2.93	106.01	102.30
3	B	401	NK4	O09-C08-C13	2.76	108.53	104.98
3	C	401	NK4	C15-C10-C11	-2.74	108.28	114.93
3	C	401	NK4	C02-C03-C48	2.71	105.06	100.98
3	C	401	NK4	C02-C05-C06	-2.71	111.53	115.74
3	B	401	NK4	C02-C03-C48	2.57	104.84	100.98
3	B	401	NK4	O47-C05-C02	2.49	108.94	104.27
3	A	401	NK4	C15-C10-C11	-2.38	109.15	114.93
3	D	401	NK4	C02-C05-C06	-2.27	112.21	115.74
3	B	401	NK4	C15-C10-C11	-2.26	109.45	114.93
3	A	401	NK4	O09-C08-C13	2.18	107.79	104.98
3	D	401	NK4	C15-C10-C11	-2.14	109.74	114.93
3	D	401	NK4	C54-C55-N51	-2.14	118.60	123.31

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	NK4	C20-C21-C22-C23
3	A	401	NK4	C13-C08-O07-C06

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Mol	Chain	Res	Type	Atoms
3	B	401	NK4	C20-C21-C22-C23
3	C	401	NK4	C20-C21-C22-C23
3	C	401	NK4	C13-C08-O07-C06
3	D	401	NK4	C20-C21-C22-C23
3	D	401	NK4	C13-C08-O07-C06
3	D	401	NK4	C32-C33-C34-C35
3	A	401	NK4	C32-C33-C34-C35
3	C	401	NK4	C32-C33-C34-C35
3	B	401	NK4	C32-C33-C34-C35
3	B	401	NK4	C21-C22-C23-C24
3	D	401	NK4	C24-C25-C26-C27
3	C	401	NK4	C24-C25-C26-C27
3	B	401	NK4	C25-C26-C27-C28
3	A	401	NK4	C24-C25-C26-C27
3	D	401	NK4	C25-C26-C27-C28
3	B	401	NK4	C24-C25-C26-C27
3	C	401	NK4	C25-C26-C27-C28
3	A	401	NK4	O09-C08-O07-C06
3	C	401	NK4	O09-C08-O07-C06
3	D	401	NK4	O09-C08-O07-C06
3	A	401	NK4	C27-C28-C29-C30
3	D	401	NK4	C27-C28-C29-C30
3	D	401	NK4	C34-C35-C36-C37
3	C	401	NK4	C29-C30-C31-C32
3	D	401	NK4	C35-C36-C37-C38
3	A	401	NK4	C25-C26-C27-C28
3	B	401	NK4	C22-C23-C24-C25
3	B	401	NK4	C29-C30-C31-C32
3	B	401	NK4	C27-C28-C29-C30
3	C	401	NK4	C22-C23-C24-C25
3	C	401	NK4	C35-C36-C37-C38
3	A	401	NK4	C35-C36-C37-C38
3	A	401	NK4	C21-C22-C23-C24
3	D	401	NK4	C22-C23-C24-C25
3	A	401	NK4	C39-C21-C22-C23
3	B	401	NK4	C39-C21-C22-C23
3	D	401	NK4	C39-C21-C22-C23
3	A	401	NK4	C29-C30-C31-C32
3	A	401	NK4	C28-C29-C30-C31
3	C	401	NK4	C27-C28-C29-C30
3	B	401	NK4	C13-C08-O07-C06
3	D	401	NK4	C29-C30-C31-C32

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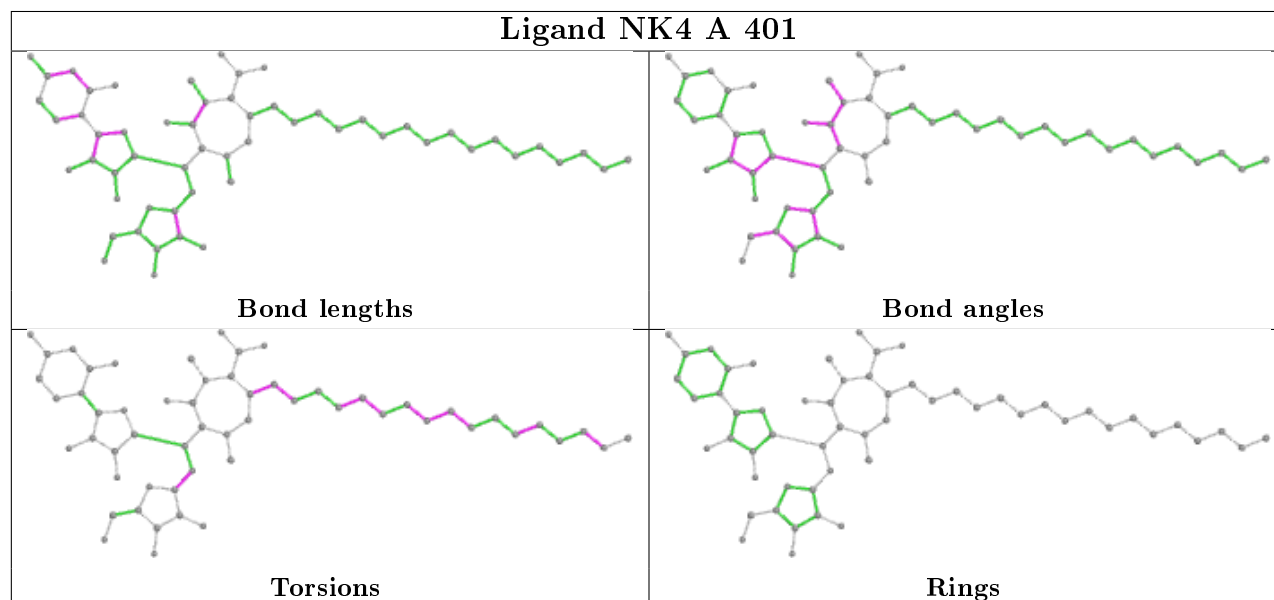
Mol	Chain	Res	Type	Atoms
3	D	401	NK4	C28-C29-C30-C31

There are no ring outliers.

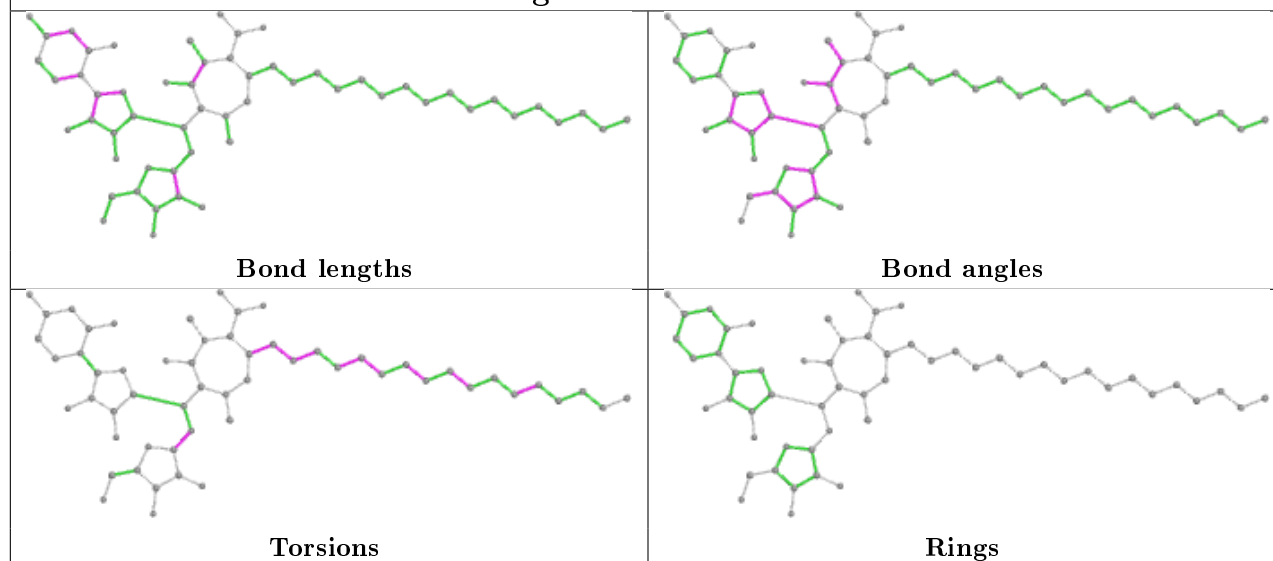
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	NK4	1	0
3	B	401	NK4	1	0
3	C	401	NK4	3	0

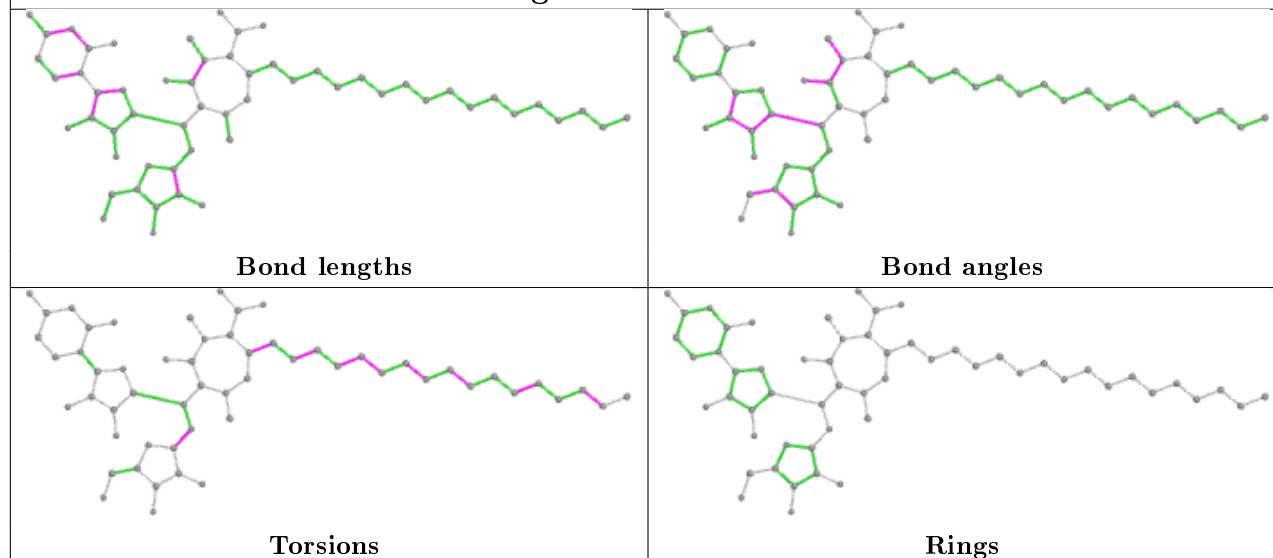
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

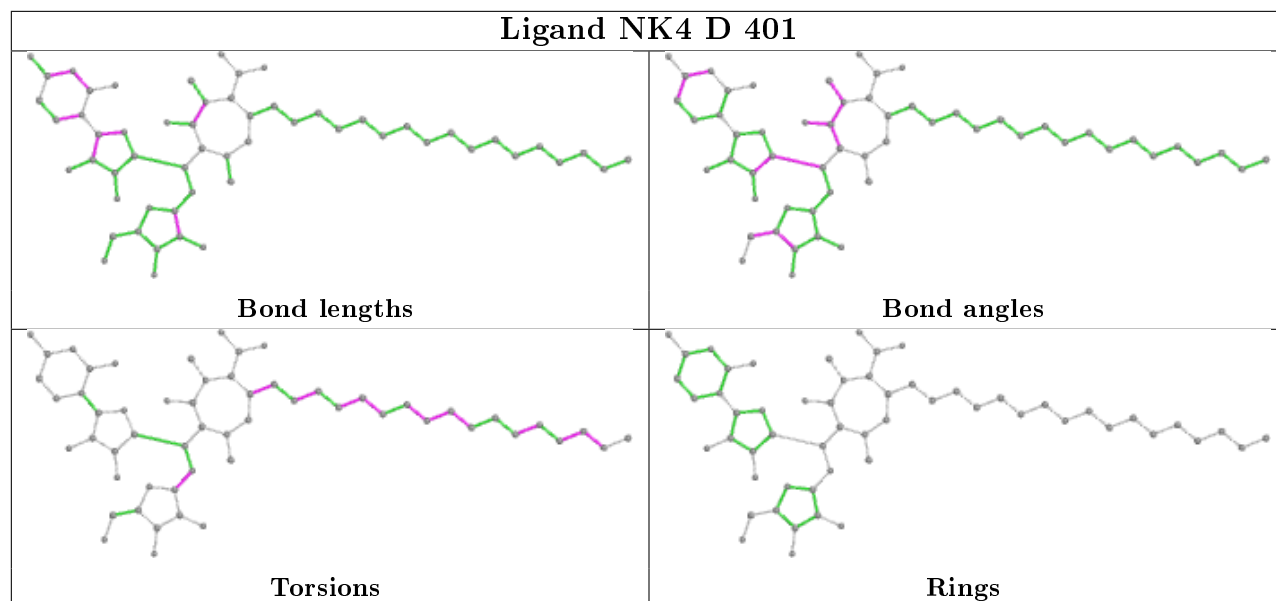


Ligand NK4 B 401



Ligand NK4 C 401





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	E	124/137 (90%)	0.69	8 (6%) 18 11	50, 68, 90, 110	0
1	F	125/137 (91%)	0.53	3 (2%) 59 42	53, 68, 94, 114	0
1	G	125/137 (91%)	0.59	7 (5%) 24 15	46, 63, 85, 106	0
1	H	126/137 (91%)	0.55	8 (6%) 20 11	60, 81, 103, 125	0
2	A	326/365 (89%)	0.66	14 (4%) 35 22	50, 67, 102, 135	0
2	B	330/365 (90%)	0.81	32 (9%) 7 4	60, 87, 136, 161	0
2	C	328/365 (89%)	0.73	31 (9%) 8 5	55, 77, 116, 137	0
2	D	337/365 (92%)	0.82	40 (11%) 4 2	62, 85, 128, 162	0
All	All	1821/2008 (90%)	0.71	143 (7%) 12 7	46, 76, 120, 162	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	358	LEU	7.8
2	D	59	VAL	7.7
2	B	49	ARG	7.4
2	C	127	GLY	6.8
2	C	125	LYS	6.7
2	D	52	GLN	6.6
2	B	126	LYS	6.3
2	D	162	PHE	6.0
2	B	191	LEU	5.7
2	C	119	TYR	5.7
2	B	127	GLY	5.3
2	B	358	LEU	4.8
2	A	309	PHE	4.7
2	C	126	LYS	4.7
2	B	166	LEU	4.5
2	D	161	PRO	4.4

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Mol	Chain	Res	Type	RSRZ
1	G	74	ALA	4.3
2	D	67	HIS	4.3
1	E	73	ASN	4.3
2	D	60	ARG	4.2
2	B	321	ALA	4.2
2	D	163	PHE	4.2
2	A	99	TYR	3.9
2	D	127	GLY	3.7
1	F	18	LEU	3.7
2	B	165	GLU	3.6
2	B	46	ASN	3.6
2	B	52	GLN	3.5
1	H	18	LEU	3.5
1	G	75	ALA	3.5
2	C	152	ALA	3.5
2	D	63	THR	3.4
2	B	130	ILE	3.4
2	C	24	PHE	3.4
2	C	123	LYS	3.4
2	D	200	ILE	3.3
2	C	281	LEU	3.2
2	A	14	PHE	3.2
2	D	269	LEU	3.1
2	B	97	ILE	3.1
2	B	316	ARG	3.1
2	D	233	TYR	3.1
2	D	119	TYR	3.1
2	C	356	LEU	3.0
1	E	24	THR	3.0
2	C	346	ILE	2.9
2	C	170	LEU	2.9
2	B	233	TYR	2.9
2	D	320	ARG	2.9
2	A	153	ASP	2.9
2	B	76	MET	2.9
2	B	119	TYR	2.8
2	C	122	LEU	2.8
2	C	70	LYS	2.8
1	E	25	SER	2.8
2	B	323	PHE	2.8
2	D	240	PHE	2.8
2	D	21	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	51	ILE	2.7
1	G	48	VAL	2.7
1	G	101	ALA	2.7
2	D	125	LYS	2.7
2	C	155	ASP	2.7
2	C	339	VAL	2.7
1	E	79	TYR	2.6
1	H	17	SER	2.6
1	E	14	THR	2.6
2	D	126	LYS	2.6
2	C	274	SER	2.6
2	C	342	TRP	2.6
2	B	232	PRO	2.5
1	H	71	ARG	2.5
2	D	62	TYR	2.5
2	B	303	ILE	2.5
2	C	107	PHE	2.5
1	E	26	GLY	2.5
2	D	74	PRO	2.5
1	G	103	THR	2.5
2	C	270	SER	2.5
2	B	216	ALA	2.5
2	A	72	TYR	2.5
2	D	68	GLU	2.5
2	D	76	MET	2.5
2	D	135	LEU	2.5
2	B	160	PHE	2.5
1	H	55	GLY	2.4
2	D	48	LEU	2.4
1	E	70	SER	2.4
2	C	128	ILE	2.4
2	D	99	TYR	2.4
2	C	22	ILE	2.4
2	B	125	LYS	2.4
1	H	111	ASN	2.4
2	C	278	VAL	2.4
2	B	27	PHE	2.4
2	A	166	LEU	2.4
2	C	23	THR	2.3
2	B	353	ILE	2.3
2	B	356	LEU	2.3
2	D	317	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	75	ALA	2.3
1	H	77	THR	2.3
2	C	130	ILE	2.3
2	D	190	ASN	2.3
2	C	271	ILE	2.3
1	G	100	VAL	2.3
2	C	79	ILE	2.3
2	A	75	THR	2.3
2	A	205	THR	2.3
2	C	115	PHE	2.3
2	B	335	PRO	2.2
2	A	281	LEU	2.2
2	D	158	LEU	2.2
2	B	261	MET	2.2
1	G	102	VAL	2.2
2	D	75	THR	2.2
2	B	44	PHE	2.2
2	D	318	PHE	2.2
2	C	195	LEU	2.2
2	D	337	ILE	2.2
1	H	20	LEU	2.2
2	C	112	THR	2.2
2	B	148	ILE	2.2
1	F	102	VAL	2.2
1	H	51	VAL	2.2
2	A	354	SER	2.2
2	D	123	LYS	2.1
2	B	99	TYR	2.1
2	A	97	ILE	2.1
2	B	337	ILE	2.1
2	D	342	TRP	2.1
2	D	286	PHE	2.1
2	D	306	ILE	2.1
2	B	257	PHE	2.1
2	A	17	ASN	2.1
1	E	124	VAL	2.1
2	C	99	TYR	2.1
2	A	177	PHE	2.1
2	D	329	LEU	2.1
2	D	244	LEU	2.0
2	C	136	LEU	2.0
2	A	268	SER	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	203	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

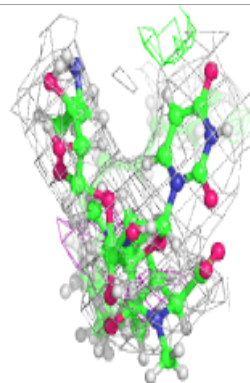
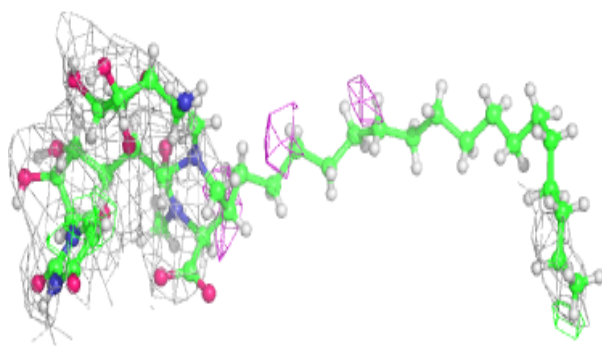
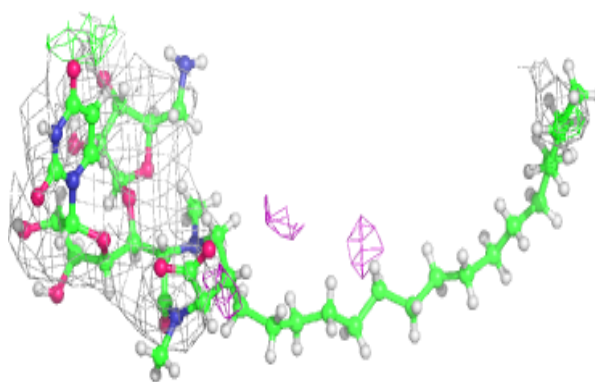
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NK4	B	401	56/56	0.82	0.46	99,133,153,158	0
3	NK4	A	401	56/56	0.88	0.30	63,83,111,113	0
3	NK4	D	401	56/56	0.88	0.39	83,107,130,133	0
3	NK4	C	401	56/56	0.91	0.23	79,104,112,115	0

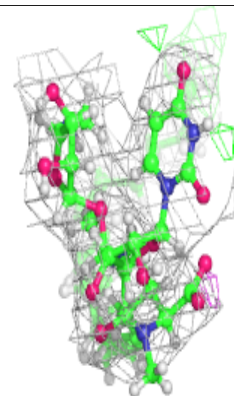
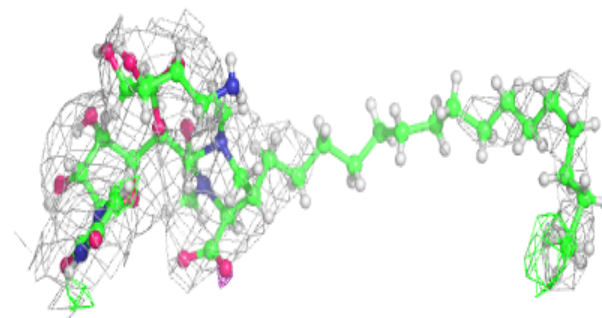
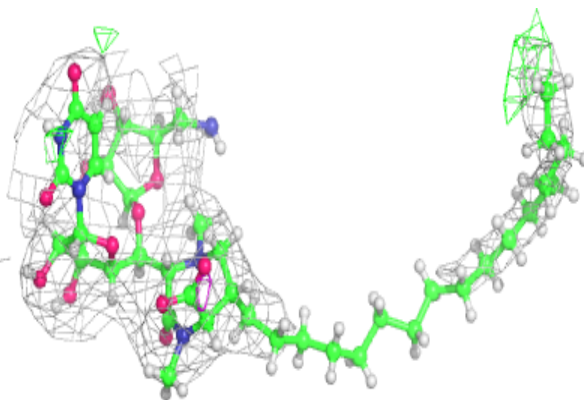
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NK4 B 401:

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

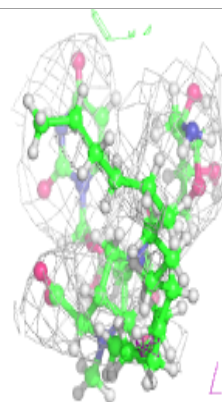
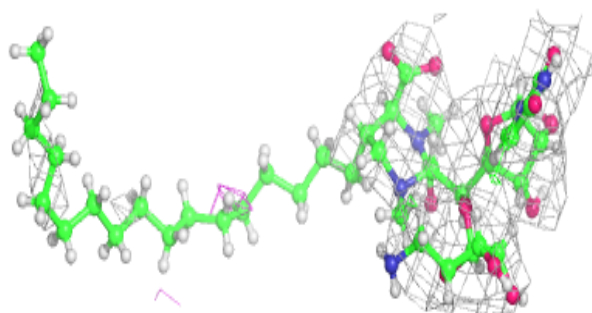
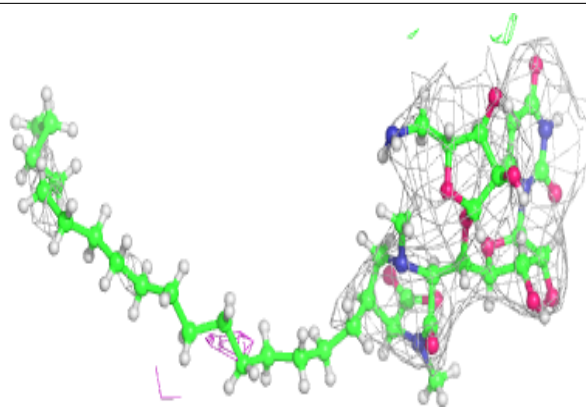
**Electron density around NK4 A 401:**

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

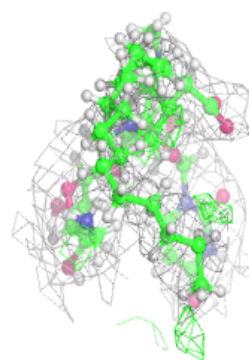
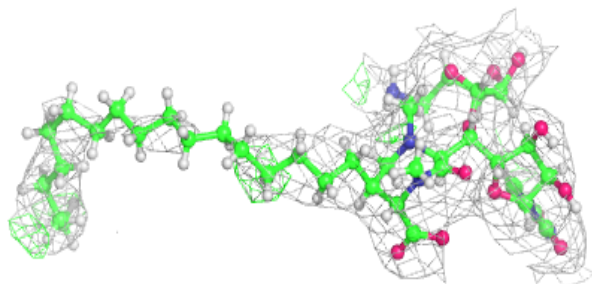
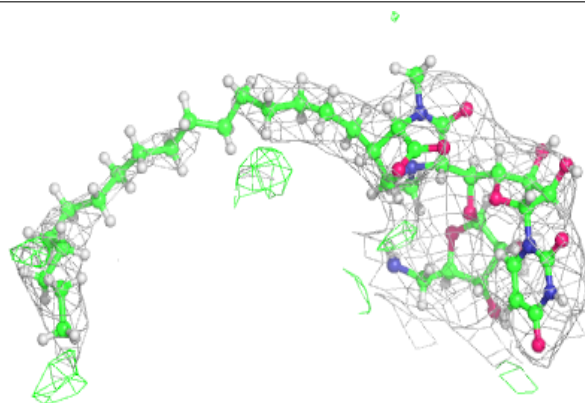


Electron density around NK4 D 401:

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

**Electron density around NK4 C 401:**

$2mF_o-DF_c$ (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.