



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:25 AM UTC

PDB ID : 8CXR / pdb_00008cxr
Title : Crystal structure of MraY bound to a sphaerimicin analogue
Authors : Mashalidis, E.H.; Lee, S.Y.
Deposited on : 2022-05-22
Resolution : 3.65 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

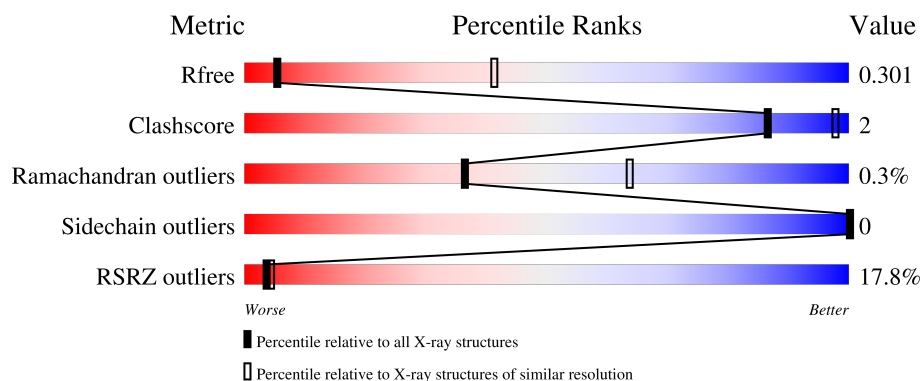
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.65 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 (3.78-3.54)
Clashscore	190562	1009 (3.76-3.56)
Ramachandran outliers	187476	1054 (3.78-3.54)
Sidechain outliers	187428	1052 (3.78-3.54)
RSRZ outliers	180081	1061 (3.78-3.54)

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	23% 91% 8%
1	F	137	8% 91% 8%
1	G	137	17% 89% 8%
1	H	137	15% 91% 9%
2	A	365	15% 80% 6% 14%

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Mol	Chain	Length	Quality of chain
2	B	365	18% 84% 7% 10%
2	C	365	14% 81% 7% 12%
2	D	365	15% 76% 6% 18%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 26549 atoms, of which 13185 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	126	Total	C	H	N	O	S	0	0	0
			1805	584	871	161	185	4			
1	G	126	Total	C	H	N	O	S	0	0	0
			1800	583	867	160	186	4			
1	F	126	Total	C	H	N	O	S	0	0	0
			1810	585	873	161	187	4			
1	H	124	Total	C	H	N	O	S	0	0	0
			1788	577	863	160	184	4			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	A	315	Total	C	H	N	O	S	0	0	0
			4828	1618	2431	363	408	8			
2	C	320	Total	C	H	N	O	S	0	0	0
			4788	1613	2391	367	409	8			
2	B	330	Total	C	H	N	O	S	0	0	0
			4933	1664	2465	379	418	7			
2	D	300	Total	C	H	N	O	S	0	0	0
			4569	1529	2306	341	385	8			

There are 24 discrepancies between the modelled and reference sequences:

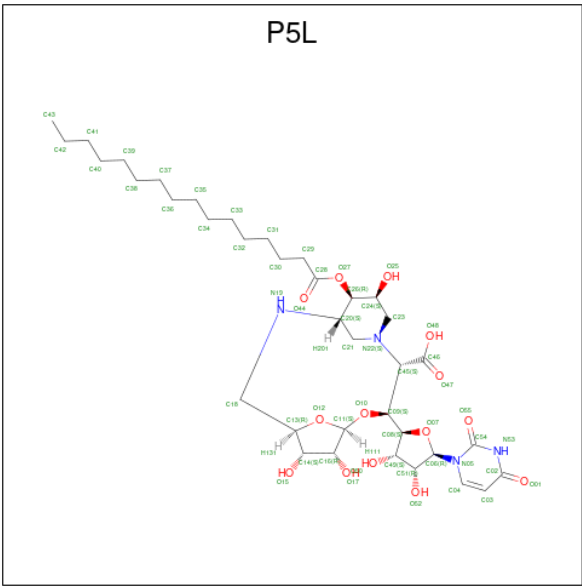
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP O66465
A	-4	PRO	-	expression tag	UNP O66465
A	-3	ALA	-	expression tag	UNP O66465
A	-2	VAL	-	expression tag	UNP O66465
A	-1	PRO	-	expression tag	UNP O66465
A	0	ARG	-	expression tag	UNP O66465
C	-5	GLY	-	expression tag	UNP O66465
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 (1S,4R,5S,6R,7S,9S,10S,11S,13S,14R)-9-[(2S,3S,4R,5R)-5-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)-3,4-dihydroxyoxolan-2-yl]-14-(hexadecanoyloxy)-5,6,13-trihydroxy-8,16-dioxo-2,11-diazatricyclo[9.3.1.1 4,7]hexadecane-10-carboxylic acid (CCD ID: P5L) (formula: C₃₇H₆₀N₄O₁₄) (labeled as "Ligand of Interest" by depositor).

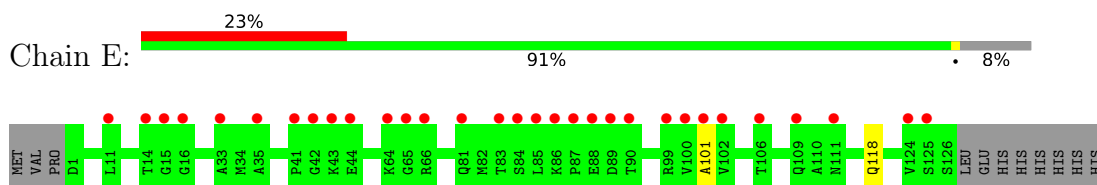


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			114	37	59	4	14		
3	C	1	Total	C	H	N	O	0	0
			114	37	59	4	14		

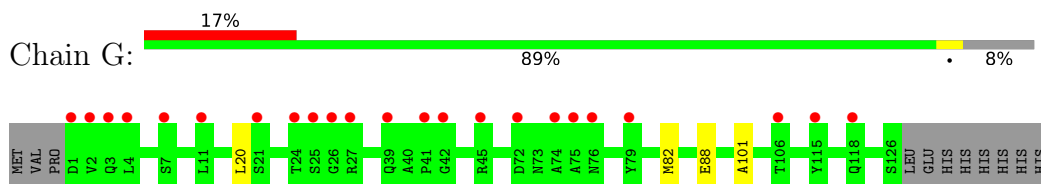
3 Residue-property plots [i](#)

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.

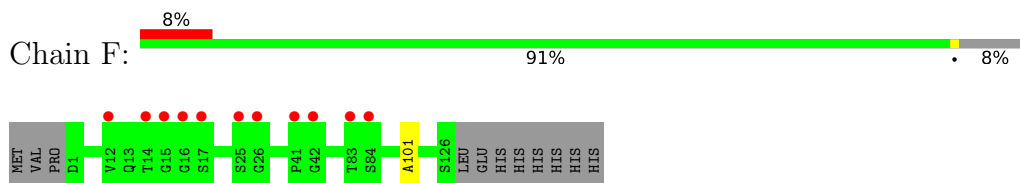
- Molecule 1: MraYAA nanobody



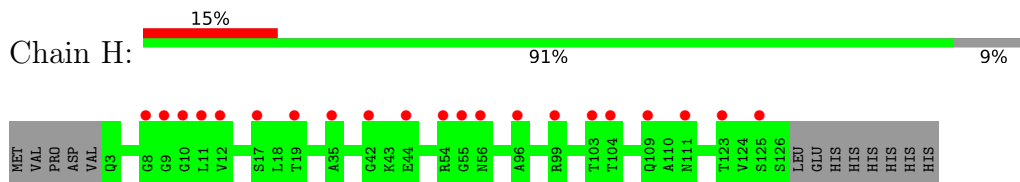
- Molecule 1: MraYAA nanobody



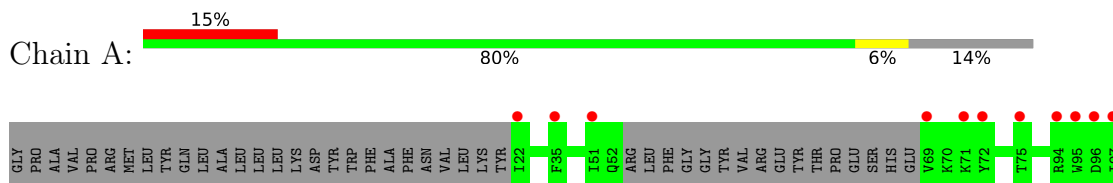
- Molecule 1: MraYAA nanobody

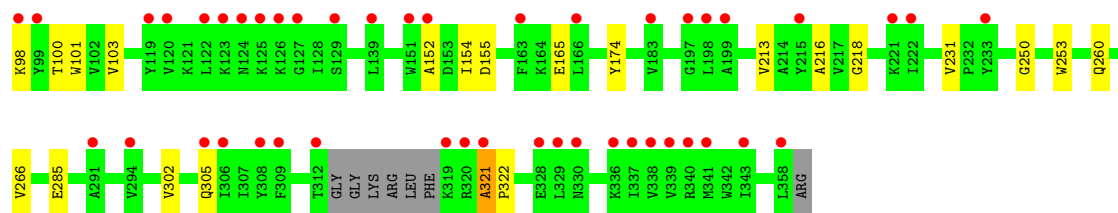


- Molecule 1: MraYAA nanobody

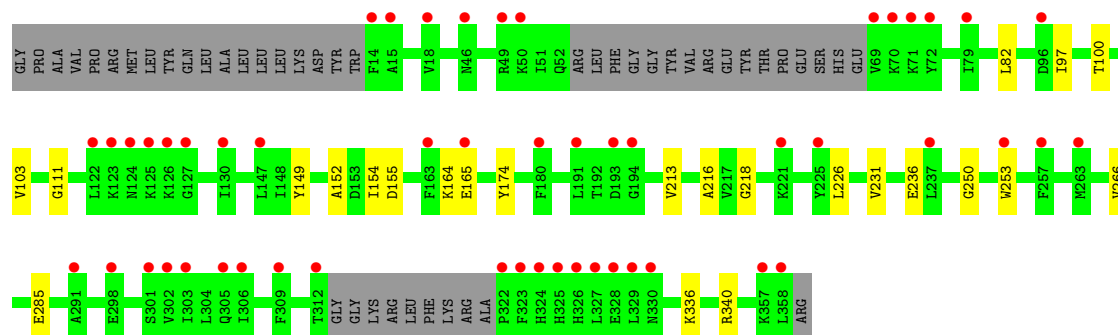
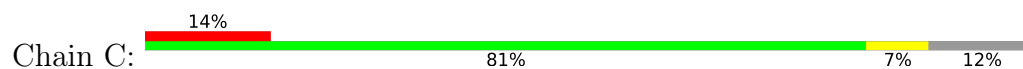


- Molecule 2: Phospho-N-acetylmuramoyl-pentapeptide-transferase

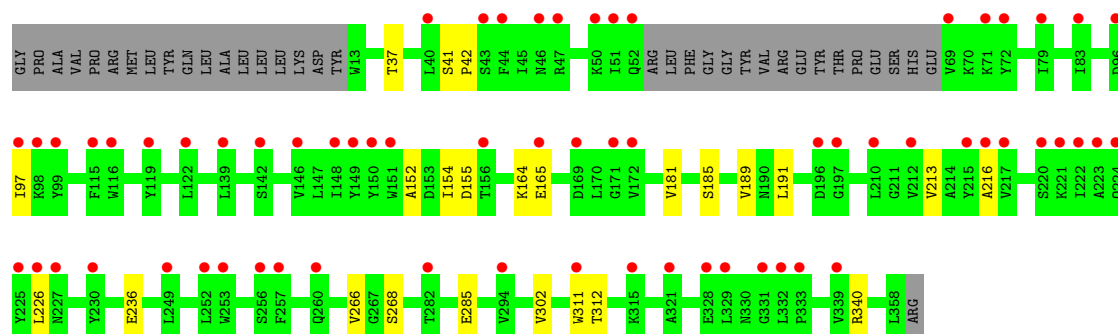
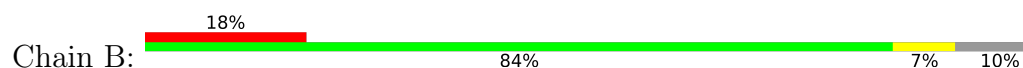




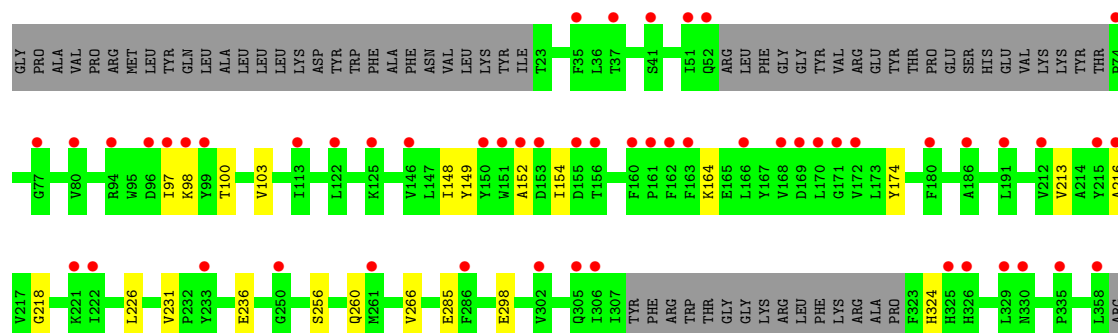
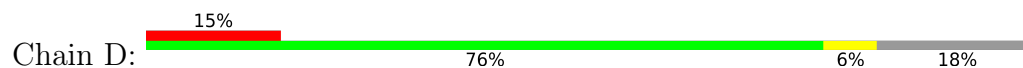
● Molecule 2: Phospho-N-acetylmuramoyl-pentapeptide-transferase



● 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	93.88Å 127.70Å 130.15Å 90.00° 111.39° 90.00°	Depositor
Resolution (Å)	87.91 – 3.65 87.91 – 3.65	Depositor EDS
% Data completeness (in resolution range)	99.5 (87.91-3.65) 99.4 (87.91-3.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 3.67Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.249 , 0.295 0.257 , 0.301	Depositor DCC
R_{free} test set	1385 reflections (4.33%)	wwPDB-VP
Wilson B-factor (Å ²)	116.7	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 91.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	26549	wwPDB-VP
Average B, all atoms (Å ²)	131.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: P5L

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	0.13	0/952	0.28	0/1294
1	F	0.12	0/955	0.27	0/1298
1	G	0.12	0/951	0.27	0/1293
1	H	0.10	0/943	0.28	0/1281
2	A	0.12	0/2458	0.29	0/3358
2	B	0.12	0/2532	0.27	0/3464
2	C	0.11	0/2457	0.27	0/3358
2	D	0.12	0/2319	0.27	0/3169
All	All	0.12	0/13567	0.28	0/18515

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	321	ALA	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	934	871	873	2	0
1	F	937	873	875	1	0
1	G	933	867	869	3	0
1	H	925	863	863	0	0
2	A	2397	2431	2431	12	0
2	B	2468	2465	2463	15	0
2	C	2397	2391	2391	15	0
2	D	2263	2306	2306	14	0
3	A	55	59	0	0	0
3	C	55	59	0	0	0
All	All	13364	13185	13071	56	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 2.

All (56) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:101:ALA:O	2:C:155:ASP:N	2.28	0.66
1:F:101:ALA:O	2:B:155:ASP:N	2.29	0.66
1:E:101:ALA:O	2:A:155:ASP:N	2.30	0.65
2:D:298:GLU:OE1	2:D:324:HIS:ND1	2.33	0.62
2:C:285:GLU:N	2:C:285:GLU:OE1	2.33	0.61
2:A:174:TYR:OH	2:A:285:GLU:OE2	2.17	0.60
2:D:285:GLU:N	2:D:285:GLU:OE1	2.38	0.56
2:A:260:GLN:OE1	2:B:340:ARG:NH2	2.40	0.54
2:C:149:TYR:HH	2:C:174:TYR:HE1	1.56	0.53
2:C:340:ARG:NH2	2:D:260:GLN:OE1	2.43	0.52
1:G:88:GLU:OE1	1:G:88:GLU:N	2.39	0.52
2:C:336:LYS:NZ	2:D:256:SER:OG	2.42	0.51
2:B:164:LYS:NZ	2:B:226:LEU:O	2.44	0.51
1:G:20:LEU:HD13	1:G:82:MET:HE2	1.93	0.50
2:D:213:VAL:O	2:D:216:ALA:N	2.44	0.50
2:C:165:GLU:OE1	2:C:165:GLU:N	2.42	0.50
2:D:152:ALA:O	2:D:154:ILE:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:164:LYS:NZ	2:D:226:LEU:O	2.45	0.49
2:B:213:VAL:O	2:B:216:ALA:N	2.45	0.49
2:B:165:GLU:OE1	2:B:165:GLU:N	2.42	0.48
1:E:118:GLN:OE1	1:E:118:GLN:N	2.40	0.48
2:C:152:ALA:O	2:C:154:ILE:N	2.47	0.48
2:A:165:GLU:OE1	2:A:165:GLU:N	2.42	0.46
2:C:213:VAL:O	2:C:216:ALA:N	2.48	0.46
2:A:213:VAL:O	2:A:216:ALA:N	2.50	0.45
2:D:174:TYR:OH	2:D:285:GLU:OE2	2.35	0.45
2:A:152:ALA:O	2:A:154:ILE:N	2.49	0.45
2:D:148:ILE:HG22	2:D:149:TYR:CE1	2.52	0.45
2:B:285:GLU:OE1	2:B:285:GLU:N	2.50	0.44
2:B:97:ILE:HG13	2:B:236:GLU:HG3	2.00	0.44
2:C:97:ILE:HG13	2:C:236:GLU:HG3	1.99	0.44
2:B:189:VAL:HG12	2:B:268:SER:HB2	2.00	0.43
2:A:302:VAL:HG22	2:A:321:ALA:O	2.19	0.43
2:D:149:TYR:CE1	2:D:174:TYR:HE2	2.37	0.43
2:B:152:ALA:O	2:B:154:ILE:N	2.51	0.43
2:A:100:THR:O	2:A:103:VAL:HG12	2.19	0.42
2:B:37:THR:O	2:B:41:SER:OG	2.24	0.42
2:D:218:GLY:HA2	2:D:231:VAL:O	2.19	0.42
2:D:97:ILE:O	2:D:98:LYS:HG2	2.20	0.42
2:D:97:ILE:HG13	2:D:236:GLU:HG3	2.02	0.42
2:A:98:LYS:HA	2:A:101:TRP:HD1	1.85	0.41
2:A:305:GLN:CB	2:A:321:ALA:CB	2.97	0.41
2:C:218:GLY:HA2	2:C:231:VAL:O	2.20	0.41
2:C:174:TYR:OH	2:C:285:GLU:OE2	2.39	0.41
2:B:311:TRP:O	2:B:311:TRP:CG	2.73	0.41
2:A:250:GLY:O	2:A:253:TRP:HB3	2.21	0.41
2:C:164:LYS:NZ	2:C:226:LEU:O	2.53	0.41
2:C:250:GLY:O	2:C:253:TRP:HB3	2.21	0.41
2:B:181:VAL:O	2:B:185:SER:N	2.49	0.41
2:C:100:THR:HA	2:C:103:VAL:HG12	2.03	0.41
2:B:41:SER:N	2:B:42:PRO:CD	2.84	0.41
2:A:218:GLY:HA2	2:A:231:VAL:O	2.21	0.41
2:B:189:VAL:HG11	2:B:268:SER:O	2.21	0.41
2:D:100:THR:O	2:D:103:VAL:HG12	2.21	0.40
2:C:82:LEU:HD21	2:C:111:GLY:HA3	2.04	0.40
2:B:191:LEU:HD11	2:B:302:VAL:HG21	2.03	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	124/137 (90%)	123 (99%)	1 (1%)	0	100	100
1	F	124/137 (90%)	123 (99%)	1 (1%)	0	100	100
1	G	124/137 (90%)	122 (98%)	2 (2%)	0	100	100
1	H	122/137 (89%)	121 (99%)	1 (1%)	0	100	100
2	A	309/365 (85%)	291 (94%)	16 (5%)	2 (1%)	21	51
2	B	326/365 (89%)	308 (94%)	16 (5%)	2 (1%)	21	51
2	C	314/365 (86%)	294 (94%)	19 (6%)	1 (0%)	36	64
2	D	294/365 (80%)	278 (95%)	15 (5%)	1 (0%)	36	64
All	All	1737/2008 (86%)	1660 (96%)	71 (4%)	6 (0%)	36	64

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	312	THR
2	A	322	PRO
2	C	266	VAL
2	B	266	VAL
2	D	266	VAL
2	A	266	VAL

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	92/110 (84%)	92 (100%)	0	100	100
1	F	93/110 (84%)	93 (100%)	0	100	100
1	G	92/110 (84%)	92 (100%)	0	100	100
1	H	92/110 (84%)	92 (100%)	0	100	100
2	A	247/309 (80%)	247 (100%)	0	100	100
2	B	246/309 (80%)	246 (100%)	0	100	100
2	C	240/309 (78%)	240 (100%)	0	100	100
2	D	234/309 (76%)	234 (100%)	0	100	100
All	All	1336/1676 (80%)	1336 (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 (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	111	ASN
2	B	219	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 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	P5L	A	401	-	57,59,59	2.82	15 (26%)	66,82,82	1.52	11 (16%)
3	P5L	C	401	-	57,59,59	2.83	15 (26%)	66,82,82	1.53	11 (16%)

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	P5L	A	401	-	-	16/48/96/96	0/3/5/5
3	P5L	C	401	-	-	16/48/96/96	0/3/5/5

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	P5L	C54-N05	9.46	1.53	1.38
3	A	401	P5L	C54-N05	9.42	1.53	1.38
3	C	401	P5L	C51-C49	-9.39	1.27	1.53
3	A	401	P5L	C51-C49	-9.36	1.28	1.53
3	C	401	P5L	C54-N53	8.78	1.53	1.38
3	A	401	P5L	C54-N53	8.71	1.53	1.38
3	A	401	P5L	C49-C08	6.30	1.66	1.53
3	C	401	P5L	C49-C08	6.27	1.66	1.53
3	A	401	P5L	C06-N05	-5.14	1.33	1.47
3	C	401	P5L	C06-N05	-5.05	1.33	1.47
3	C	401	P5L	C04-C03	4.77	1.46	1.35
3	A	401	P5L	C04-C03	4.72	1.46	1.35
3	C	401	P5L	C02-N53	3.66	1.44	1.38
3	A	401	P5L	C02-N53	3.61	1.44	1.38
3	A	401	P5L	O27-C28	3.39	1.43	1.34
3	C	401	P5L	O27-C28	3.34	1.43	1.34
3	A	401	P5L	C23-N22	3.23	1.52	1.47
3	C	401	P5L	C45-N22	-3.22	1.44	1.47
3	C	401	P5L	C23-N22	3.21	1.52	1.47
3	C	401	P5L	O52-C51	3.09	1.50	1.43
3	A	401	P5L	O52-C51	3.04	1.50	1.43
3	A	401	P5L	C45-N22	-3.04	1.44	1.47
3	C	401	P5L	C16-C14	-2.90	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	P5L	C16-C14	-2.86	1.45	1.53
3	A	401	P5L	O01-C02	-2.50	1.19	1.24
3	C	401	P5L	O01-C02	-2.41	1.19	1.24
3	C	401	P5L	O55-C54	-2.40	1.18	1.23
3	A	401	P5L	O55-C54	-2.39	1.18	1.23
3	A	401	P5L	C23-C24	2.17	1.55	1.52
3	C	401	P5L	C23-C24	2.15	1.55	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	P5L	O48-C46-C45	5.19	120.52	111.92
3	C	401	P5L	O48-C46-C45	5.19	120.51	111.92
3	A	401	P5L	C02-N53-C54	-4.44	121.10	126.61
3	C	401	P5L	C02-N53-C54	-4.36	121.19	126.61
3	A	401	P5L	C23-N22-C21	-4.21	105.59	110.20
3	C	401	P5L	C23-N22-C21	-4.15	105.66	110.20
3	A	401	P5L	O27-C28-C29	3.80	119.69	111.48
3	C	401	P5L	O27-C28-C29	3.79	119.69	111.48
3	A	401	P5L	C03-C02-N53	3.25	119.36	114.80
3	C	401	P5L	C03-C02-N53	3.16	119.22	114.80
3	A	401	P5L	O01-C02-C03	-2.99	120.01	125.16
3	C	401	P5L	O01-C02-C03	-2.92	120.13	125.16
3	C	401	P5L	C46-C45-N22	-2.89	110.13	112.16
3	C	401	P5L	O47-C46-C45	-2.84	119.34	123.45
3	A	401	P5L	O47-C46-C45	-2.76	119.45	123.45
3	A	401	P5L	C46-C45-N22	-2.50	110.40	112.16
3	C	401	P5L	C23-C24-C26	2.26	115.44	111.53
3	A	401	P5L	C23-C24-C26	2.26	115.44	111.53
3	C	401	P5L	C49-C51-C06	2.25	105.71	101.46
3	C	401	P5L	O07-C06-N05	2.19	113.31	108.36
3	A	401	P5L	O07-C06-N05	2.17	113.27	108.36
3	A	401	P5L	C49-C51-C06	2.14	105.52	101.46

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	P5L	C14-C13-C18-N19
3	A	401	P5L	O12-C13-C18-N19
3	A	401	P5L	C29-C28-O27-C26
3	A	401	P5L	O44-C28-O27-C26

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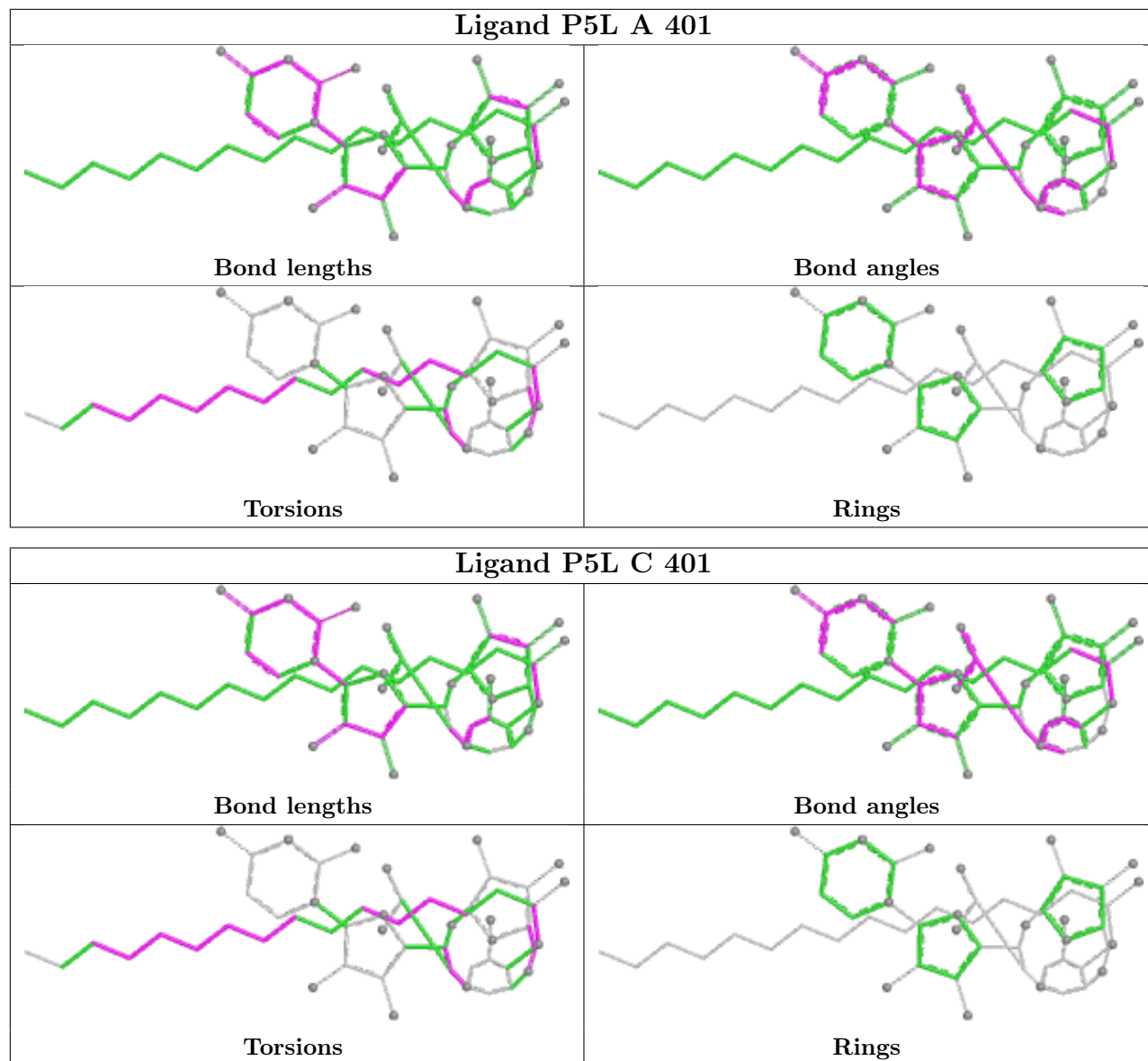
Mol	Chain	Res	Type	Atoms
3	A	401	P5L	C13-C18-N19-C20
3	A	401	P5L	C46-C45-N22-C21
3	C	401	P5L	C14-C13-C18-N19
3	C	401	P5L	O12-C13-C18-N19
3	C	401	P5L	C29-C28-O27-C26
3	C	401	P5L	O44-C28-O27-C26
3	C	401	P5L	C13-C18-N19-C20
3	C	401	P5L	C46-C45-N22-C21
3	C	401	P5L	C34-C35-C36-C37
3	A	401	P5L	C34-C35-C36-C37
3	A	401	P5L	C35-C36-C37-C38
3	C	401	P5L	C35-C36-C37-C38
3	C	401	P5L	C29-C30-C31-C32
3	A	401	P5L	C29-C30-C31-C32
3	A	401	P5L	C38-C39-C40-C41
3	C	401	P5L	C38-C39-C40-C41
3	C	401	P5L	C39-C40-C41-C42
3	A	401	P5L	C39-C40-C41-C42
3	A	401	P5L	C08-C09-C45-C46
3	C	401	P5L	C08-C09-C45-C46
3	C	401	P5L	C36-C37-C38-C39
3	A	401	P5L	C36-C37-C38-C39
3	C	401	P5L	C31-C32-C33-C34
3	A	401	P5L	C31-C32-C33-C34
3	C	401	P5L	C30-C31-C32-C33
3	A	401	P5L	C30-C31-C32-C33
3	C	401	P5L	C37-C38-C39-C40
3	A	401	P5L	C37-C38-C39-C40

There are no ring outliers.

No monomer is involved in short contacts.

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	126/137 (91%)	1.49	31 (24%) 2 2	78, 113, 148, 174	0
1	F	126/137 (91%)	0.54	11 (8%) 16 12	94, 131, 167, 201	0
1	G	126/137 (91%)	0.90	23 (18%) 3 4	85, 111, 160, 185	0
1	H	124/137 (90%)	1.03	21 (16%) 4 5	107, 137, 177, 209	0
2	A	315/365 (86%)	0.83	56 (17%) 4 4	69, 106, 162, 196	0
2	B	330/365 (90%)	1.19	66 (20%) 3 3	70, 146, 205, 235	0
2	C	320/365 (87%)	0.96	52 (16%) 4 5	84, 130, 182, 227	0
2	D	300/365 (82%)	1.02	54 (18%) 3 4	93, 142, 191, 211	0
All	All	1767/2008 (87%)	1.00	314 (17%) 4 4	69, 128, 184, 235	0

All (314) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	163	PHE	14.0
1	G	1	ASP	13.3
2	B	51	ILE	12.8
2	C	126	LYS	11.6
1	E	44	GLU	10.9
2	A	319	LYS	10.8
2	B	150	TYR	10.7
2	C	72	TYR	10.2
2	D	162	PHE	10.0
2	C	165	GLU	9.9
2	C	325	HIS	9.6
1	E	65	GLY	9.4
2	A	329	LEU	9.4
2	A	96	ASP	8.8
1	H	11	LEU	8.5
1	G	75	ALA	8.4

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Mol	Chain	Res	Type	RSRZ
2	B	72	TYR	8.1
1	E	87	PRO	7.8
2	C	324	HIS	7.6
2	A	72	TYR	7.3
1	E	42	GLY	7.1
2	B	221	LYS	7.0
1	H	111	ASN	7.0
2	D	169	ASP	6.9
2	C	125	LYS	6.8
1	E	88	GLU	6.8
2	C	309	PHE	6.7
2	B	146	VAL	6.7
2	B	119	TYR	6.7
1	E	43	LYS	6.6
1	G	74	ALA	6.5
2	C	130	ILE	6.5
2	C	328	GLU	6.5
2	C	69	VAL	6.4
2	B	222	ILE	6.4
1	H	54	ARG	6.4
1	H	109	GLN	6.3
2	D	330	ASN	6.3
2	C	302	VAL	6.3
2	A	97	ILE	6.3
2	C	326	HIS	6.2
2	A	123	LYS	6.1
2	C	124	ASN	6.0
1	H	125	SER	6.0
2	B	216	ALA	5.9
2	D	96	ASP	5.9
2	A	321	ALA	5.9
2	B	331	GLY	5.8
2	B	44	PHE	5.8
2	A	306	ILE	5.7
2	D	150	TYR	5.6
2	D	305	GLN	5.6
1	G	25	SER	5.5
2	D	151	TRP	5.5
2	B	46	ASN	5.5
2	C	225	TYR	5.3
2	D	98	LYS	5.3
2	A	320	ARG	5.2

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Mol	Chain	Res	Type	RSRZ
2	C	127	GLY	5.2
2	C	323	PHE	5.2
1	F	17	SER	5.2
2	B	52	GLN	5.2
2	C	50	LYS	5.1
1	F	15	GLY	5.1
1	H	44	GLU	5.0
2	B	40	LEU	5.0
2	D	160	PHE	5.0
2	C	221	LYS	5.0
2	C	322	PRO	4.9
2	D	99	TYR	4.9
1	E	124	VAL	4.9
2	D	155	ASP	4.9
2	C	71	LYS	4.8
1	H	103	THR	4.8
1	H	10	GLY	4.8
1	E	84	SER	4.7
2	A	99	TYR	4.7
2	B	151	TRP	4.7
2	C	329	LEU	4.6
2	C	312	THR	4.6
2	B	71	LYS	4.6
2	A	330	ASN	4.6
2	A	119	TYR	4.6
1	G	2	VAL	4.5
2	B	50	LYS	4.5
2	A	69	VAL	4.5
2	A	308	TYR	4.5
2	A	221	LYS	4.4
2	D	166	LEU	4.4
1	E	111	ASN	4.3
2	B	98	LYS	4.3
1	G	76	ASN	4.3
1	E	81	GLN	4.3
2	D	306	ILE	4.3
1	E	66	ARG	4.3
1	G	21	SER	4.3
2	B	96	ASP	4.3
2	B	223	ALA	4.3
1	H	55	GLY	4.2
1	G	26	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
1	F	42	GLY	4.2
1	H	56	ASN	4.2
2	A	22	ILE	4.2
1	E	14	THR	4.2
2	A	126	LYS	4.2
2	D	97	ILE	4.1
2	B	215	TYR	4.1
2	D	233	TYR	4.1
1	E	86	LYS	4.1
1	H	19	THR	4.1
2	B	256	SER	4.1
2	A	129	SER	4.0
2	A	125	LYS	4.0
2	B	282	THR	3.9
1	E	15	GLY	3.9
2	D	122	LEU	3.9
2	B	226	LEU	3.9
1	H	8	GLY	3.9
2	A	312	THR	3.9
2	D	216	ALA	3.9
1	E	85	LEU	3.8
1	E	109	GLN	3.8
2	A	124	ASN	3.8
2	C	122	LEU	3.8
2	B	212	VAL	3.8
2	C	306	ILE	3.8
2	C	291	ALA	3.8
2	D	171	GLY	3.8
2	D	146	VAL	3.8
2	D	191	LEU	3.7
2	D	94	ARG	3.7
2	A	309	PHE	3.7
2	A	215	TYR	3.7
2	B	225	TYR	3.7
2	A	98	LYS	3.7
2	A	122	LEU	3.7
1	G	11	LEU	3.6
1	E	90	THR	3.6
2	C	301	SER	3.6
2	B	328	GLU	3.6
1	E	83	THR	3.6
2	C	46	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	64	LYS	3.6
1	F	83	THR	3.6
2	B	210	LEU	3.5
2	A	120	VAL	3.5
2	C	357	LYS	3.5
1	E	33	ALA	3.5
2	D	161	PRO	3.5
2	D	221	LYS	3.5
2	C	298	GLU	3.4
1	H	9	GLY	3.4
1	H	123	THR	3.4
2	C	79	ILE	3.4
2	A	94	ARG	3.4
2	B	122	LEU	3.4
2	B	149	TYR	3.3
2	D	74	PRO	3.3
2	A	127	GLY	3.3
2	D	152	ALA	3.2
2	D	153	ASP	3.2
2	A	339	VAL	3.2
2	B	69	VAL	3.2
2	B	333	PRO	3.2
2	D	156	THR	3.2
2	C	163	PHE	3.2
2	B	83	ILE	3.2
2	D	329	LEU	3.2
2	A	340	ARG	3.2
1	H	42	GLY	3.1
2	B	172	VAL	3.1
1	E	125	SER	3.1
2	B	43	SER	3.1
2	D	168	VAL	3.1
1	G	118	GLN	3.1
2	C	18	VAL	3.1
2	A	51	ILE	3.1
2	D	326	HIS	3.1
2	A	151	TRP	3.0
2	B	253	TRP	3.0
2	B	169	ASP	3.0
2	B	97	ILE	3.0
1	H	12	VAL	3.0
2	A	152	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
2	A	166	LEU	3.0
2	A	95	TRP	3.0
2	D	335	PRO	3.0
2	C	257	PHE	3.0
2	B	332	LEU	3.0
1	G	115	TYR	3.0
2	A	341	MET	3.0
2	B	217	VAL	3.0
2	D	125	LYS	2.9
1	G	27	ARG	2.9
1	E	106	THR	2.9
2	D	222	ILE	2.9
2	A	163	PHE	2.9
2	A	305	GLN	2.9
2	C	237	LEU	2.8
2	B	220	SER	2.8
1	E	16	GLY	2.8
2	C	193	ASP	2.8
2	C	194	GLY	2.8
2	B	197	GLY	2.8
2	B	148	ILE	2.8
2	C	49	ARG	2.8
1	E	11	LEU	2.8
2	C	303	ILE	2.8
2	D	170	LEU	2.8
2	A	222	ILE	2.8
2	A	294	VAL	2.8
1	E	99	ARG	2.7
2	A	358	LEU	2.7
2	D	51	ILE	2.7
1	H	17	SER	2.7
2	D	80	VAL	2.7
2	D	302	VAL	2.7
2	B	252	LEU	2.7
2	A	291	ALA	2.7
2	D	113	ILE	2.7
2	D	37	THR	2.7
2	A	198	LEU	2.7
1	G	45	ARG	2.7
2	C	14	PHE	2.7
1	H	35	ALA	2.6
2	B	156	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	16	GLY	2.6
2	A	336	LYS	2.6
1	G	79	TYR	2.6
2	C	191	LEU	2.6
2	A	338	VAL	2.6
2	D	358	LEU	2.6
2	D	286	PHE	2.6
2	A	343	ILE	2.5
2	B	171	GLY	2.5
1	G	106	THR	2.5
2	B	329	LEU	2.5
2	C	70	LYS	2.5
2	B	315	LYS	2.5
1	F	84	SER	2.5
2	C	305	GLN	2.5
1	F	26	GLY	2.5
2	D	172	VAL	2.5
2	B	116	TRP	2.5
2	B	260	GLN	2.5
1	F	12	VAL	2.4
2	C	123	LYS	2.4
2	C	330	ASN	2.4
2	B	224	GLN	2.4
1	E	89	ASP	2.4
2	A	337	ILE	2.4
2	D	186	ALA	2.4
2	A	75	THR	2.4
2	B	230	TYR	2.4
2	B	47	ARG	2.4
1	G	39	GLN	2.4
1	H	96	ALA	2.4
2	D	41	SER	2.4
1	G	24	THR	2.4
2	B	321	ALA	2.4
2	D	325	HIS	2.3
2	B	115	PHE	2.3
1	E	41	PRO	2.3
2	C	15	ALA	2.3
2	A	35	PHE	2.3
1	F	25	SER	2.3
2	D	35	PHE	2.3
2	D	180	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	14	THR	2.3
2	B	227	ASN	2.3
2	C	96	ASP	2.3
2	B	165	GLU	2.2
2	A	197	GLY	2.2
1	G	3	GLN	2.2
2	D	52	GLN	2.2
2	B	139	LEU	2.2
2	B	196	ASP	2.2
2	C	263	MET	2.2
2	B	142	SER	2.2
1	G	4	LEU	2.2
2	D	250	GLY	2.2
1	G	72	ASP	2.2
2	A	139	LEU	2.2
2	B	249	LEU	2.2
1	G	42	GLY	2.2
1	F	41	PRO	2.2
1	E	100	VAL	2.1
1	E	102	VAL	2.1
2	C	327	LEU	2.1
1	E	35	ALA	2.1
2	B	99	TYR	2.1
2	A	183	VAL	2.1
2	C	180	PHE	2.1
2	B	257	PHE	2.1
2	D	77	GLY	2.1
1	G	7	SER	2.1
2	B	339	VAL	2.1
2	D	261	MET	2.1
1	H	104	THR	2.1
2	C	147	LEU	2.1
2	B	294	VAL	2.1
1	G	41	PRO	2.0
2	B	79	ILE	2.0
1	E	101	ALA	2.0
2	A	199	ALA	2.0
2	A	233	TYR	2.0
1	H	99	ARG	2.0
2	A	328	GLU	2.0
2	C	253	TRP	2.0
2	D	212	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
2	A	71	LYS	2.0
2	D	215	TYR	2.0
2	B	311	TRP	2.0
2	C	358	LEU	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](#)

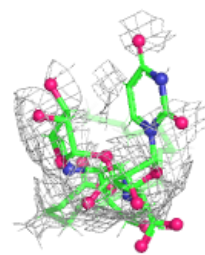
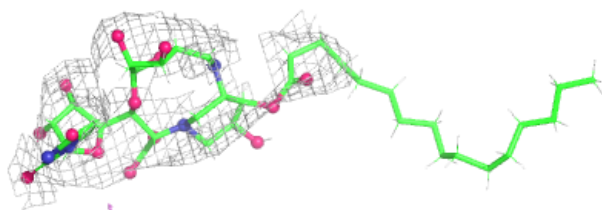
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	P5L	C	401	55/55	0.75	0.19	126,167,205,225	0
3	P5L	A	401	55/55	0.81	0.16	92,134,174,197	0

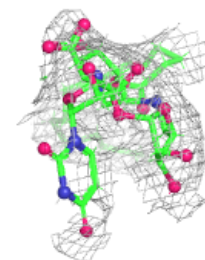
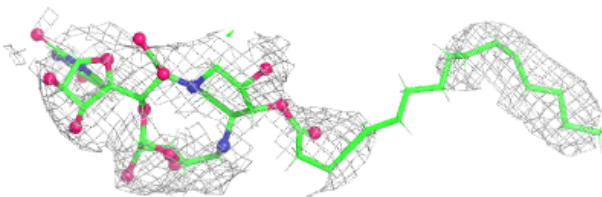
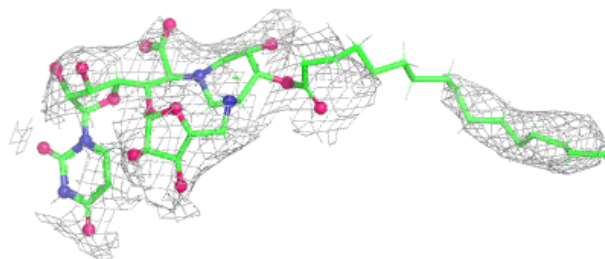
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around P5L 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)

**Electron density around P5L 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.