Full wwPDB X-ray Structure Validation Report (i)

Oct 5, 2023 – 10:16 PM EDT

PDB ID	:	6OYZ
Title	:	Crystal structure of MraY bound to capuramycin
Authors	:	Mashalidis, E.H.; Lee, S.Y.
Deposited on	:	2019-05-15
Resolution	:	3.62 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 (i) 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 (i)) were used in the production of this report:

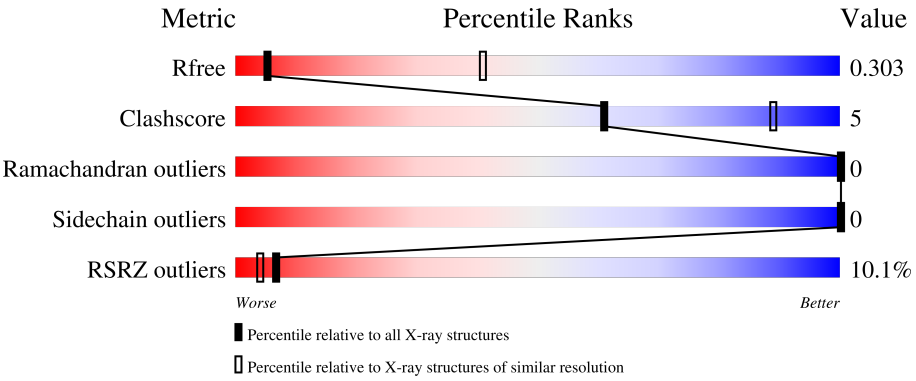
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.62 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	1290 (3.74-3.50)
Clashscore	141614	1387 (3.74-3.50)
Ramachandran outliers	138981	1339 (3.74-3.50)
Sidechain outliers	138945	1339 (3.74-3.50)
RSRZ outliers	127900	1191 (3.74-3.50)

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 <=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	14% 82% 8% 9%
1	F	137	24% 84% 7% 9%
1	G	137	11% 88% • 9%
1	H	137	27% 90% 10%
2	A	365	5% 79% 7% 14%

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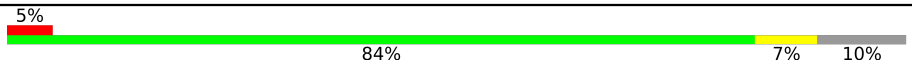
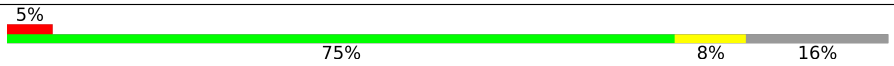
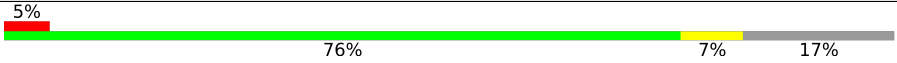
Mol	Chain	Length	Quality of chain
2	B	365	
2	C	365	
2	D	365	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 25385 atoms, of which 12441 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
			1781	577	858	159	183	4			
1	G	125	Total	C	H	N	O	S	0	0	0
			1780	577	857	158	184	4			
1	F	124	Total	C	H	N	O	S	0	0	0
			1666	551	780	153	178	4			
1	H	123	Total	C	H	N	O	S	0	0	0
			1734	566	834	153	177	4			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	A	313	Total	C	H	N	O	S	0	0	0
			4814	1620	2425	359	402	8			
2	C	306	Total	C	H	N	O	S	0	0	0
			4490	1521	2227	342	394	6			
2	B	330	Total	C	H	N	O	S	0	0	0
			4658	1604	2268	365	414	7			
2	D	304	Total	C	H	N	O	S	0	0	0
			4392	1498	2162	344	381	7			

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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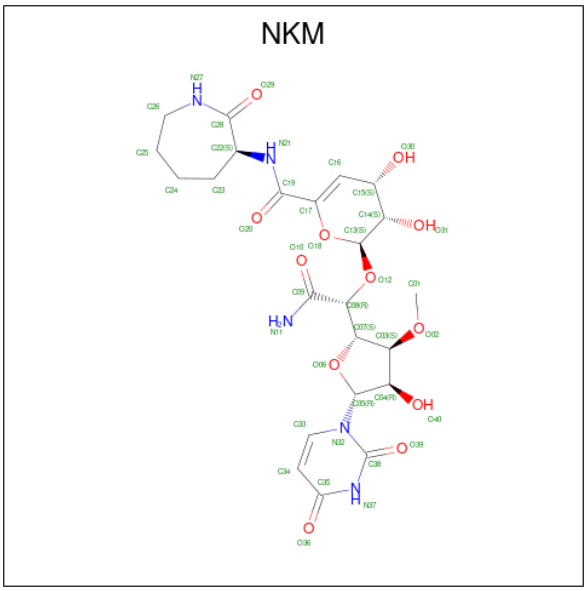
Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	ALA	-	expression tag	UNP O66465
C	-2	VAL	-	expression tag	UNP O66465
C	-1	PRO	-	expression tag	UNP O66465
C	0	ARG	-	expression tag	UNP O66465
B	-5	GLY	-	expression tag	UNP O66465
B	-4	PRO	-	expression tag	UNP O66465
B	-3	ALA	-	expression tag	UNP O66465
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 (2 {S},3 {S},4 {S})-2-[(1 {R})-2-azanyl-1-[(2 {S},3 {S},4 {R},5 {R})-5-[2,4-bis(oxidanylidene)pyrimidin-1-yl]-3-methoxy-4-oxidanyl-oxolan-2-yl]-2-oxidanylidene-ethoxy]-3,4-bis(oxidanyl)- {N}-[(3 {S})-2-oxidanylideneazepan-3-yl]-3,4-dihydro-2 {H}-pyran-6-carboxamide (three-letter code: NKM) (formula: $C_{23}H_{31}N_5O_{12}$).



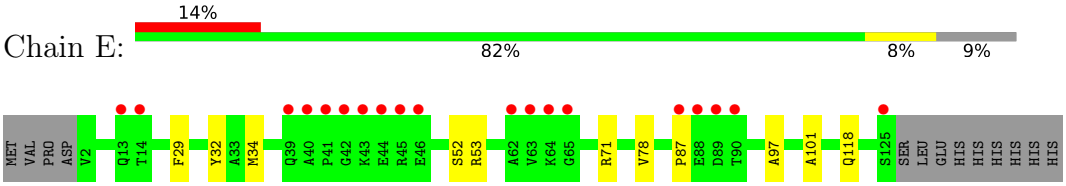
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			70	23	30	5	12		

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.

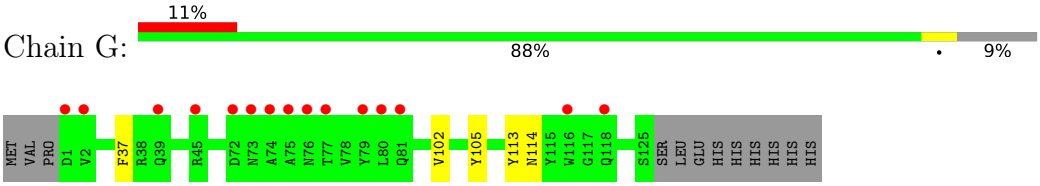
• Molecule 1: MraYAA nanobody

Chain E:



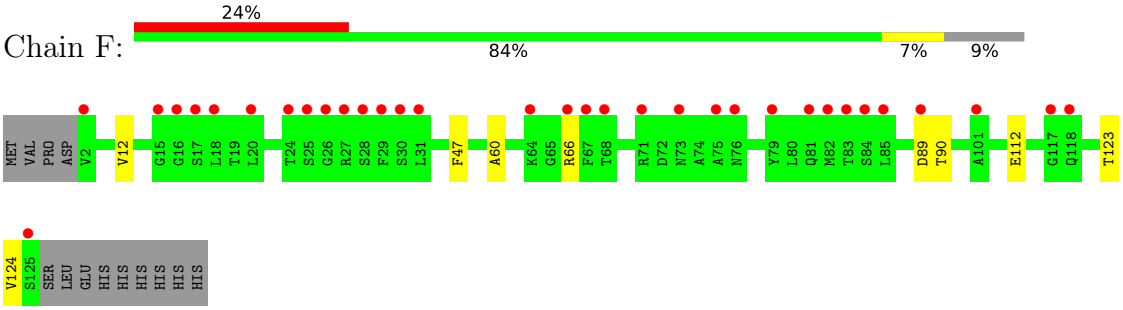
• Molecule 1: MraYAA nanobody

Chain G:



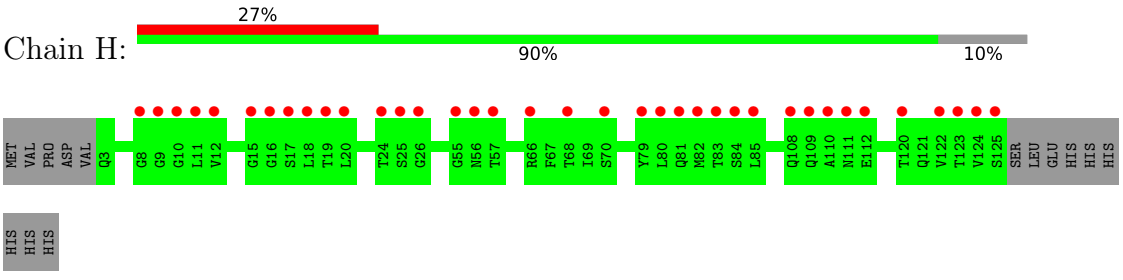
• Molecule 1: MraYAA nanobody

Chain F:



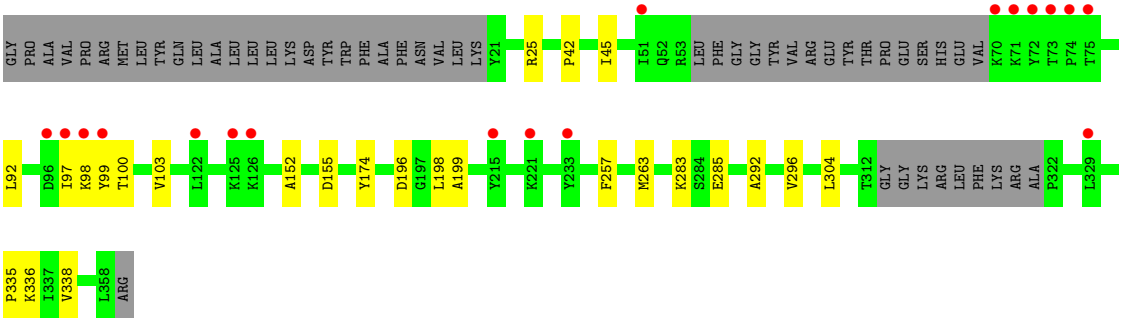
• Molecule 1: MraYAA nanobody

Chain H:

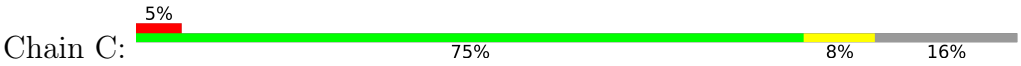


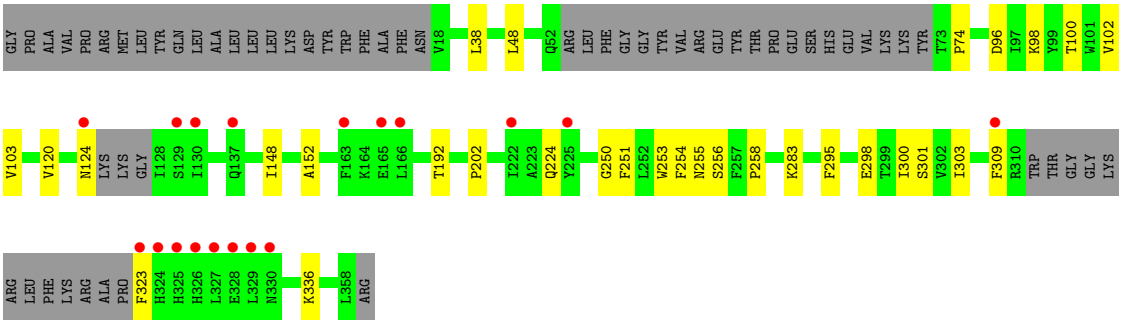
• Molecule 2: Phospho-N-acetylmuramoyl-pentapeptide-transferase

Chain A:

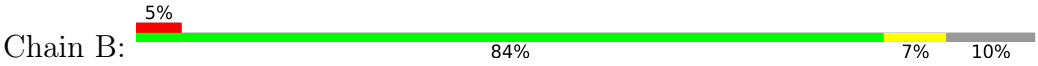


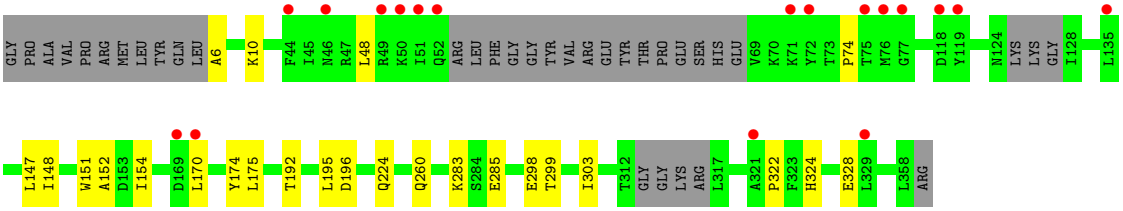
• Molecule 2: Phospho-N-acetylmuramoyl-pentapeptide-transferase



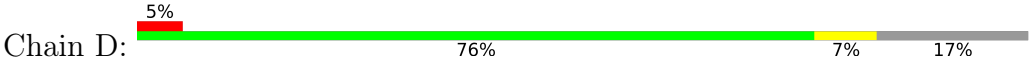


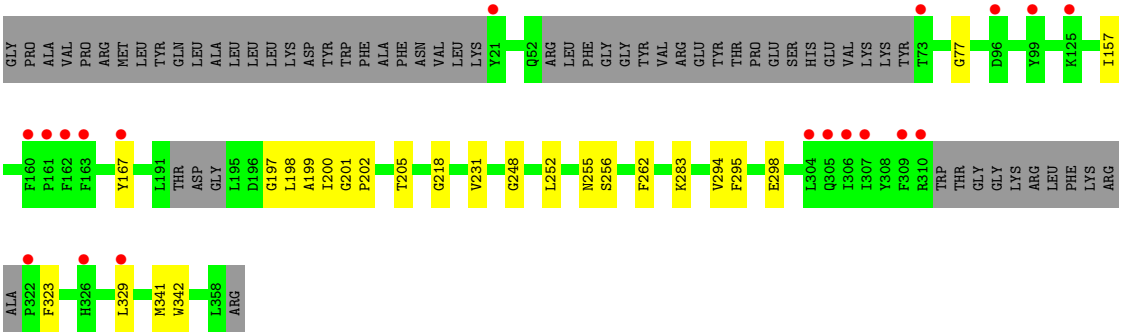
• Molecule 2: Phospho-N-acetylmuramoyl-pentapeptide-transferase





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





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	93.76Å 128.07Å 129.52Å 90.00° 110.82° 90.00°	Depositor
Resolution (Å)	87.64 – 3.62 87.97 – 3.62	Depositor EDS
% Data completeness (in resolution range)	100.0 (87.64-3.62) 92.8 (87.97-3.62)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.61 (at 3.58Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, R_{free}	0.277 , 0.301 0.279 , 0.303	Depositor DCC
R_{free} test set	1420 reflections (4.33%)	wwPDB-VP
Wilson B-factor (Å^2)	96.0	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 62.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.79	EDS
Total number of atoms	25385	wwPDB-VP
Average B, all atoms (Å^2)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NKM

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	0.27	0/941	0.46	0/1280
1	F	0.27	0/904	0.46	0/1233
1	G	0.28	0/941	0.47	0/1280
1	H	0.26	0/918	0.46	0/1250
2	A	0.29	0/2453	0.40	0/3354
2	B	0.35	0/2449	0.46	0/3361
2	C	0.35	0/2316	0.46	0/3171
2	D	0.35	0/2285	0.43	0/3126
All	All	0.32	0/13207	0.45	0/18055

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

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	923	858	858	18	0
1	F	886	780	780	5	0
1	G	923	857	859	3	0
1	H	900	834	834	0	0
2	A	2389	2425	2423	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2390	2268	2267	26	0
2	C	2263	2227	2224	31	0
2	D	2230	2162	2160	26	0
3	A	40	30	0	2	0
All	All	12944	12441	12405	115	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 5.

All (115) 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:198:LEU:O	2:D:202:PRO:CD	2.15	0.94
1:E:34:MET:HG3	1:E:78:VAL:HG21	1.55	0.86
2:D:198:LEU:O	2:D:202:PRO:HD3	1.76	0.85
2:B:192:THR:HG23	2:B:298:GLU:OE2	1.55	0.85
2:C:256:SER:O	2:C:258:PRO:O	1.94	0.84
2:D:294:VAL:HG13	2:D:341:MET:CE	2.10	0.81
2:D:198:LEU:O	2:D:202:PRO:HD2	1.82	0.78
2:D:157:ILE:O	2:D:283:LYS:NZ	2.17	0.77
1:E:87:PRO:CG	2:C:309:PHE:CZ	2.69	0.76
1:E:87:PRO:HG2	2:C:309:PHE:CZ	2.22	0.73
2:B:147:LEU:O	2:B:151:TRP:CB	2.41	0.69
2:B:175:LEU:C	2:B:175:LEU:HD23	2.14	0.68
2:C:102:VAL:HG11	2:C:148:ILE:HG23	1.75	0.68
2:B:322:PRO:CG	2:B:324:HIS:CE1	2.77	0.67
2:B:147:LEU:O	2:B:151:TRP:HB3	1.95	0.65
2:A:98:LYS:HD3	2:A:152:ALA:HB2	1.78	0.64
1:E:29:PHE:HZ	1:E:78:VAL:HG23	1.64	0.62
1:E:87:PRO:HG2	2:C:309:PHE:CE2	2.34	0.61
2:B:322:PRO:HB2	2:B:324:HIS:CE1	2.35	0.61
2:D:294:VAL:HG13	2:D:341:MET:HE2	1.84	0.60
2:A:292:ALA:O	2:A:296:VAL:HG23	2.00	0.60
1:E:34:MET:CG	1:E:78:VAL:HG21	2.30	0.59
2:C:202:PRO:HG2	2:C:295:PHE:CZ	2.37	0.59
2:D:199:ALA:O	2:D:202:PRO:HD2	2.03	0.58
2:D:202:PRO:HB2	2:D:295:PHE:CZ	2.38	0.58
2:A:97:ILE:CG2	2:A:99:TYR:HD2	2.16	0.58
1:E:118:GLN:OE1	1:E:118:GLN:N	2.36	0.57
2:A:304:LEU:C	2:A:304:LEU:HD23	2.26	0.55
2:D:200:ILE:HD11	2:D:248:GLY:HA3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:252:LEU:HD21	2:D:342:TRP:CH2	2.41	0.55
2:C:48:LEU:HB2	2:C:74:PRO:HG3	1.88	0.55
2:D:200:ILE:HD11	2:D:248:GLY:CA	2.36	0.55
2:B:322:PRO:CB	2:B:324:HIS:CE1	2.90	0.55
2:C:251:PHE:CE2	2:C:255:ASN:ND2	2.75	0.54
2:C:251:PHE:CZ	2:C:255:ASN:ND2	2.76	0.54
2:B:299:THR:O	2:B:303:ILE:HG13	2.09	0.52
2:D:294:VAL:CG1	2:D:341:MET:CE	2.87	0.52
2:B:170:LEU:HB2	2:B:174:TYR:HB2	1.92	0.52
1:E:87:PRO:CG	2:C:309:PHE:HZ	2.18	0.52
2:D:197:GLY:HA2	2:D:255:ASN:OD1	2.10	0.52
2:C:48:LEU:HB3	2:C:74:PRO:CB	2.40	0.52
2:D:298:GLU:OE1	2:D:323:PHE:HB3	2.11	0.51
2:C:102:VAL:HG11	2:C:148:ILE:CG2	2.41	0.50
1:F:112:GLU:O	2:B:224:GLN:NE2	2.38	0.49
2:C:283:LYS:HA	2:C:283:LYS:HE2	1.94	0.49
2:B:192:THR:HG22	2:B:192:THR:O	2.12	0.49
2:B:285:GLU:OE1	2:B:285:GLU:N	2.36	0.49
1:F:66:ARG:NH2	1:F:89:ASP:OD1	2.46	0.49
2:B:147:LEU:O	2:B:151:TRP:HB2	2.12	0.49
2:C:48:LEU:HB3	2:C:74:PRO:HB2	1.95	0.49
2:B:174:TYR:CD2	2:B:174:TYR:C	2.85	0.49
2:C:250:GLY:O	2:C:253:TRP:HB3	2.13	0.48
2:D:199:ALA:C	2:D:202:PRO:HD2	2.32	0.48
2:B:154:ILE:HG23	2:B:283:LYS:HD3	1.95	0.48
2:C:323:PHE:C	2:C:323:PHE:CD2	2.87	0.48
2:A:97:ILE:CG2	2:A:99:TYR:CD2	2.96	0.48
1:G:114:ASN:HB2	2:C:224:GLN:OE1	2.14	0.48
2:A:100:THR:O	2:A:103:VAL:HG12	2.14	0.47
2:B:6:ALA:HB3	2:B:10:LYS:CB	2.45	0.47
1:F:90:THR:HG23	1:F:123:THR:HA	1.96	0.46
2:D:294:VAL:HG13	2:D:341:MET:HE3	1.97	0.46
1:E:29:PHE:CZ	1:E:78:VAL:HG23	2.47	0.46
2:C:98:LYS:HE3	2:C:152:ALA:HA	1.98	0.46
2:C:120:VAL:O	2:C:124:ASN:N	2.48	0.46
2:D:201:GLY:O	2:D:205:THR:HG23	2.15	0.46
2:A:263:MET:O	3:A:401:NKM:O30	2.33	0.46
1:G:102:VAL:HB	1:G:105:TYR:HB2	1.97	0.45
2:B:148:ILE:O	2:B:152:ALA:N	2.36	0.45
2:D:198:LEU:HD21	2:D:341:MET:HG3	1.98	0.45
2:C:298:GLU:HA	2:C:301:SER:OG	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:322:PRO:HG2	2:B:324:HIS:CE1	2.50	0.45
2:A:336:LYS:HZ3	2:B:260:GLN:HG3	1.81	0.45
1:E:87:PRO:CG	2:C:309:PHE:CE2	2.99	0.45
2:C:48:LEU:HB2	2:C:74:PRO:CG	2.47	0.45
2:C:300:ILE:HA	2:C:303:ILE:HG22	1.98	0.45
1:E:101:ALA:O	2:A:155:ASP:N	2.38	0.45
2:A:25:ARG:NH1	2:A:92:LEU:O	2.50	0.45
2:D:157:ILE:HD11	2:D:167:TYR:CD2	2.51	0.44
2:B:48:LEU:HD23	2:B:74:PRO:HB2	1.99	0.44
1:E:29:PHE:HZ	1:E:78:VAL:CG2	2.30	0.44
2:D:198:LEU:CD2	2:D:341:MET:HG3	2.47	0.44
1:F:47:PHE:O	1:F:60:ALA:HB2	2.18	0.43
2:B:175:LEU:C	2:B:175:LEU:CD2	2.85	0.43
2:C:298:GLU:O	2:C:301:SER:OG	2.34	0.43
1:E:53:ARG:NH1	2:A:155:ASP:OD1	2.46	0.43
2:B:195:LEU:HD13	2:B:324:HIS:CD2	2.53	0.43
2:C:96:ASP:OD1	2:C:96:ASP:N	2.47	0.43
2:B:170:LEU:CB	2:B:174:TYR:HB2	2.49	0.43
1:E:52:SER:O	1:E:71:ARG:NH1	2.51	0.43
1:F:12:VAL:O	1:F:124:VAL:HA	2.19	0.43
2:A:42:PRO:HA	2:A:45:ILE:HG22	1.99	0.43
2:A:199:ALA:HB3	2:A:263:MET:HE1	2.01	0.43
2:B:328:GLU:HA	2:B:328:GLU:OE1	2.19	0.43
1:E:71:ARG:HB3	1:E:78:VAL:HG22	2.01	0.42
2:D:218:GLY:HA2	2:D:231:VAL:O	2.20	0.42
2:A:198:LEU:HA	2:A:338:VAL:HG13	2.02	0.42
1:G:37:PHE:HZ	1:G:113:TYR:CE2	2.36	0.42
1:E:87:PRO:HG3	2:C:309:PHE:CZ	2.53	0.42
2:A:257:PHE:CD2	2:A:335:PRO:HG3	2.55	0.42
1:E:71:ARG:CB	1:E:78:VAL:HG22	2.49	0.41
2:B:196:ASP:N	2:B:196:ASP:OD1	2.53	0.41
2:D:77:GLY:N	2:D:262:PHE:O	2.53	0.41
2:A:196:ASP:HA	3:A:401:NKM:O36	2.21	0.41
2:C:38:LEU:HD12	2:C:254:PHE:CE2	2.56	0.41
2:A:155:ASP:O	2:A:283:LYS:NZ	2.41	0.41
2:A:174:TYR:OH	2:A:285:GLU:OE2	2.37	0.41
2:C:100:THR:O	2:C:103:VAL:HG12	2.20	0.41
2:C:202:PRO:HB2	2:C:295:PHE:CE2	2.56	0.41
2:C:336:LYS:NZ	2:D:256:SER:O	2.54	0.41
2:D:294:VAL:CG1	2:D:341:MET:HE2	2.49	0.41
2:C:192:THR:HG22	2:C:192:THR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:32:TYR:HB3	1:E:97:ALA:HB1	2.01	0.40
2:D:198:LEU:HD21	2:D:341:MET:CG	2.51	0.40
2:D:329:LEU:C	2:D:329:LEU:HD13	2.41	0.40
2:B:322:PRO:HG2	2:B:324:HIS:NE2	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	122/137 (89%)	119 (98%)	3 (2%)	0	100	100
1	F	122/137 (89%)	121 (99%)	1 (1%)	0	100	100
1	G	123/137 (90%)	121 (98%)	2 (2%)	0	100	100
1	H	121/137 (88%)	119 (98%)	2 (2%)	0	100	100
2	A	307/365 (84%)	299 (97%)	8 (3%)	0	100	100
2	B	322/365 (88%)	314 (98%)	8 (2%)	0	100	100
2	C	298/365 (82%)	291 (98%)	7 (2%)	0	100	100
2	D	296/365 (81%)	289 (98%)	7 (2%)	0	100	100
All	All	1711/2008 (85%)	1673 (98%)	38 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	91/110 (83%)	91 (100%)	0	100	100
1	F	81/110 (74%)	81 (100%)	0	100	100
1	G	91/110 (83%)	91 (100%)	0	100	100
1	H	87/110 (79%)	87 (100%)	0	100	100
2	A	246/309 (80%)	246 (100%)	0	100	100
2	B	223/309 (72%)	223 (100%)	0	100	100
2	C	223/309 (72%)	223 (100%)	0	100	100
2	D	214/309 (69%)	214 (100%)	0	100	100
All	All	1256/1676 (75%)	1256 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	NKM	A	401	-	43,43,43	3.17	14 (32%)	50,62,62	1.87	12 (24%)

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	NKM	A	401	-	-	4/26/70/70	1/4/4/4

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	NKM	C22-C28	-9.81	1.40	1.52
3	A	401	NKM	C15-C16	-8.35	1.39	1.50
3	A	401	NKM	O18-C13	-6.85	1.30	1.44
3	A	401	NKM	O06-C05	-6.13	1.27	1.42
3	A	401	NKM	C26-N27	-5.83	1.34	1.46
3	A	401	NKM	C09-N11	5.66	1.47	1.32
3	A	401	NKM	C05-N32	-5.03	1.33	1.47
3	A	401	NKM	C16-C17	4.43	1.40	1.33
3	A	401	NKM	C17-C19	-4.00	1.40	1.47
3	A	401	NKM	O36-C35	-2.82	1.19	1.24
3	A	401	NKM	O40-C04	2.75	1.49	1.43
3	A	401	NKM	O39-C38	-2.30	1.18	1.23
3	A	401	NKM	C35-N37	-2.28	1.34	1.38
3	A	401	NKM	C38-N32	-2.14	1.35	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	401	NKM	C35-N37-C38	-4.93	120.08	126.58
3	A	401	NKM	O18-C17-C16	-4.68	119.15	124.61
3	A	401	NKM	N37-C38-N32	4.32	120.63	114.89
3	A	401	NKM	O36-C35-C34	-3.30	119.36	125.16
3	A	401	NKM	C15-C16-C17	-3.07	116.40	121.60
3	A	401	NKM	C34-C35-N37	3.04	119.38	114.84
3	A	401	NKM	C26-N27-C28	-2.99	121.55	127.17
3	A	401	NKM	O29-C28-N27	-2.78	118.85	122.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	401	NKM	C14-C15-C16	-2.59	107.29	111.84
3	A	401	NKM	C17-C19-N21	2.25	119.68	115.69
3	A	401	NKM	C08-C09-N11	2.04	120.07	116.73
3	A	401	NKM	C03-C04-C05	2.02	104.36	99.89

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	NKM	C23-C22-N21-C19
3	A	401	NKM	O12-C08-C09-O10
3	A	401	NKM	C09-C08-O12-C13
3	A	401	NKM	C28-C22-N21-C19

All (1) ring outliers are listed below:

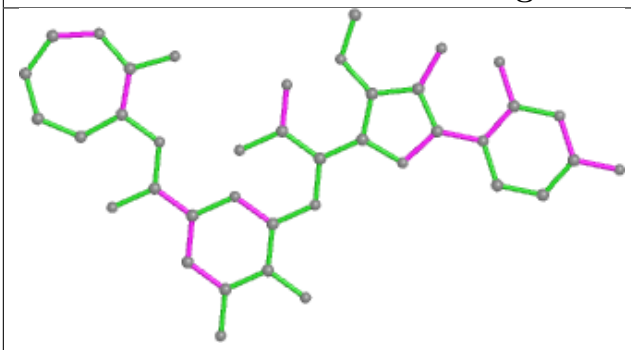
Mol	Chain	Res	Type	Atoms
3	A	401	NKM	C22-C23-C24-C25-C26-C28-N27

1 monomer is involved in 2 short contacts:

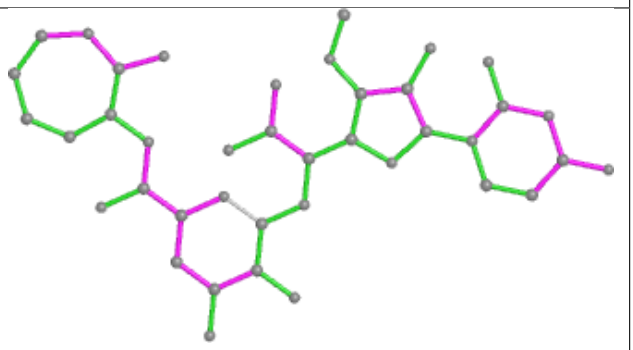
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	NKM	2	0

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 then 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.

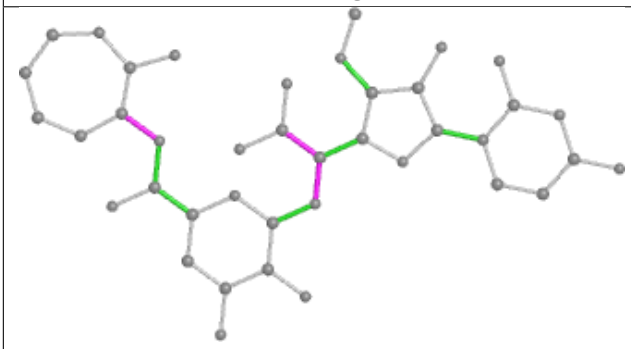
Ligand NKM A 401



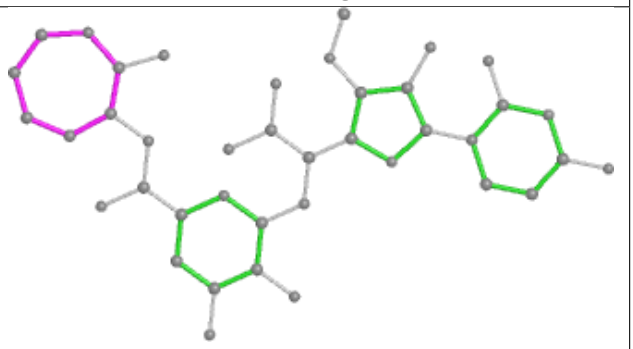
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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%)	0.55	19 (15%)	2	1	76, 95, 124, 147	0
1	F	124/137 (90%)	1.33	33 (26%)	0	0	86, 109, 133, 161	0
1	G	125/137 (91%)	0.50	15 (12%)	4	3	80, 95, 123, 134	0
1	H	123/137 (89%)	1.46	37 (30%)	0	0	93, 114, 140, 152	0
2	A	313/365 (85%)	0.08	18 (5%)	23	14	62, 87, 122, 141	0
2	B	330/365 (90%)	0.15	18 (5%)	25	15	69, 120, 152, 181	0
2	C	306/365 (83%)	0.17	18 (5%)	22	13	75, 110, 151, 176	0
2	D	304/365 (83%)	-0.03	19 (6%)	20	12	76, 116, 150, 164	0
All	All	1749/2008 (87%)	0.34	177 (10%)	7	4	62, 107, 146, 181	0

All (177) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	26	GLY	7.0
1	H	10	GLY	7.0
1	H	17	SER	6.9
1	E	44	GLU	6.8
2	C	325	HIS	6.7
2	C	130	ILE	6.7
2	D	162	PHE	6.7
2	B	51	ILE	6.4
1	H	16	GLY	6.4
1	G	1	ASP	6.0
1	H	85	LEU	6.0
1	F	83	THR	5.9
1	F	17	SER	5.8
2	B	50	LYS	5.8
1	F	27	ARG	5.6
2	D	163	PHE	5.4

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Mol	Chain	Res	Type	RSRZ
1	H	11	LEU	5.4
1	H	9	GLY	5.3
1	H	81	GLN	5.3
1	F	25	SER	5.3
1	H	123	THR	5.3
2	C	329	LEU	5.2
1	E	42	GLY	5.2
2	C	324	HIS	5.2
2	A	72	TYR	5.1
1	H	84	SER	5.0
1	H	83	THR	5.0
1	H	18	LEU	4.9
1	H	19	THR	4.9
1	F	85	LEU	4.9
1	E	90	THR	4.8
2	D	160	PHE	4.6
1	F	24	THR	4.6
1	H	125	SER	4.5
1	F	28	SER	4.5
1	H	111	ASN	4.4
2	C	309	PHE	4.4
1	F	84	SER	4.4
1	E	41	PRO	4.3
2	D	161	PRO	4.3
2	A	99	TYR	4.3
2	B	77	GLY	4.3
2	B	52	GLN	4.2
2	D	73	THR	4.2
2	C	328	GLU	4.2
1	E	40	ALA	4.1
1	G	74	ALA	4.1
1	F	66	ARG	4.1
1	F	16	GLY	4.0
1	H	82	MET	4.0
1	F	125	SER	3.9
2	C	225	TYR	3.9
1	F	2	VAL	3.8
1	H	55	GLY	3.8
2	C	326	HIS	3.8
2	D	309	PHE	3.8
2	C	165	GLU	3.7
1	H	66	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	H	15	GLY	3.7
1	F	68	THR	3.6
2	C	327	LEU	3.5
2	B	329	LEU	3.5
1	F	82	MET	3.4
2	B	76	MET	3.4
2	A	329	LEU	3.4
1	F	81	GLN	3.4
1	E	14	THR	3.4
1	H	57	THR	3.4
1	G	79	TYR	3.4
1	F	15	GLY	3.4
2	A	97	ILE	3.4
1	F	118	GLN	3.4
1	F	29	PHE	3.3
1	G	75	ALA	3.3
2	C	163	PHE	3.3
1	F	64	LYS	3.2
2	D	322	PRO	3.2
2	B	46	ASN	3.2
1	E	43	LYS	3.1
1	H	112	GLU	3.1
2	C	129	SER	3.1
1	F	73	ASN	3.1
2	A	126	LYS	3.1
1	H	109	GLN	3.1
2	C	222	ILE	3.0
1	E	45	ARG	3.0
2	A	233	TYR	3.0
1	F	31	LEU	2.9
2	B	170	LEU	2.9
2	A	98	LYS	2.9
1	E	65	GLY	2.9
1	H	110	ALA	2.9
1	E	46	GLU	2.9
1	G	39	GLN	2.9
2	B	71	LYS	2.9
2	D	305	GLN	2.8
1	G	72	ASP	2.8
2	D	21	TYR	2.8
1	H	68	THR	2.8
1	E	125	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	80	LEU	2.8
1	H	12	VAL	2.8
1	G	2	VAL	2.7
2	D	304	LEU	2.7
1	H	25	SER	2.7
1	E	89	ASP	2.7
1	G	81	GLN	2.7
1	H	20	LEU	2.6
2	D	326	HIS	2.6
1	F	89	ASP	2.6
1	H	70	SER	2.6
2	A	125	LYS	2.6
1	G	116	TRP	2.6
2	C	166	LEU	2.6
2	B	135	LEU	2.6
1	E	13	GLN	2.6
1	H	56	ASN	2.6
1	H	24	THR	2.6
1	G	76	ASN	2.6
2	A	51	ILE	2.6
1	H	124	VAL	2.6
1	G	45	ARG	2.5
1	E	87	PRO	2.5
2	C	323	PHE	2.5
2	D	310	ARG	2.5
2	B	169	ASP	2.5
2	D	306	ILE	2.5
2	A	74	PRO	2.5
2	B	75	THR	2.5
2	B	44	PHE	2.5
1	H	8	GLY	2.4
1	H	122	VAL	2.4
1	E	64	LYS	2.4
2	C	124	ASN	2.4
2	D	125	LYS	2.4
1	G	77	THR	2.4
1	F	101	ALA	2.4
1	F	30	SER	2.4
2	A	221	LYS	2.4
1	G	73	ASN	2.4
2	D	307	ILE	2.4
1	F	18	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	76	ASN	2.4
2	A	71	LYS	2.4
1	E	88	GLU	2.4
1	H	120	THR	2.4
2	D	167	TYR	2.4
2	B	72	TYR	2.3
1	F	117	GLY	2.3
2	C	137	GLN	2.3
2	B	119	TYR	2.3
1	H	26	GLY	2.3
1	H	108	GLN	2.3
2	C	330	ASN	2.2
1	F	79	TYR	2.2
2	D	96	ASP	2.2
2	A	75	THR	2.2
2	D	329	LEU	2.2
2	A	73	THR	2.2
2	B	49	ARG	2.2
2	B	321	ALA	2.2
2	D	99	TYR	2.1
1	H	79	TYR	2.1
1	E	39	GLN	2.1
1	F	67	PHE	2.1
2	A	96	ASP	2.1
2	A	122	LEU	2.1
2	B	118	ASP	2.1
1	G	118	GLN	2.1
1	G	80	LEU	2.1
1	F	75	ALA	2.1
1	E	63	VAL	2.1
1	E	62	ALA	2.0
2	A	215	TYR	2.0
1	F	20	LEU	2.0
1	F	71	ARG	2.0
2	A	70	LYS	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)

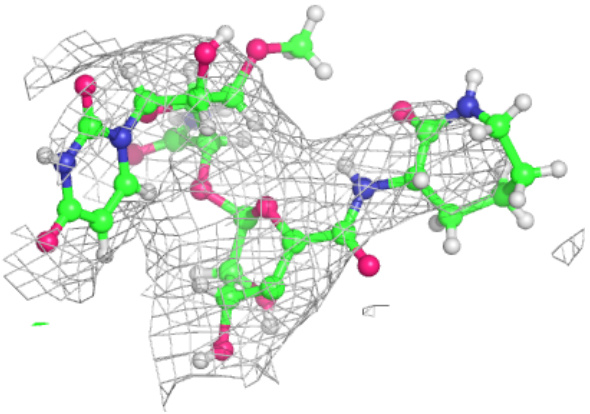
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

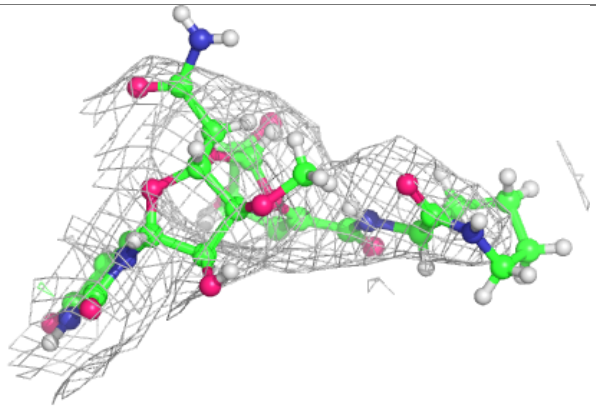
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NKM	A	401	40/40	0.86	0.39	120,139,181,186	0

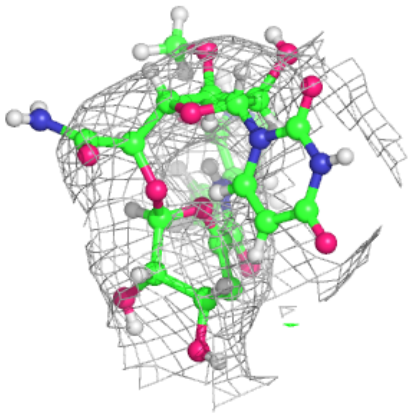
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NKM 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)







6.5 Other polymers (i)

There are no such residues in this entry.