



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 06:23 PM UTC

PDB ID : 6OYZ / pdb_00006oyz
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 ⓘ symbol.

The types of validation reports are described at

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

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

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

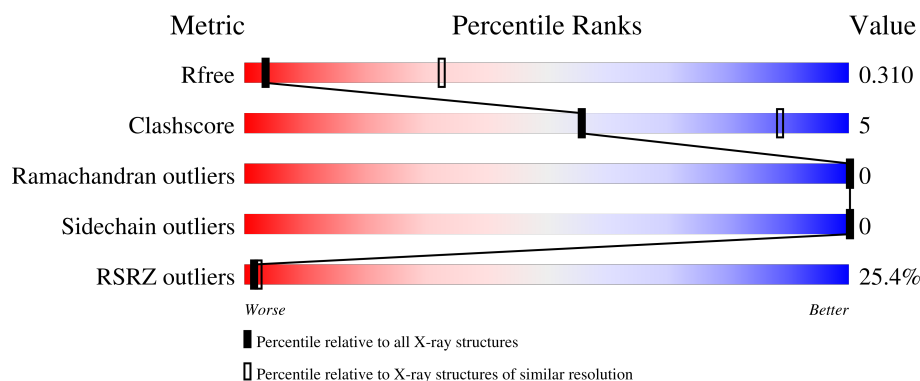
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1062 (3.72-3.52)
Clashscore	190562	1092 (3.72-3.52)
Ramachandran outliers	187476	1057 (3.72-3.52)
Sidechain outliers	187428	1055 (3.72-3.52)
RSRZ outliers	180081	1060 (3.72-3.52)

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	E	137	32% 81% 9% 9%
1	F	137	24% 84% 7% 9%
1	G	137	18% 88% • 9%
1	H	137	20% 90% 10%
2	A	365	18% 79% 7% 14%

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Mol	Chain	Length	Quality of chain
2	B	365	33% 83% 7% 10%
2	C	365	12% 75% 8% 16%
2	D	365	24% 76% 7% 17%

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:

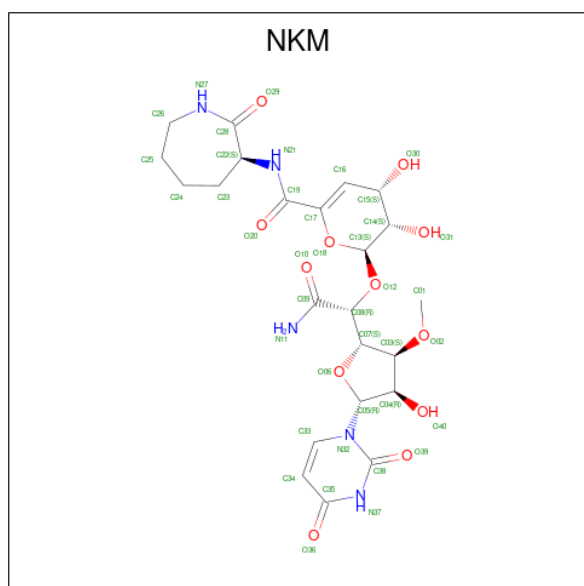
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP O66465
A	-4	PRO	-	expression tag	UNP O66465
A	-3	ALA	-	expression tag	UNP O66465
A	-2	VAL	-	expression tag	UNP O66465
A	-1	PRO	-	expression tag	UNP O66465
A	0	ARG	-	expression tag	UNP O66465
C	-5	GLY	-	expression tag	UNP O66465
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 (CCD ID: NKM) (formula: C₂₃H₃₁N₅O₁₂).

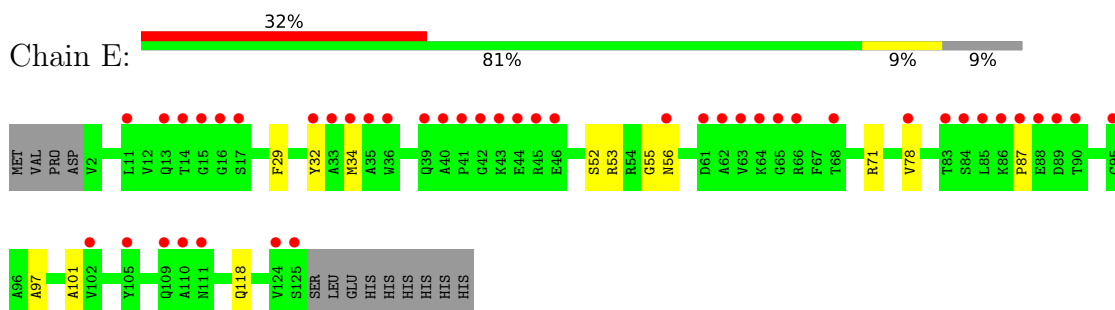


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			70	23	30	5	12		

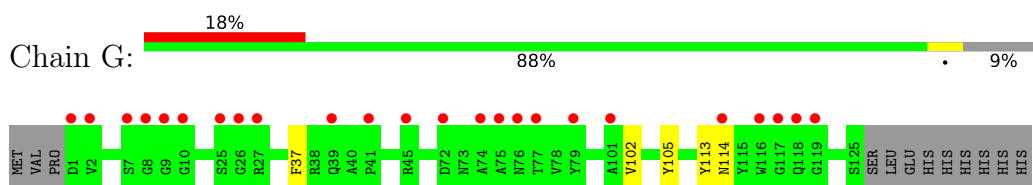
3 Residue-property plots [i](#)

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.

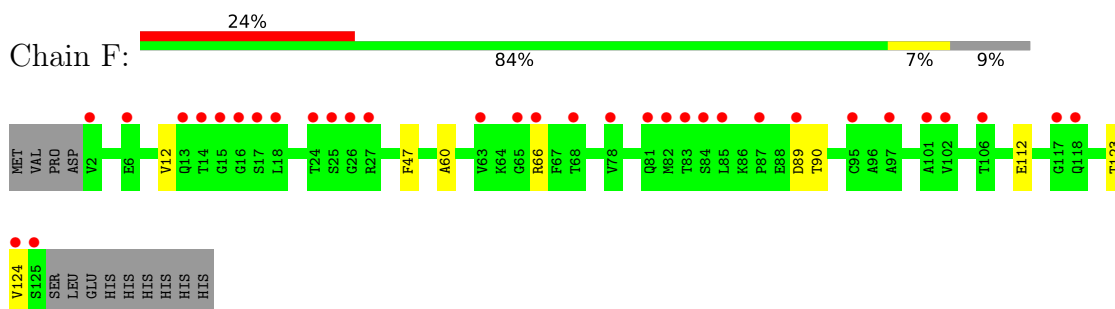
- Molecule 1: MraYAA nanobody



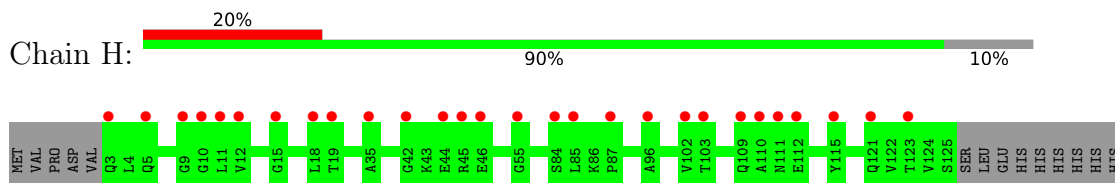
- Molecule 1: MraYAA nanobody



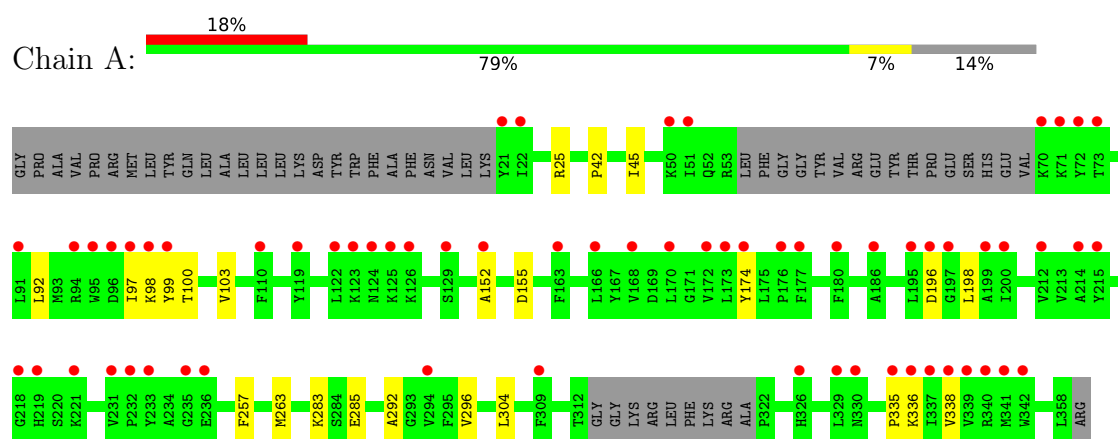
- Molecule 1: MraYAA nanobody



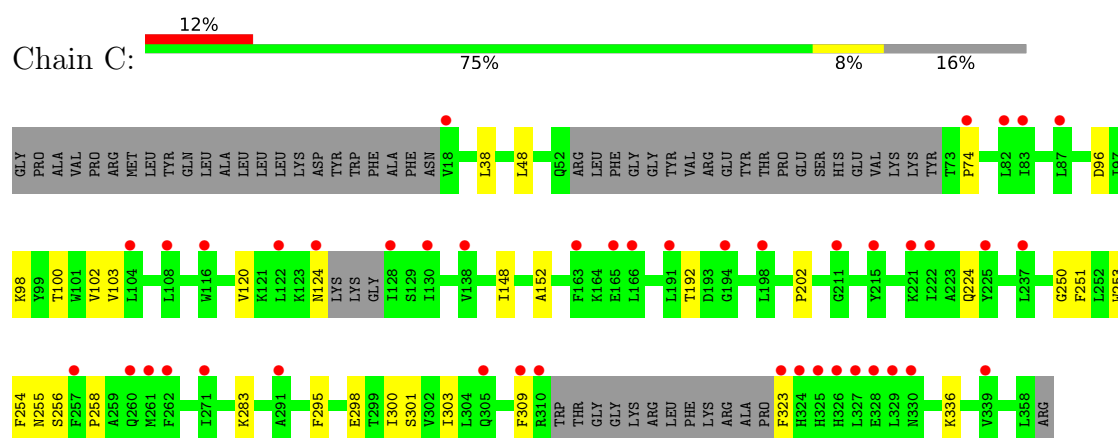
- Molecule 1: MraYAA nanobody



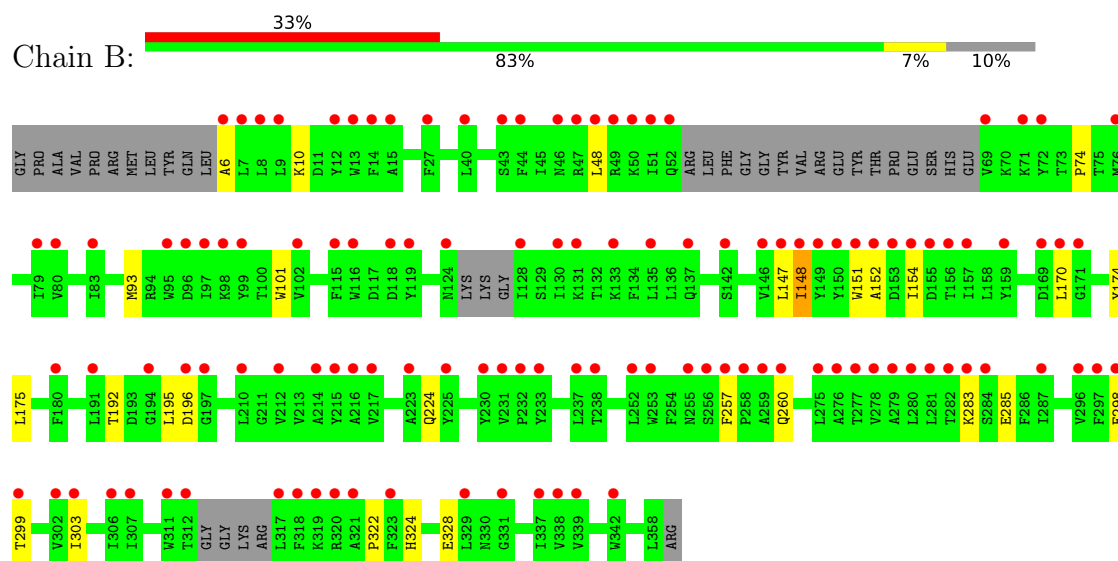
- Molecule 2: Phospho-N-acetylmuramoyl-pentapeptide-transferase



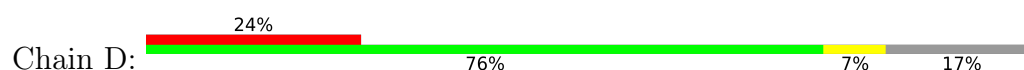
• Molecule 2: Phospho-N-acetylmuramoyl-pentapeptide-transferase

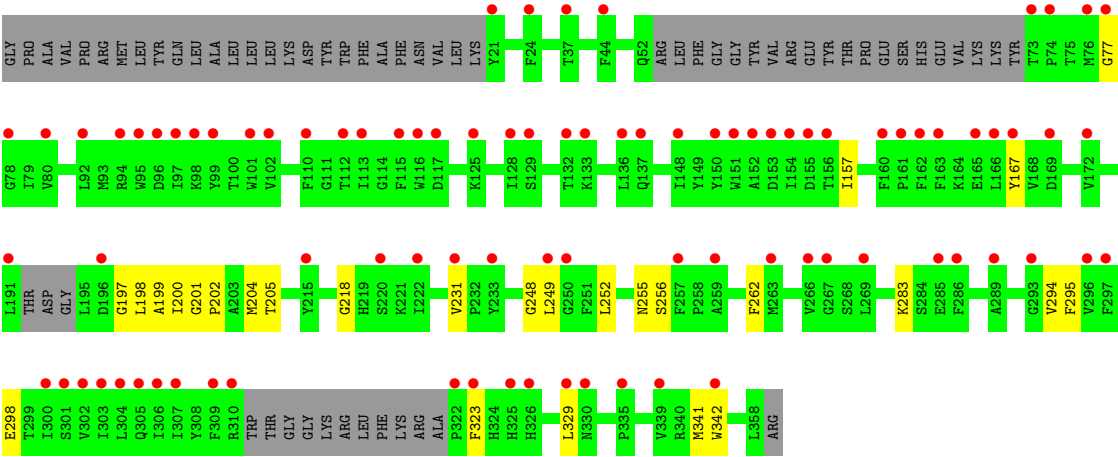


• Molecule 2: Phospho-N-acetylmuramoyl-pentapeptide-transferase



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





4 Data and refinement statistics

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 87.64 – 3.62	Depositor EDS
% Data completeness (in resolution range)	100.0 (87.64-3.62) 92.8 (87.64-3.62)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.61 (at 3.58Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, R_{free}	0.277 , 0.301 0.286 , 0.310	Depositor DCC
R_{free} test set	1420 reflections (2.15%)	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)	0.29 , 65.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.80	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.*

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: 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	0.12	0/941	0.25	0/1280
1	F	0.15	0/904	0.27	0/1233
1	G	0.21	0/941	0.36	0/1280
1	H	0.11	0/918	0.28	0/1250
2	A	0.26	0/2453	0.47	0/3354
2	B	0.41	0/2449	0.72	2/3361 (0.1%)
2	C	0.42	0/2316	0.68	0/3171
2	D	0.40	0/2285	0.68	0/3126
All	All	0.33	0/13207	0.57	2/18055 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	148	ILE	CA-C-N	5.56	130.01	120.72
2	B	148	ILE	C-N-CA	5.56	130.01	120.72

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	923	858	858	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	886	780	780	5	0
1	G	923	857	859	4	0
1	H	900	834	834	0	0
2	A	2389	2425	2423	18	0
2	B	2390	2268	2267	28	0
2	C	2263	2227	2224	32	0
2	D	2230	2162	2160	27	0
3	A	40	30	0	2	0
All	All	12944	12441	12405	120	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 (120) 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: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
2:B:192:THR:HG23	2:B:298:GLU:OE2	1.55	0.76
2:B:175:LEU:C	2:B:175:LEU:HD23	2.14	0.73
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: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:A:304:LEU:C	2:A:304:LEU:HD23	2.26	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:294:VAL:HG13	2:D:341:MET:HE2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:200:ILE:HD11	2:D:248:GLY:HA3	1.88	0.55
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:D:199:ALA:C	2:D:202:PRO:HD2	2.32	0.53
2:B:174:TYR:CD2	2:B:174:TYR:C	2.85	0.53
2:C:323:PHE:C	2:C:323:PHE:CD2	2.87	0.52
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
2:B:175:LEU:C	2:B:175:LEU:CD2	2.85	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:C:250:GLY:O	2:C:253:TRP:HB3	2.13	0.48
2:D:294:VAL:HG13	2:D:341:MET:HE3	1.94	0.48
2:B:154:ILE:HG23	2:B:283:LYS:HD3	1.95	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:B:93:MET:HE1	2:B:101:TRP:CE2	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:322:PRO:HG2	2:B:324:HIS:CE1	2.50	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
2:D:329:LEU:C	2:D:329:LEU:HD13	2.41	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:A:336:LYS:HZ3	2:B:260:GLN:HG3	1.82	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: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: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
2:D:294:VAL:CG1	2:D:341:MET:HE3	2.50	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:257:PHE:CD2	2:A:257:PHE:C	2.98	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:204:MET:HE1	2:D:249:LEU:CD2	2.50	0.41
1:G:114:ASN:HB2	2:C:224:GLN:CD	2.46	0.41
2:C:192:THR:HG22	2:C:192:THR:O	2.20	0.41
1:E:32:TYR:HB3	1:E:97:ALA:HB1	2.01	0.40
1:E:55:GLY:O	1:E:56:ASN:C	2.65	0.40
2:B:257:PHE:CD2	2:B:257:PHE:C	3.00	0.40
2:D:198:LEU:HD21	2:D:341:MET:CG	2.51	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 ⓘ

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%)	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 ⓘ

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. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	73	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 [i](#)

There are no oligosaccharides 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	3.18	15 (34%)	52,62,62	1.90	12 (23%)

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 (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	NKM	C22-C28	-9.75	1.40	1.52
3	A	401	NKM	C15-C16	-8.56	1.39	1.50
3	A	401	NKM	O18-C13	-6.66	1.30	1.44
3	A	401	NKM	O06-C05	-6.29	1.27	1.42
3	A	401	NKM	C09-N11	6.07	1.47	1.32
3	A	401	NKM	C26-N27	-5.81	1.34	1.46
3	A	401	NKM	C05-N32	-5.10	1.33	1.47
3	A	401	NKM	C16-C17	3.90	1.40	1.33
3	A	401	NKM	C17-C19	-3.63	1.40	1.47
3	A	401	NKM	O36-C35	-2.81	1.19	1.24
3	A	401	NKM	O40-C04	2.62	1.49	1.43
3	A	401	NKM	C35-N37	-2.42	1.34	1.38
3	A	401	NKM	O39-C38	-2.39	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	NKM	C38-N32	-2.21	1.35	1.38
3	A	401	NKM	O18-C17	-2.12	1.29	1.37

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	NKM	C35-N37-C38	-5.26	120.08	126.61
3	A	401	NKM	O18-C17-C16	-4.89	119.15	124.62
3	A	401	NKM	N37-C38-N32	4.41	120.63	114.89
3	A	401	NKM	O36-C35-C34	-3.36	119.36	125.16
3	A	401	NKM	C34-C35-N37	3.27	119.38	114.80
3	A	401	NKM	C15-C16-C17	-2.98	116.40	121.45
3	A	401	NKM	C26-N27-C28	-2.74	121.55	126.98
3	A	401	NKM	C14-C15-C16	-2.59	107.29	111.80
3	A	401	NKM	O29-C28-N27	-2.56	118.85	121.96
3	A	401	NKM	C08-C09-N11	2.45	120.07	116.64
3	A	401	NKM	C17-C19-N21	2.31	119.68	115.73
3	A	401	NKM	C03-C04-C05	2.03	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	C09-C08-O12-C13
3	A	401	NKM	O12-C08-C09-O10
3	A	401	NKM	C28-C22-N21-C19

All (1) ring outliers are listed below:

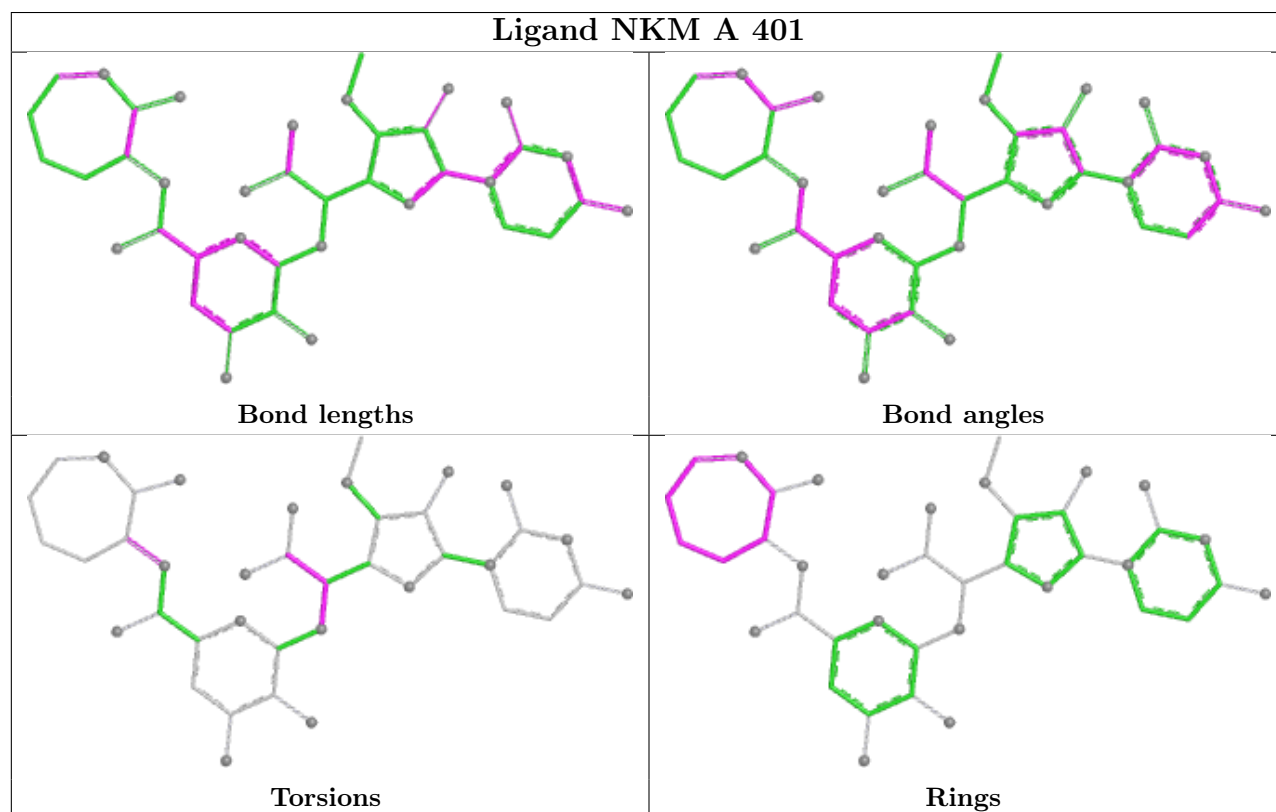
Mol	Chain	Res	Type	Atoms
3	A	401	NKM	C22-C23-C24-C25-C26-C28-N27

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	E	124/137 (90%)	2.05	44 (35%) 1 1	82, 103, 137, 158	0
1	F	124/137 (90%)	1.53	33 (26%) 1 2	94, 119, 146, 179	0
1	G	125/137 (91%)	1.03	24 (19%) 3 3	86, 104, 135, 145	0
1	H	123/137 (89%)	1.46	28 (22%) 2 2	100, 125, 152, 167	0
2	A	313/365 (85%)	1.13	64 (20%) 3 3	68, 96, 137, 153	0
2	B	330/365 (90%)	1.79	120 (36%) 1 1	74, 130, 165, 207	0
2	C	306/365 (83%)	0.97	43 (14%) 6 7	85, 119, 163, 190	0
2	D	304/365 (83%)	1.61	89 (29%) 1 1	84, 127, 163, 178	0
All	All	1749/2008 (87%)	1.42	445 (25%) 1 2	68, 118, 159, 207	0

All (445) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	51	ILE	18.6
2	D	162	PHE	14.8
2	D	163	PHE	12.9
2	D	96	ASP	12.0
2	B	119	TYR	11.0
1	G	1	ASP	10.7
2	B	50	LYS	10.6
1	E	44	GLU	10.6
1	F	17	SER	10.5
1	E	88	GLU	10.5
2	A	99	TYR	10.4
1	E	64	LYS	9.7
1	E	87	PRO	9.2
2	A	72	TYR	9.1
1	E	65	GLY	9.0
2	C	130	ILE	8.9

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Mol	Chain	Res	Type	RSRZ
1	G	74	ALA	8.7
1	H	111	ASN	8.7
2	C	325	HIS	8.7
2	B	72	TYR	8.6
2	A	97	ILE	8.5
2	D	160	PHE	8.5
2	D	73	THR	8.3
1	H	55	GLY	8.2
2	B	52	GLN	8.2
2	D	286	PHE	8.2
2	A	96	ASP	8.1
2	B	146	VAL	8.0
2	C	225	TYR	7.9
1	E	14	THR	7.9
2	D	94	ARG	7.8
2	A	126	LYS	7.8
2	C	324	HIS	7.4
2	B	99	TYR	7.3
1	F	16	GLY	7.3
1	F	83	THR	7.1
2	B	329	LEU	7.1
2	D	326	HIS	7.0
2	B	281	LEU	7.0
1	E	90	THR	6.9
1	F	26	GLY	6.9
1	F	15	GLY	6.9
2	D	306	ILE	6.9
1	E	109	GLN	6.9
2	A	233	TYR	6.9
2	D	233	TYR	6.8
1	E	111	ASN	6.8
1	H	10	GLY	6.6
2	D	161	PRO	6.5
2	B	282	THR	6.4
1	G	118	GLN	6.4
2	B	71	LYS	6.3
1	F	84	SER	6.2
2	A	51	ILE	6.2
2	A	94	ARG	6.2
2	D	99	TYR	6.1
2	A	173	LEU	6.1
2	C	222	ILE	6.1

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Mol	Chain	Res	Type	RSRZ
2	C	163	PHE	6.1
1	E	46	GLU	6.0
2	B	44	PHE	6.0
2	A	177	PHE	6.0
1	H	11	LEU	5.9
1	G	75	ALA	5.9
2	B	47	ARG	5.9
1	H	109	GLN	5.9
2	A	98	LYS	5.9
2	D	329	LEU	5.9
2	A	125	LYS	5.9
2	B	233	TYR	5.8
2	D	21	TYR	5.8
1	H	9	GLY	5.8
2	B	154	ILE	5.6
2	C	165	GLU	5.6
2	A	215	TYR	5.6
2	D	322	PRO	5.6
2	A	329	LEU	5.4
1	E	62	ALA	5.4
2	A	71	LYS	5.3
2	D	152	ALA	5.3
2	D	325	HIS	5.3
2	B	46	ASN	5.3
2	B	115	PHE	5.3
1	H	123	THR	5.3
1	E	83	THR	5.2
2	D	304	LEU	5.1
2	A	122	LEU	5.1
2	B	151	TRP	5.1
2	A	172	VAL	5.0
1	F	85	LEU	4.9
1	G	116	TRP	4.9
2	B	14	PHE	4.9
1	E	61	ASP	4.9
1	G	79	TYR	4.8
2	D	335	PRO	4.8
1	E	42	GLY	4.7
2	D	297	PHE	4.7
2	C	221	LYS	4.7
2	B	142	SER	4.7
2	D	98	LYS	4.6

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Mol	Chain	Res	Type	RSRZ
1	F	118	GLN	4.6
2	D	150	TYR	4.6
2	D	196	ASP	4.5
2	C	309	PHE	4.5
2	B	135	LEU	4.5
1	F	6	GLU	4.5
2	B	312	THR	4.4
2	B	216	ALA	4.4
2	B	150	TYR	4.4
1	F	25	SER	4.4
2	B	116	TRP	4.4
2	B	299	THR	4.3
1	E	15	GLY	4.3
1	F	101	ALA	4.3
2	C	327	LEU	4.3
2	D	309	PHE	4.3
1	F	27	ARG	4.2
2	D	302	VAL	4.2
2	B	15	ALA	4.2
1	E	41	PRO	4.1
2	D	266	VAL	4.1
2	B	149	TYR	4.1
2	D	155	ASP	4.1
2	A	197	GLY	4.0
2	D	293	GLY	4.0
1	H	15	GLY	4.0
2	D	330	ASN	4.0
2	B	69	VAL	4.0
2	D	97	ILE	4.0
2	A	123	LYS	4.0
1	E	85	LEU	4.0
2	D	257	PHE	4.0
2	C	18	VAL	3.9
2	D	222	ILE	3.9
2	D	169	ASP	3.9
2	B	232	PRO	3.9
1	G	119	GLY	3.9
2	D	156	THR	3.9
2	B	49	ARG	3.9
1	F	102	VAL	3.9
2	B	319	LYS	3.9
2	C	108	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
2	C	261	MET	3.9
2	C	323	PHE	3.8
2	A	339	VAL	3.8
2	C	191	LEU	3.8
2	D	128	ILE	3.7
2	B	256	SER	3.7
1	H	103	THR	3.7
2	B	277	THR	3.7
2	D	78	GLY	3.7
2	D	167	TYR	3.7
2	B	194	GLY	3.7
2	B	342	TRP	3.7
2	C	329	LEU	3.7
2	A	180	PHE	3.7
2	D	125	LYS	3.6
2	B	96	ASP	3.6
2	B	48	LEU	3.6
2	A	221	LYS	3.6
1	E	11	LEU	3.6
1	E	66	ARG	3.6
2	B	275	LEU	3.6
2	C	257	PHE	3.6
2	B	280	LEU	3.6
2	D	101	TRP	3.6
2	B	210	LEU	3.6
2	A	235	GLY	3.6
2	D	300	ILE	3.5
2	C	166	LEU	3.5
1	E	56	ASN	3.5
2	A	219	HIS	3.5
2	B	283	LYS	3.5
2	D	116	TRP	3.5
2	D	305	GLN	3.5
2	D	95	TRP	3.5
2	B	118	ASP	3.5
2	A	22	ILE	3.5
2	D	307	ILE	3.5
2	D	102	VAL	3.5
2	D	339	VAL	3.5
2	A	119	TYR	3.5
2	A	166	LEU	3.5
2	A	232	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	278	VAL	3.4
2	C	124	ASN	3.4
2	C	326	HIS	3.4
2	D	151	TRP	3.4
2	D	165	GLU	3.4
1	E	95	CYS	3.4
2	B	279	ALA	3.4
1	E	17	SER	3.4
2	B	7	LEU	3.3
2	B	196	ASP	3.3
2	B	152	ALA	3.3
1	F	82	MET	3.3
2	D	296	VAL	3.3
2	B	148	ILE	3.3
2	B	297	PHE	3.3
2	B	338	VAL	3.3
2	A	212	VAL	3.2
2	A	218	GLY	3.2
1	H	44	GLU	3.2
2	A	163	PHE	3.2
2	D	110	PHE	3.2
2	D	113	ILE	3.2
1	E	16	GLY	3.2
1	E	89	ASP	3.2
2	B	153	ASP	3.2
2	B	155	ASP	3.2
1	H	3	GLN	3.2
2	C	291	ALA	3.2
1	E	84	SER	3.2
2	C	339	VAL	3.2
1	G	9	GLY	3.2
2	D	310	ARG	3.2
1	E	40	ALA	3.2
2	C	271	ILE	3.2
2	D	153	ASP	3.1
2	D	259	ALA	3.1
2	C	82	LEU	3.1
2	C	194	GLY	3.1
2	D	215	TYR	3.1
2	C	104	LEU	3.1
1	G	45	ARG	3.1
1	E	124	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	H	84	SER	3.1
2	A	21	TYR	3.1
2	B	12	TYR	3.1
1	H	45	ARG	3.1
2	B	98	LYS	3.1
1	E	34	MET	3.1
1	E	125	SER	3.1
2	D	285	GLU	3.1
1	E	43	LYS	3.1
2	C	122	LEU	3.1
1	F	125	SER	3.0
2	B	9	LEU	3.0
2	D	166	LEU	3.0
2	B	284	SER	3.0
2	B	215	TYR	3.0
2	A	236	GLU	3.0
2	A	70	LYS	3.0
2	C	116	TRP	3.0
1	H	12	VAL	3.0
1	H	110	ALA	3.0
2	A	174	TYR	3.0
1	F	87	PRO	3.0
2	B	128	ILE	3.0
2	B	339	VAL	3.0
1	H	18	LEU	2.9
2	B	212	VAL	2.9
2	B	320	ARG	2.9
1	E	32	TYR	2.9
2	B	83	ILE	2.9
2	B	217	VAL	2.9
1	G	76	ASN	2.9
2	A	326	HIS	2.9
1	E	86	LYS	2.9
1	F	14	THR	2.9
2	A	309	PHE	2.9
2	B	124	ASN	2.9
2	B	302	VAL	2.9
2	B	259	ALA	2.9
1	G	25	SER	2.8
2	A	176	PRO	2.8
2	A	330	ASN	2.8
2	B	197	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
2	C	262	PHE	2.8
2	B	97	ILE	2.8
1	G	114	ASN	2.8
2	B	276	ALA	2.8
2	B	287	ILE	2.8
1	F	106	THR	2.8
2	A	231	VAL	2.8
2	A	335	PRO	2.8
2	D	80	VAL	2.8
1	G	26	GLY	2.7
1	H	5	GLN	2.7
1	E	68	THR	2.7
2	B	169	ASP	2.7
2	B	40	LEU	2.7
1	H	102	VAL	2.7
2	B	257	PHE	2.7
2	B	170	LEU	2.7
2	B	156	THR	2.7
2	B	306	ILE	2.7
2	B	43	SER	2.7
1	H	87	PRO	2.7
1	G	8	GLY	2.7
1	F	65	GLY	2.7
1	H	85	LEU	2.7
2	D	133	LYS	2.6
2	B	191	LEU	2.6
2	A	129	SER	2.6
2	A	168	VAL	2.6
2	A	338	VAL	2.6
1	H	42	GLY	2.6
1	G	39	GLN	2.6
1	F	13	GLN	2.6
2	A	195	LEU	2.6
2	B	237	LEU	2.6
1	G	27	ARG	2.6
2	B	6	ALA	2.6
2	A	200	ILE	2.6
2	B	255	ASN	2.6
2	D	74	PRO	2.6
1	F	68	THR	2.5
2	A	50	LYS	2.5
2	B	252	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	191	LEU	2.5
1	E	39	GLN	2.5
2	B	137	GLN	2.5
2	D	289	ALA	2.5
2	C	83	ILE	2.5
2	B	79	ILE	2.5
2	D	132	THR	2.5
1	H	46	GLU	2.5
2	D	172	VAL	2.5
1	F	95	CYS	2.5
2	D	323	PHE	2.5
1	G	41	PRO	2.5
2	D	154	ILE	2.5
2	D	267	GLY	2.5
1	E	36	TRP	2.5
2	B	130	ILE	2.5
1	G	77	THR	2.5
2	D	37	THR	2.5
2	D	220	SER	2.5
2	A	294	VAL	2.5
2	C	260	GLN	2.5
1	F	66	ARG	2.5
2	D	136	LEU	2.5
2	B	76	MET	2.5
2	C	328	GLU	2.4
2	C	128	ILE	2.4
1	F	18	LEU	2.4
1	G	72	ASP	2.4
1	H	19	THR	2.4
2	B	13	TRP	2.4
2	B	133	LYS	2.4
2	D	115	PHE	2.4
2	B	311	TRP	2.4
1	F	24	THR	2.4
2	B	307	ILE	2.4
2	D	303	ILE	2.4
2	A	91	LEU	2.4
1	G	7	SER	2.4
2	B	102	VAL	2.4
2	D	148	ILE	2.4
2	D	231	VAL	2.4
1	E	35	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	96	ALA	2.4
2	B	95	TRP	2.3
2	B	157	ILE	2.3
2	B	303	ILE	2.3
1	F	78	VAL	2.3
2	A	341	MET	2.3
1	F	117	GLY	2.3
2	C	215	TYR	2.3
2	B	321	ALA	2.3
1	G	117	GLY	2.3
2	A	340	ARG	2.3
2	A	170	LEU	2.3
2	C	87	LEU	2.3
2	D	301	SER	2.3
1	F	124	VAL	2.3
1	H	35	ALA	2.3
2	B	214	ALA	2.3
2	B	260	GLN	2.3
2	C	330	ASN	2.3
2	B	223	ALA	2.3
2	B	80	VAL	2.3
2	D	117	ASP	2.3
2	A	95	TRP	2.2
1	E	110	ALA	2.2
1	H	115	TYR	2.2
2	D	263	MET	2.2
2	A	196	ASP	2.2
2	B	253	TRP	2.2
1	G	2	VAL	2.2
2	B	258	PRO	2.2
2	B	337	ILE	2.2
1	E	63	VAL	2.2
2	D	112	THR	2.2
1	F	97	ALA	2.2
2	D	342	TRP	2.2
1	E	13	GLN	2.2
2	C	305	GLN	2.2
1	E	45	ARG	2.2
2	C	198	LEU	2.2
2	D	129	SER	2.2
2	B	159	TYR	2.2
1	F	63	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	331	GLY	2.2
2	D	269	LEU	2.2
2	D	250	GLY	2.2
2	B	323	PHE	2.2
1	F	89	ASP	2.1
2	B	230	TYR	2.1
1	G	10	GLY	2.1
2	B	180	PHE	2.1
2	A	199	ALA	2.1
1	E	102	VAL	2.1
2	A	342	TRP	2.1
2	B	231	VAL	2.1
2	B	225	TYR	2.1
2	C	74	PRO	2.1
2	B	171	GLY	2.1
2	D	76	MET	2.1
2	A	337	ILE	2.1
2	D	77	GLY	2.1
1	H	112	GLU	2.1
2	D	249	LEU	2.1
2	A	124	ASN	2.1
2	C	138	VAL	2.1
2	B	317	LEU	2.1
2	B	298	GLU	2.1
1	G	101	ALA	2.1
2	A	214	ALA	2.1
2	B	131	LYS	2.1
1	F	81	GLN	2.1
2	B	318	PHE	2.1
2	D	44	PHE	2.1
2	B	147	LEU	2.1
2	C	211	GLY	2.1
2	A	73	THR	2.1
2	A	110	PHE	2.1
2	D	92	LEU	2.1
2	A	336	LYS	2.0
1	E	78	VAL	2.0
1	F	2	VAL	2.0
1	H	121	GLN	2.0
2	C	237	LEU	2.0
2	D	137	GLN	2.0
2	B	238	THR	2.0

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Mol	Chain	Res	Type	RSRZ
2	A	152	ALA	2.0
2	A	186	ALA	2.0
2	B	27	PHE	2.0
2	D	24	PHE	2.0
1	E	105	TYR	2.0
2	C	310	ARG	2.0
2	B	8	LEU	2.0
1	E	33	ALA	2.0
2	B	296	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

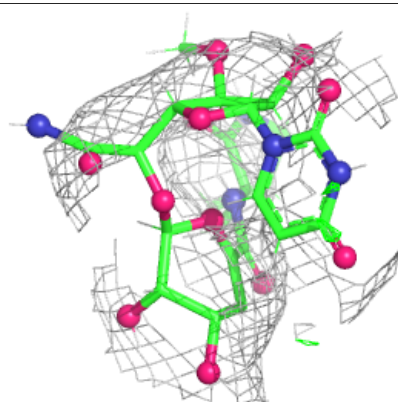
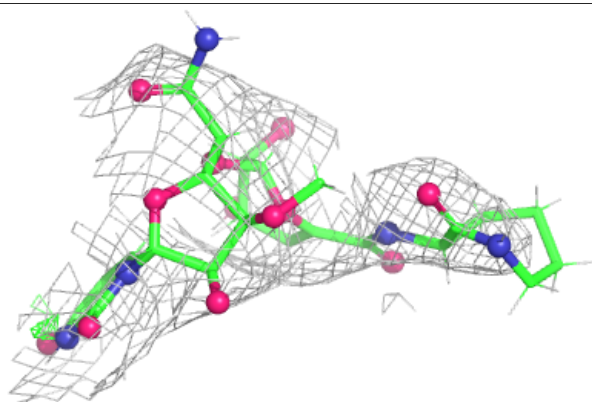
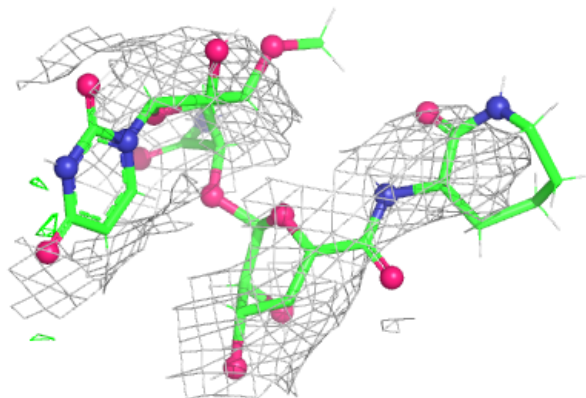
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NKM	A	401	40/40	0.82	0.22	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.