



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 20, 2024 – 12:04 PM EDT

PDB ID : 8UE9
Title : Structure of TREK-1CG*:CAT335
Authors : Mondal, A.; Lee, H.; Minor, D.L.
Deposited on : 2023-09-29
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.37.1
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) : 2.37.1

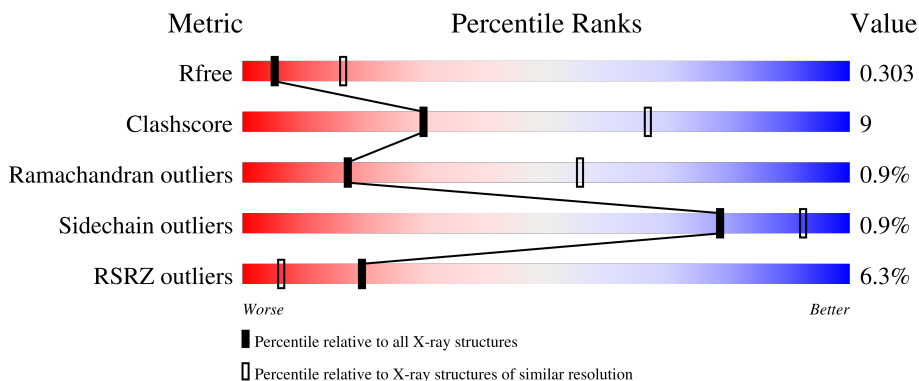
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	287	
1	B	287	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	R16	A	615	-	-	-	X
2	R16	B	403	-	-	-	X

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 4643 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Potassium channel subfamily K member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	274	Total	C	N	O	S	0	0	0
			2150	1433	339	372	6			
1	B	282	Total	C	N	O	S	0	0	0
			2190	1457	347	380	6			

There are 28 discrepancies between the modelled and reference sequences:

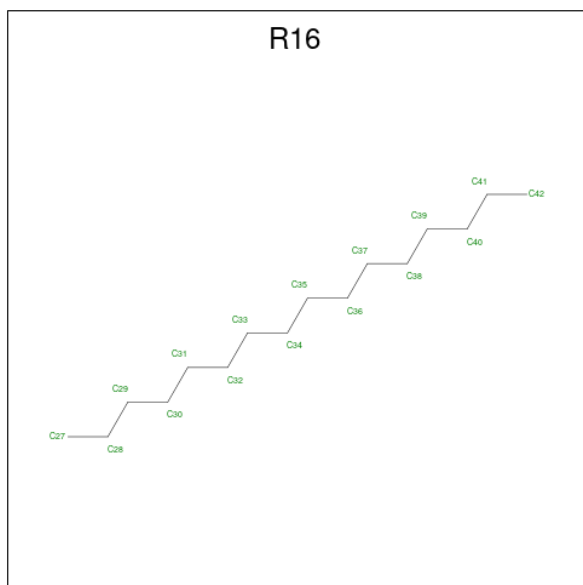
Chain	Residue	Modelled	Actual	Comment	Reference
A	84	ARG	LYS	engineered mutation	UNP P97438
A	85	GLU	GLN	engineered mutation	UNP P97438
A	86	LYS	THR	engineered mutation	UNP P97438
A	88	LEU	ILE	engineered mutation	UNP P97438
A	89	ARG	ALA	engineered mutation	UNP P97438
A	90	ALA	GLN	engineered mutation	UNP P97438
A	92	PRO	ALA	engineered mutation	UNP P97438
A	95	SER	ASN	engineered mutation	UNP P97438
A	96	ASP	SER	engineered mutation	UNP P97438
A	97	GLN	THR	engineered mutation	UNP P97438
A	119	ALA	ASN	engineered mutation	UNP P97438
A	131	CYS	SER	engineered mutation	UNP P97438
A	300	ALA	SER	engineered mutation	UNP P97438
A	306	ALA	GLU	engineered mutation	UNP P97438
B	84	ARG	LYS	engineered mutation	UNP P97438
B	85	GLU	GLN	engineered mutation	UNP P97438
B	86	LYS	THR	engineered mutation	UNP P97438
B	88	LEU	ILE	engineered mutation	UNP P97438
B	89	ARG	ALA	engineered mutation	UNP P97438
B	90	ALA	GLN	engineered mutation	UNP P97438
B	92	PRO	ALA	engineered mutation	UNP P97438
B	95	SER	ASN	engineered mutation	UNP P97438
B	96	ASP	SER	engineered mutation	UNP P97438
B	97	GLN	THR	engineered mutation	UNP P97438
B	119	ALA	ASN	engineered mutation	UNP P97438

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Chain	Residue	Modelled	Actual	Comment	Reference
B	131	CYS	SER	engineered mutation	UNP P97438
B	300	ALA	SER	engineered mutation	UNP P97438
B	306	ALA	GLU	engineered mutation	UNP P97438

- Molecule 2 is HEXADECANE (three-letter code: R16) (formula: C₁₆H₃₄).



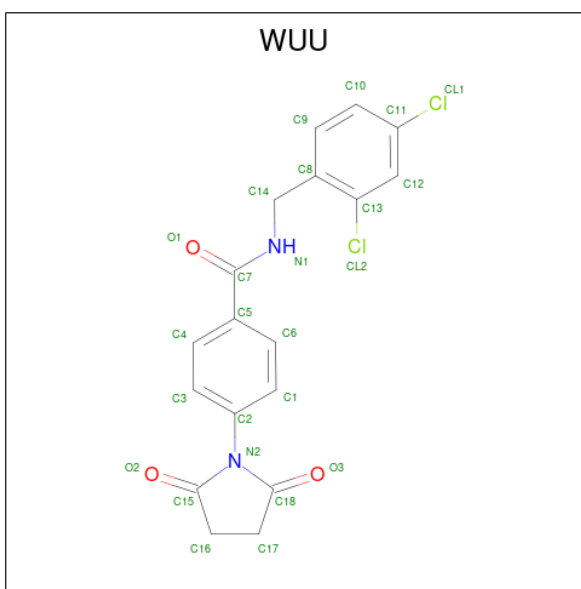
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 16 16	0	0
2	A	1	Total C 16 16	0	0
2	A	1	Total C 16 16	0	0
2	A	1	Total C 16 16	0	0
2	A	1	Total C 16 16	0	0
2	A	1	Total C 16 16	0	0
2	A	1	Total C 16 16	0	0
2	A	1	Total C 16 16	0	0
2	B	1	Total C 16 16	0	0
2	B	1	Total C 16 16	0	0

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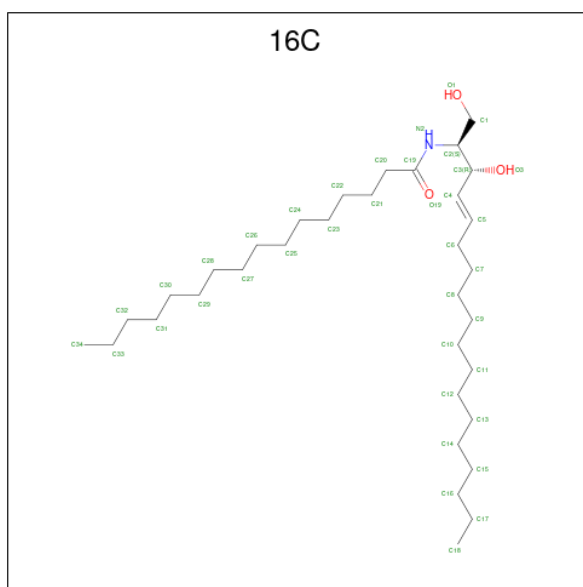
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C 16 16	0	0
2	B	1	Total C 16 16	0	0
2	B	1	Total C 16 16	0	0

- Molecule 3 is N-[(2,4-dichlorophenyl)methyl]-4-(2,5-dioxopyrrolidin-1-yl)benzamide (three-letter code: WUU) (formula: C₁₈H₁₄Cl₂N₂O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C Cl N O 25 18 2 2 3	0	0
3	B	1	Total C Cl N O 25 18 2 2 3	0	0

- Molecule 4 is N-((E,2S,3R)-1,3-DIHYDROXYOCTADEC-4-EN-2-YL)PALMITAMIDE (three-letter code: 16C) (formula: C₃₄H₆₇NO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
4	A	1	38	34	1	3	0	0

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
5	A	5	5	5	0	0

- Molecule 6 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cd		
6	B	1	1	1	0	0

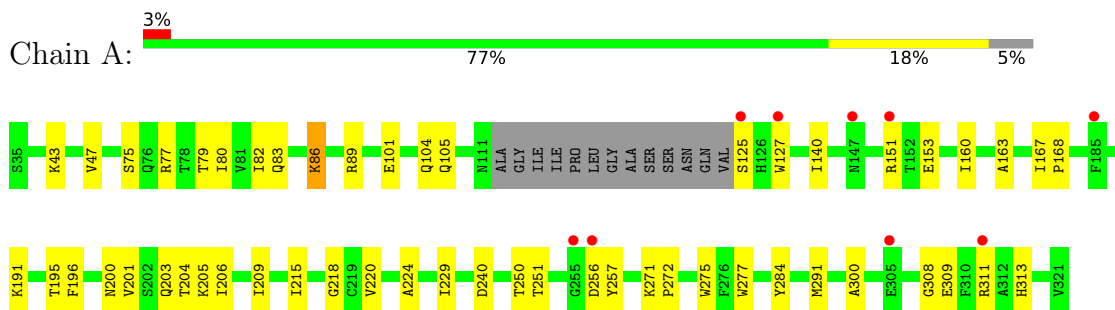
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	B	1	1	1	0	0

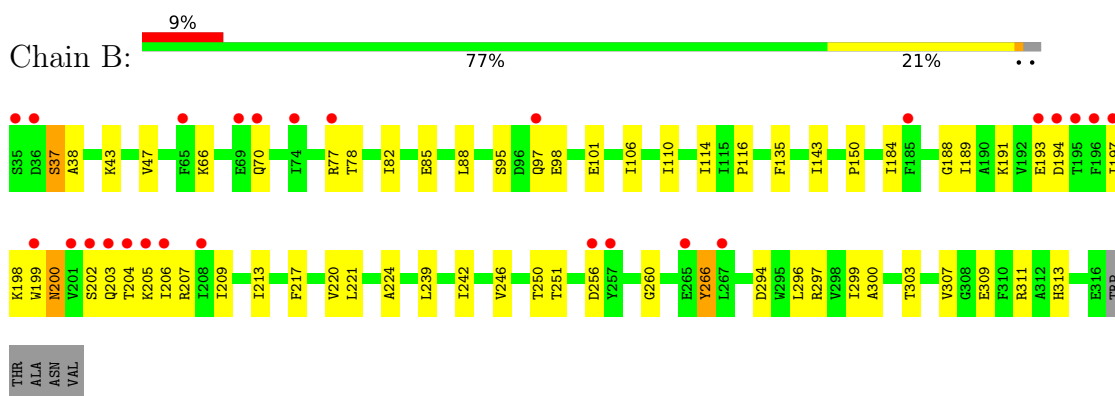
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Potassium channel subfamily K member 2



- Molecule 1: Potassium channel subfamily K member 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.07Å 119.78Å 129.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.62 – 3.00 46.62 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.62-3.00) 99.9 (46.62-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.81Å)	Xtrriage
Refinement program	PHENIX 1.20.1-4487	Depositor
R, R_{free}	0.268 , 0.306 0.265 , 0.303	Depositor DCC
R_{free} test set	1295 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	105.9	Xtrriage
Anisotropy	0.315	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 113.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	4643	wwPDB-VP
Average B, all atoms (Å ²)	157.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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: K, WUU, CD, R16, 16C

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.24	0/2203	0.42	0/2996
1	B	0.24	0/2243	0.46	0/3051
All	All	0.24	0/4446	0.44	0/6047

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	A	2150	0	2197	37	0
1	B	2190	0	2246	42	0
2	A	128	0	272	16	0
2	B	80	0	170	6	0
3	A	25	0	0	0	0
3	B	25	0	0	0	0
4	A	38	0	67	4	0
5	A	5	0	0	0	0
6	B	1	0	0	0	0
7	B	1	0	0	0	0
All	All	4643	0	4952	90	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 9.

All (90) 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:B:307:VAL:HG12	1:B:311:ARG:HD3	1.65	0.78
1:B:309:GLU:OE2	1:B:313:HIS:NE2	2.28	0.67
1:B:204:THR:HA	1:B:207:ARG:HH11	1.59	0.66
1:B:198:LYS:HG2	1:B:199:TRP:H	1.61	0.66
1:B:220:VAL:HA	1:B:224:ALA:HB3	1.79	0.64
1:A:308:GLY:HA2	1:A:311:ARG:NH1	2.15	0.61
1:A:220:VAL:HA	1:A:224:ALA:HB3	1.84	0.59
2:A:612:R16:H322	2:A:612:R16:H382	1.85	0.59
1:B:95:SER:O	1:B:97:GLN:N	2.34	0.59
1:A:309:GLU:OE2	1:A:313:HIS:NE2	2.35	0.58
1:B:199:TRP:O	1:B:200:ASN:HB2	2.05	0.57
1:B:106:ILE:O	1:B:110:ILE:HG12	2.05	0.56
1:B:95:SER:HB2	1:B:98:GLU:HB2	1.86	0.56
1:A:160:ILE:HG12	1:B:246:VAL:HG21	1.85	0.56
1:A:125:SER:HA	1:B:77:ARG:HH22	1.71	0.56
1:B:143:ILE:HG12	1:B:251:THR:HA	1.89	0.54
2:A:611:R16:H291	1:B:184:ILE:HG12	1.90	0.53
1:A:271:LYS:HB2	2:A:612:R16:H412	1.91	0.53
1:B:256:ASP:OD1	1:B:256:ASP:N	2.43	0.52
1:A:256:ASP:N	1:A:256:ASP:OD1	2.43	0.52
1:B:135:PHE:CZ	1:B:150:PRO:HD3	2.45	0.52
1:A:275:TRP:HE1	2:A:612:R16:H332	1.75	0.51
1:A:215:ILE:HD11	1:A:291:MET:HE1	1.93	0.50
1:B:37:SER:OG	1:B:38:ALA:N	2.44	0.49
1:A:125:SER:OG	1:B:70:GLN:OE1	2.30	0.49
1:B:260:GLY:HA2	1:B:266:TYR:CZ	2.48	0.49
1:B:114:ILE:HG13	1:B:116:PRO:HD3	1.93	0.49
2:B:403:R16:H331	2:B:403:R16:H281	1.94	0.48
1:B:203:GLN:O	1:B:207:ARG:NH1	2.46	0.48
1:B:294:ASP:OD1	1:B:297:ARG:NH2	2.46	0.48
1:B:220:VAL:HG13	1:B:221:LEU:HD22	1.95	0.48
2:A:612:R16:H322	2:A:612:R16:H352	1.63	0.48
1:A:308:GLY:HA2	1:A:311:ARG:HH11	1.79	0.48
2:A:610:R16:H322	2:A:610:R16:H291	1.57	0.48
2:B:401:R16:H382	2:B:401:R16:H412	1.63	0.47
1:A:79:THR:HA	1:A:82:ILE:HG12	1.96	0.47
1:A:300:ALA:HA	2:A:602:R16:H321	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:SER:HB2	1:B:205:LYS:HE2	1.96	0.47
1:A:77:ARG:HA	1:A:80:ILE:HG12	1.96	0.46
1:B:296:LEU:HA	1:B:299:ILE:HG22	1.98	0.45
4:A:604:16C:H132	4:A:604:16C:H162	1.53	0.45
2:A:615:R16:H372	2:A:615:R16:H341	1.52	0.45
1:B:188:GLY:HA2	1:B:191:LYS:HE2	1.97	0.45
1:A:196:PHE:O	1:A:200:ASN:HB3	2.16	0.45
1:A:203:GLN:O	1:A:204:THR:OG1	2.25	0.45
1:A:82:ILE:HG13	1:A:83:GLN:N	2.31	0.45
2:A:602:R16:H361	2:A:602:R16:H391	1.67	0.45
4:A:604:16C:H122	4:A:604:16C:H71	1.98	0.45
4:A:604:16C:H4	4:A:604:16C:H11	1.57	0.45
1:B:300:ALA:HB1	2:B:403:R16:H391	1.99	0.45
2:A:612:R16:H382	2:A:612:R16:H352	1.47	0.44
1:A:167:ILE:HB	1:A:168:PRO:HD3	1.98	0.44
1:A:191:LYS:O	1:A:195:THR:HG23	2.16	0.44
1:A:125:SER:HA	1:B:77:ARG:NH2	2.32	0.44
2:A:612:R16:H371	2:A:612:R16:H401	1.73	0.44
1:A:43:LYS:O	1:A:47:VAL:HG23	2.18	0.43
1:A:163:ALA:O	1:A:167:ILE:HG12	2.19	0.43
1:A:140:ILE:HA	1:A:167:ILE:HD13	2.00	0.43
1:A:86:LYS:HE3	1:A:86:LYS:HB3	1.77	0.43
1:B:189:ILE:O	1:B:193:GLU:HG3	2.19	0.43
4:A:604:16C:H302	4:A:604:16C:H271	1.87	0.43
1:B:303:THR:O	1:B:307:VAL:HG23	2.19	0.43
1:B:213:ILE:O	1:B:217:PHE:HB2	2.19	0.43
2:B:401:R16:H352	2:B:401:R16:H322	1.43	0.42
1:B:296:LEU:HD22	2:B:403:R16:H272	2.01	0.42
1:A:272:PRO:HD3	2:A:612:R16:H392	2.01	0.42
1:B:194:ASP:OD1	1:B:194:ASP:N	2.48	0.42
1:A:229:ILE:HG21	2:A:614:R16:H322	2.02	0.42
1:B:78:THR:O	1:B:82:ILE:HG13	2.20	0.42
2:B:406:R16:H423	2:B:406:R16:H392	1.81	0.42
1:A:277:TRP:HB2	2:A:614:R16:H371	2.01	0.42
1:B:95:SER:O	1:B:97:GLN:HG2	2.20	0.42
1:A:127:TRP:O	1:B:66:LYS:HD2	2.21	0.41
1:B:242:ILE:O	1:B:246:VAL:HG22	2.20	0.41
1:A:153:GLU:HB2	1:B:239:LEU:HD23	2.03	0.41
1:A:240:ASP:N	1:A:240:ASP:OD1	2.54	0.41
1:A:206:ILE:HA	1:A:209:ILE:HD12	2.03	0.41
1:A:101:GLU:O	1:A:104:GLN:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:GLN:C	1:A:205:LYS:H	2.24	0.41
1:B:98:GLU:O	1:B:101:GLU:HB3	2.20	0.41
1:B:250:THR:O	1:B:251:THR:OG1	2.38	0.41
1:A:250:THR:O	1:A:251:THR:OG1	2.39	0.41
1:B:206:ILE:HA	1:B:209:ILE:HD12	2.03	0.41
1:A:240:ASP:OD2	1:A:257:TYR:OH	2.37	0.40
1:B:43:LYS:O	1:B:47:VAL:HG23	2.20	0.40
2:A:610:R16:H311	2:A:610:R16:H341	1.74	0.40
1:B:85:GLU:HA	1:B:88:LEU:HB2	2.02	0.40
1:A:218:GLY:HA3	1:A:284:TYR:CE1	2.57	0.40
2:A:613:R16:H352	2:A:613:R16:H322	1.74	0.40
1:A:75:SER:O	1:A:79:THR:HG23	2.21	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	A	270/287 (94%)	263 (97%)	6 (2%)	1 (0%)	34	72
1	B	280/287 (98%)	263 (94%)	13 (5%)	4 (1%)	11	43
All	All	550/574 (96%)	526 (96%)	19 (4%)	5 (1%)	17	55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	200	ASN
1	B	37	SER
1	B	266	TYR
1	A	201	VAL
1	B	197	ILE

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	A	227/236 (96%)	223 (98%)	4 (2%)	59	85
1	B	231/236 (98%)	231 (100%)	0	100	100
All	All	458/472 (97%)	454 (99%)	4 (1%)	78	92

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	LYS
1	A	89	ARG
1	A	105	GLN
1	A	151	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	40	ASN
1	B	70	GLN

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

Of 22 ligands modelled in this entry, 6 are monoatomic - leaving 16 for Mogul analysis.

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
2	R16	A	611	-	15,15,15	0.29	0	14,14,14	0.39	0
2	R16	A	614	-	15,15,15	0.30	0	14,14,14	0.33	0
2	R16	B	402	-	15,15,15	0.29	0	14,14,14	0.31	0
3	WUU	A	603	1	27,27,27	2.66	7 (25%)	38,38,38	2.02	7 (18%)
3	WUU	B	404	1	27,27,27	2.68	7 (25%)	38,38,38	2.08	8 (21%)
2	R16	A	612	-	15,15,15	0.29	0	14,14,14	0.34	0
2	R16	A	601	-	15,15,15	0.30	0	14,14,14	0.36	0
2	R16	A	602	-	15,15,15	0.30	0	14,14,14	0.35	0
2	R16	A	610	-	15,15,15	0.29	0	14,14,14	0.36	0
2	R16	B	403	-	15,15,15	0.29	0	14,14,14	0.39	0
2	R16	B	406	-	15,15,15	0.29	0	14,14,14	0.36	0
2	R16	A	615	-	15,15,15	0.29	0	14,14,14	0.34	0
4	16C	A	604	-	36,37,37	1.62	5 (13%)	37,39,39	1.28	5 (13%)
2	R16	B	405	-	15,15,15	0.30	0	14,14,14	0.36	0
2	R16	A	613	-	15,15,15	0.30	0	14,14,14	0.34	0
2	R16	B	401	-	15,15,15	0.31	0	14,14,14	0.30	0

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
2	R16	A	611	-	-	12/13/13/13	-
2	R16	A	614	-	-	8/13/13/13	-
2	R16	B	402	-	-	6/13/13/13	-
3	WUU	A	603	1	-	0/13/26/26	0/3/3/3
3	WUU	B	404	1	-	0/13/26/26	0/3/3/3
2	R16	A	612	-	-	10/13/13/13	-
2	R16	A	601	-	-	10/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	R16	A	602	-	-	9/13/13/13	-
2	R16	A	610	-	-	11/13/13/13	-
2	R16	B	403	-	-	9/13/13/13	-
2	R16	B	406	-	-	9/13/13/13	-
2	R16	A	615	-	-	9/13/13/13	-
4	16C	A	604	-	-	34/40/40/40	-
2	R16	B	405	-	-	8/13/13/13	-
2	R16	A	613	-	-	10/13/13/13	-
2	R16	B	401	-	-	12/13/13/13	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	404	WUU	C15-N2	8.29	1.50	1.40
3	A	603	WUU	C15-N2	8.19	1.50	1.40
3	B	404	WUU	C18-N2	8.16	1.50	1.40
3	A	603	WUU	C18-N2	8.00	1.50	1.40
4	A	604	16C	C19-N2	6.87	1.48	1.34
3	A	603	WUU	C7-N1	5.32	1.45	1.33
3	B	404	WUU	C7-N1	5.26	1.45	1.33
4	A	604	16C	C3-C4	3.09	1.55	1.50
4	A	604	16C	C20-C19	2.63	1.56	1.51
3	A	603	WUU	C13-CL2	2.28	1.79	1.73
3	A	603	WUU	O1-C7	-2.24	1.18	1.23
3	B	404	WUU	C13-CL2	2.22	1.78	1.73
4	A	604	16C	O19-C19	-2.20	1.18	1.23
3	B	404	WUU	O1-C7	-2.15	1.18	1.23
3	A	603	WUU	C11-CL1	2.11	1.79	1.74
4	A	604	16C	O3-C3	-2.10	1.39	1.43
3	B	404	WUU	C17-C16	-2.09	1.47	1.52
3	A	603	WUU	C17-C16	-2.08	1.47	1.52
3	B	404	WUU	C11-CL1	2.03	1.78	1.74

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	404	WUU	C18-N2-C15	-9.01	106.77	112.80
3	A	603	WUU	C18-N2-C15	-8.80	106.91	112.80
4	A	604	16C	C20-C19-N2	4.78	124.12	115.83
3	B	404	WUU	C8-C14-N1	-3.97	104.66	113.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	603	WUU	C8-C14-N1	-3.82	104.96	113.03
3	B	404	WUU	O2-C15-N2	3.05	126.74	124.01
4	A	604	16C	O19-C19-N2	-2.99	117.90	122.95
3	A	603	WUU	O2-C15-N2	2.89	126.60	124.01
3	A	603	WUU	O3-C18-N2	2.87	126.58	124.01
4	A	604	16C	C2-N2-C19	2.82	128.23	123.48
3	B	404	WUU	O3-C18-N2	2.81	126.52	124.01
3	A	603	WUU	C17-C18-N2	-2.76	105.43	107.81
3	A	603	WUU	C12-C13-C8	-2.70	120.02	122.42
3	B	404	WUU	C2-N2-C15	2.67	127.88	123.05
3	B	404	WUU	C12-C13-C8	-2.65	120.06	122.42
3	B	404	WUU	C17-C18-N2	-2.55	105.62	107.81
3	A	603	WUU	C2-N2-C15	2.49	127.56	123.05
4	A	604	16C	O19-C19-C20	-2.21	117.97	122.02
4	A	604	16C	C3-C4-C5	-2.19	119.90	124.79
3	B	404	WUU	C9-C8-C13	2.11	120.38	116.91

There are no chirality outliers.

All (157) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	604	16C	N2-C2-C3-C4
4	A	604	16C	N2-C2-C3-O3
4	A	604	16C	C1-C2-C3-C4
4	A	604	16C	C1-C2-C3-O3
4	A	604	16C	C2-C3-C4-C5
4	A	604	16C	C19-C20-C21-C22
4	A	604	16C	C20-C19-N2-C2
2	B	401	R16	C32-C33-C34-C35
4	A	604	16C	O19-C19-N2-C2
2	B	401	R16	C34-C35-C36-C37
2	A	612	R16	C35-C36-C37-C38
2	B	402	R16	C30-C31-C32-C33
2	A	602	R16	C36-C37-C38-C39
2	B	402	R16	C28-C29-C30-C31
2	A	613	R16	C32-C33-C34-C35
2	A	615	R16	C34-C35-C36-C37
4	A	604	16C	C13-C14-C15-C16
2	B	402	R16	C32-C33-C34-C35
2	A	615	R16	C36-C37-C38-C39
2	A	612	R16	C37-C38-C39-C40
2	A	614	R16	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
2	A	602	R16	C31-C32-C33-C34
2	A	610	R16	C37-C38-C39-C40
2	A	615	R16	C32-C33-C34-C35
2	B	401	R16	C33-C34-C35-C36
2	B	405	R16	C28-C29-C30-C31
2	B	405	R16	C29-C30-C31-C32
4	A	604	16C	C9-C10-C11-C12
2	A	611	R16	C29-C30-C31-C32
2	A	611	R16	C30-C31-C32-C33
2	A	613	R16	C30-C31-C32-C33
2	B	405	R16	C30-C31-C32-C33
4	A	604	16C	C24-C25-C26-C27
2	A	610	R16	C34-C35-C36-C37
2	B	405	R16	C32-C33-C34-C35
2	A	610	R16	C29-C30-C31-C32
2	A	613	R16	C28-C29-C30-C31
4	A	604	16C	C22-C23-C24-C25
2	A	615	R16	C33-C34-C35-C36
2	A	615	R16	C35-C36-C37-C38
2	A	615	R16	C38-C39-C40-C41
2	B	406	R16	C30-C31-C32-C33
2	A	601	R16	C29-C30-C31-C32
2	A	601	R16	C38-C39-C40-C41
2	A	611	R16	C34-C35-C36-C37
2	A	612	R16	C36-C37-C38-C39
2	A	615	R16	C30-C31-C32-C33
2	B	403	R16	C38-C39-C40-C41
4	A	604	16C	C12-C13-C14-C15
2	A	601	R16	C36-C37-C38-C39
2	A	611	R16	C31-C32-C33-C34
2	A	612	R16	C28-C29-C30-C31
2	A	613	R16	C38-C39-C40-C41
2	A	614	R16	C37-C38-C39-C40
2	B	403	R16	C29-C30-C31-C32
2	A	614	R16	C32-C33-C34-C35
2	A	614	R16	C36-C37-C38-C39
2	B	405	R16	C34-C35-C36-C37
2	B	406	R16	C32-C33-C34-C35
4	A	604	16C	C11-C10-C9-C8
2	A	611	R16	C38-C39-C40-C41
2	A	612	R16	C38-C39-C40-C41
2	A	615	R16	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
2	B	401	R16	C31-C32-C33-C34
2	A	610	R16	C28-C29-C30-C31
2	A	602	R16	C32-C33-C34-C35
4	A	604	16C	C6-C7-C8-C9
2	B	403	R16	C36-C37-C38-C39
2	A	611	R16	C37-C38-C39-C40
2	A	613	R16	C37-C38-C39-C40
2	B	401	R16	C38-C39-C40-C41
2	B	405	R16	C37-C38-C39-C40
2	A	602	R16	C34-C35-C36-C37
2	A	613	R16	C29-C30-C31-C32
2	A	613	R16	C33-C34-C35-C36
2	A	602	R16	C35-C36-C37-C38
2	A	601	R16	C27-C28-C29-C30
2	A	610	R16	C32-C33-C34-C35
4	A	604	16C	C1-C2-N2-C19
4	A	604	16C	O1-C1-C2-C3
4	A	604	16C	C20-C21-C22-C23
4	A	604	16C	C26-C27-C28-C29
2	A	611	R16	C35-C36-C37-C38
2	B	406	R16	C39-C40-C41-C42
2	A	612	R16	C33-C34-C35-C36
2	A	614	R16	C30-C31-C32-C33
2	B	403	R16	C28-C29-C30-C31
2	A	614	R16	C28-C29-C30-C31
4	A	604	16C	C14-C15-C16-C17
2	A	612	R16	C34-C35-C36-C37
4	A	604	16C	O1-C1-C2-N2
2	A	613	R16	C36-C37-C38-C39
2	B	406	R16	C28-C29-C30-C31
2	A	612	R16	C32-C33-C34-C35
2	A	601	R16	C28-C29-C30-C31
4	A	604	16C	C3-C2-N2-C19
2	B	406	R16	C38-C39-C40-C41
2	A	610	R16	C38-C39-C40-C41
2	A	602	R16	C38-C39-C40-C41
4	A	604	16C	C11-C12-C13-C14
2	A	611	R16	C36-C37-C38-C39
2	B	405	R16	C36-C37-C38-C39
2	A	614	R16	C38-C39-C40-C41
2	A	610	R16	C27-C28-C29-C30
2	B	403	R16	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
4	A	604	16C	C5-C6-C7-C8
2	A	610	R16	C30-C31-C32-C33
2	B	403	R16	C32-C33-C34-C35
2	B	406	R16	C27-C28-C29-C30
2	A	601	R16	C32-C33-C34-C35
2	A	612	R16	C39-C40-C41-C42
2	A	610	R16	C35-C36-C37-C38
2	B	403	R16	C39-C40-C41-C42
2	A	601	R16	C39-C40-C41-C42
2	B	401	R16	C36-C37-C38-C39
2	B	402	R16	C35-C36-C37-C38
2	A	613	R16	C39-C40-C41-C42
2	A	602	R16	C33-C34-C35-C36
2	A	602	R16	C30-C31-C32-C33
4	A	604	16C	C4-C5-C6-C7
4	A	604	16C	C15-C16-C17-C18
2	A	611	R16	C28-C29-C30-C31
2	A	613	R16	C35-C36-C37-C38
2	A	610	R16	C33-C34-C35-C36
2	B	405	R16	C27-C28-C29-C30
4	A	604	16C	C25-C26-C27-C28
2	A	610	R16	C31-C32-C33-C34
4	A	604	16C	O3-C3-C4-C5
2	B	401	R16	C28-C29-C30-C31
2	A	602	R16	C27-C28-C29-C30
4	A	604	16C	C27-C28-C29-C30
4	A	604	16C	C21-C22-C23-C24
4	A	604	16C	C30-C31-C32-C33
4	A	604	16C	C23-C24-C25-C26
2	B	401	R16	C29-C30-C31-C32
2	A	612	R16	C27-C28-C29-C30
2	B	401	R16	C35-C36-C37-C38
2	A	614	R16	C34-C35-C36-C37
2	A	611	R16	C33-C34-C35-C36
2	A	615	R16	C39-C40-C41-C42
2	A	611	R16	C27-C28-C29-C30
2	A	611	R16	C32-C33-C34-C35
2	B	406	R16	C34-C35-C36-C37
4	A	604	16C	C7-C8-C9-C10
2	A	601	R16	C31-C32-C33-C34
2	A	601	R16	C33-C34-C35-C36
2	B	406	R16	C31-C32-C33-C34

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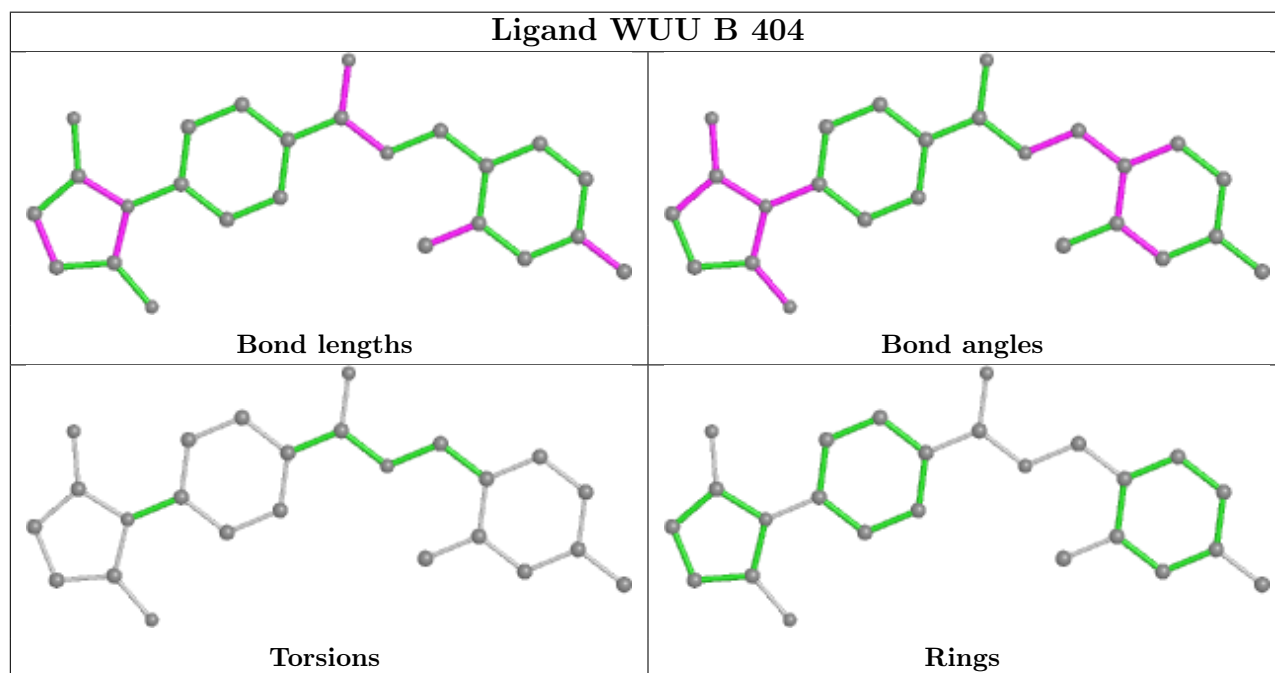
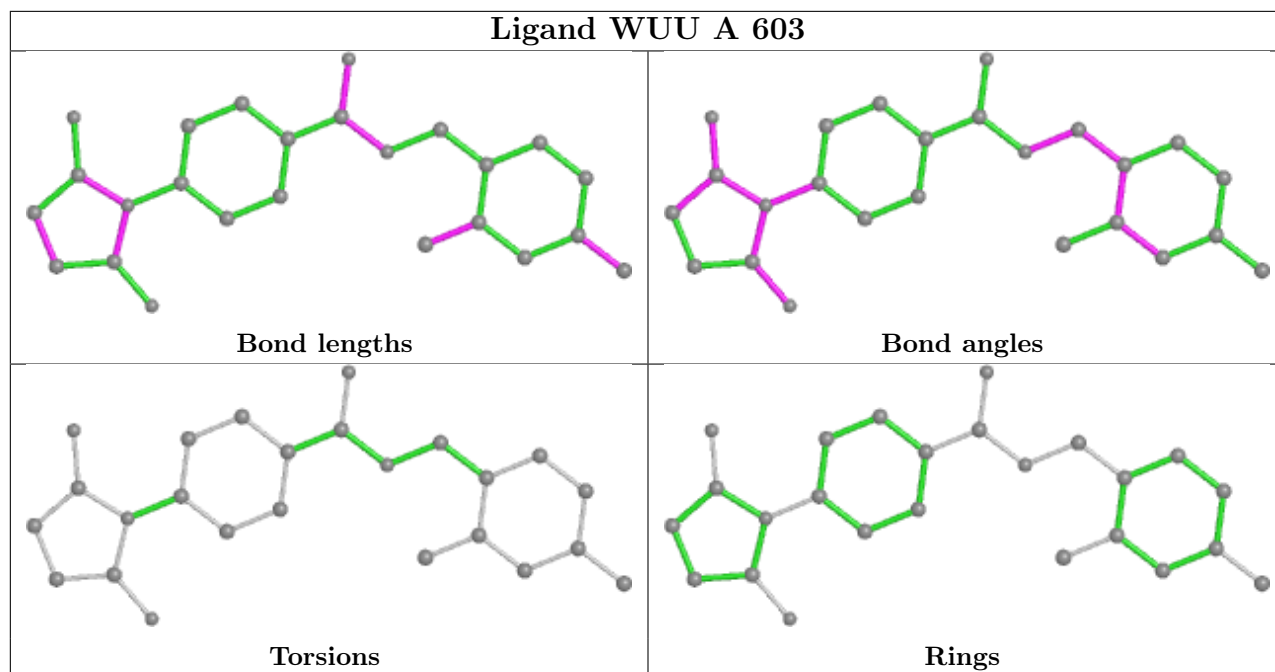
Mol	Chain	Res	Type	Atoms
4	A	604	16C	C10-C11-C12-C13
2	B	403	R16	C33-C34-C35-C36
2	B	403	R16	C31-C32-C33-C34
2	B	401	R16	C39-C40-C41-C42
2	B	401	R16	C30-C31-C32-C33
2	B	402	R16	C36-C37-C38-C39
2	B	401	R16	C27-C28-C29-C30
2	B	406	R16	C37-C38-C39-C40
2	B	402	R16	C38-C39-C40-C41
2	A	601	R16	C30-C31-C32-C33

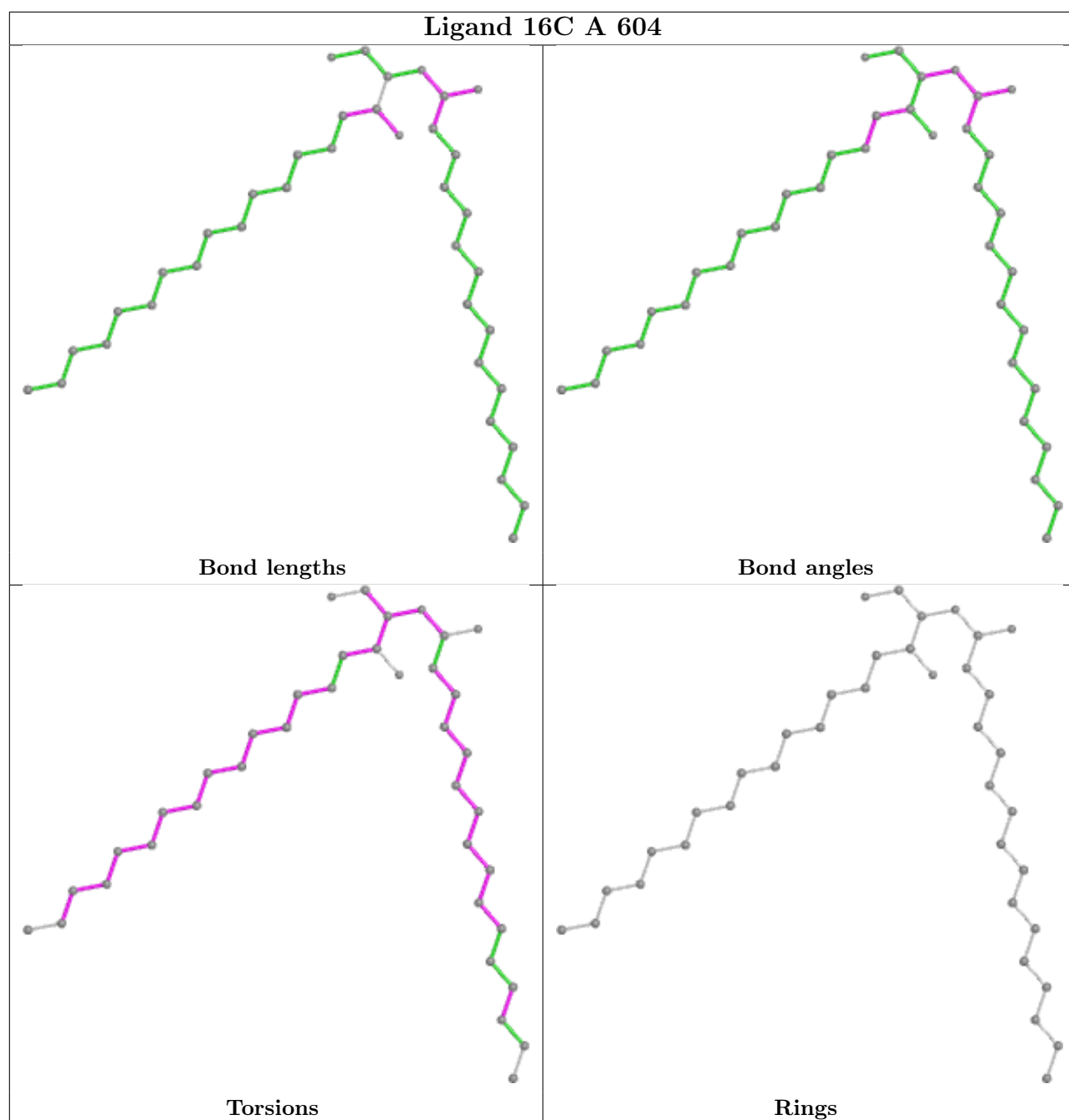
There are no ring outliers.

11 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	611	R16	1	0
2	A	614	R16	2	0
2	A	612	R16	7	0
2	A	602	R16	2	0
2	A	610	R16	2	0
2	B	403	R16	3	0
2	B	406	R16	1	0
2	A	615	R16	1	0
4	A	604	16C	4	0
2	A	613	R16	1	0
2	B	401	R16	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	A	274/287 (95%)	-0.02	9 (3%) 46 20	79, 132, 258, 318	0
1	B	282/287 (98%)	0.25	26 (9%) 9 3	86, 145, 268, 340	0
All	All	556/574 (96%)	0.12	35 (6%) 20 6	79, 138, 264, 340	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	204	THR	7.3
1	B	267	LEU	6.3
1	B	201	VAL	5.3
1	B	265	GLU	5.1
1	B	202	SER	5.1
1	B	196	PHE	5.0
1	B	69	GLU	4.9
1	B	35	SER	4.4
1	A	127	TRP	4.4
1	B	65	PHE	4.3
1	A	151	ARG	4.2
1	B	205	LYS	4.2
1	B	199	TRP	3.9
1	B	203	GLN	3.9
1	B	194	ASP	3.8
1	B	97	GLN	3.8
1	A	125	SER	3.6
1	B	193	GLU	3.6
1	B	256	ASP	3.2
1	A	305	GLU	3.0
1	A	147	ASN	2.9
1	A	255	GLY	2.8
1	B	36	ASP	2.7
1	A	311	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	185	PHE	2.5
1	B	206	ILE	2.5
1	B	74	ILE	2.4
1	B	70	GLN	2.4
1	B	195	THR	2.4
1	B	197	ILE	2.3
1	B	77	ARG	2.2
1	B	257	TYR	2.2
1	B	185	PHE	2.1
1	A	256	ASP	2.1
1	B	208	ILE	2.1

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

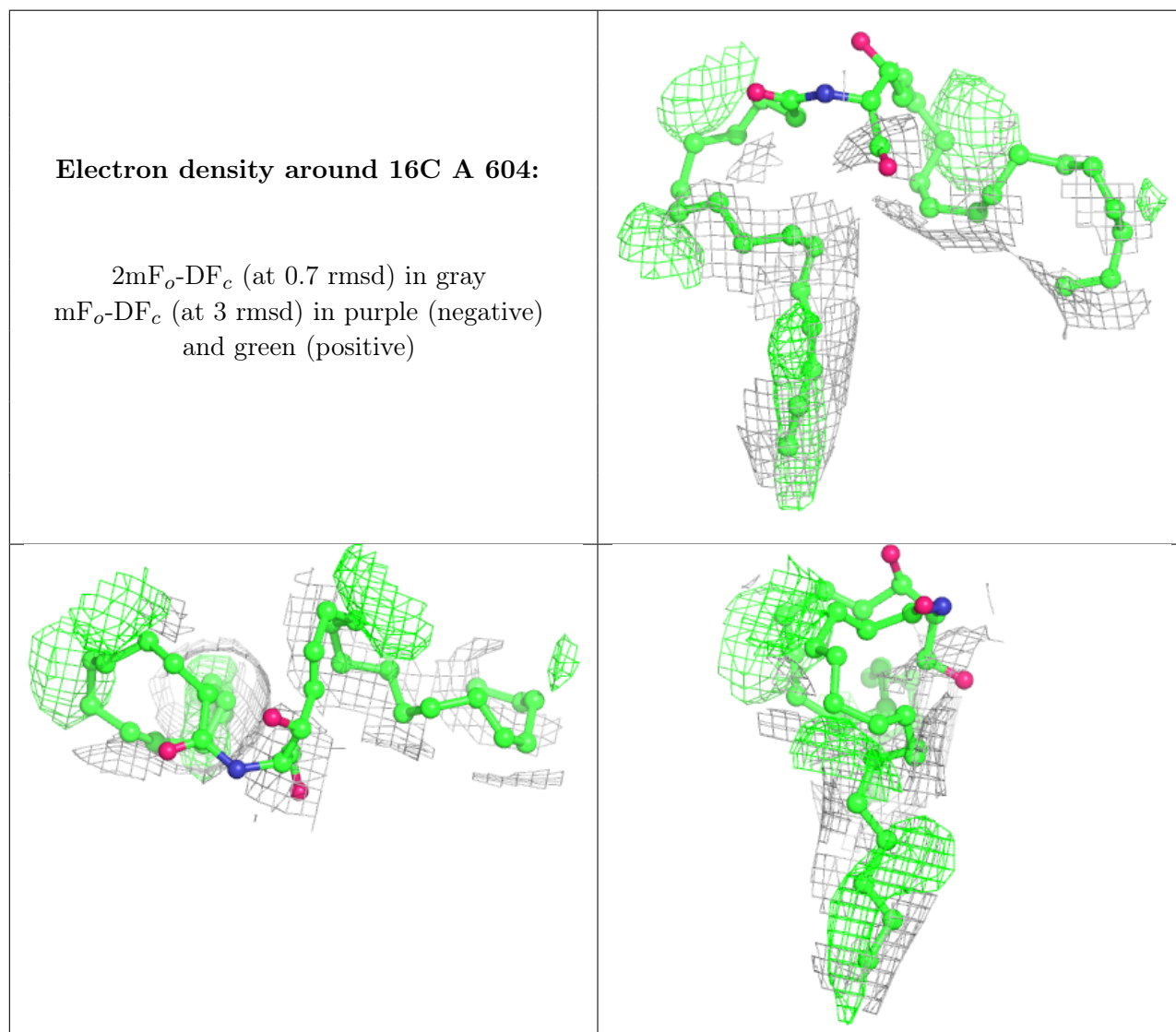
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	R16	A	610	16/16	0.42	0.31	125,157,175,177	0
2	R16	A	613	16/16	0.43	0.26	135,175,212,216	0
6	CD	B	407	1/1	0.50	0.18	338,338,338,338	0
4	16C	A	604	38/38	0.54	0.31	144,199,223,229	0
2	R16	A	612	16/16	0.63	0.39	113,126,147,151	0
2	R16	B	406	16/16	0.64	0.31	128,161,179,180	0
2	R16	A	614	16/16	0.65	0.30	103,126,165,166	0
2	R16	A	611	16/16	0.65	0.23	129,141,156,158	0
2	R16	A	615	16/16	0.68	0.53	98,143,195,199	0
2	R16	B	403	16/16	0.76	0.50	114,132,140,143	0
2	R16	B	405	16/16	0.78	0.29	84,128,148,154	0
2	R16	B	401	16/16	0.78	0.30	144,166,185,186	0

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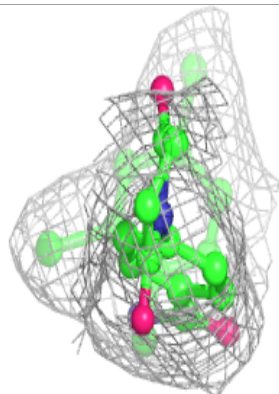
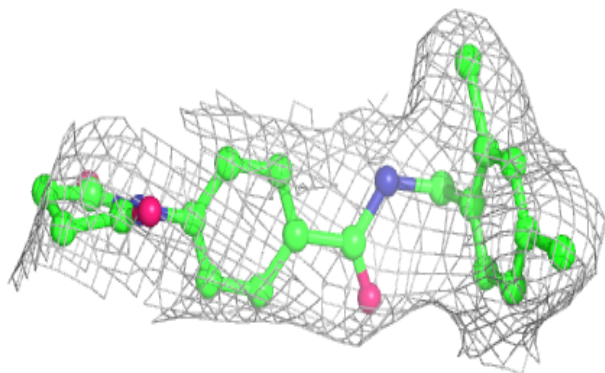
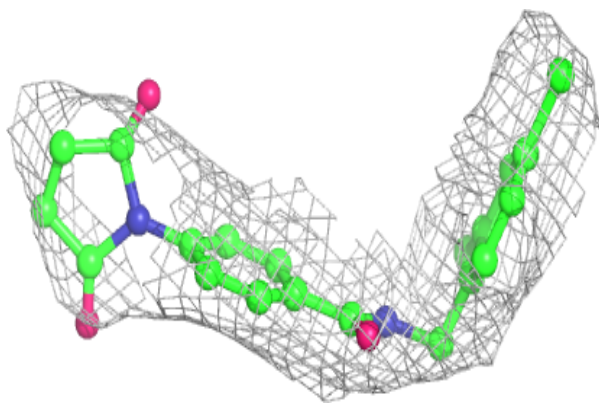
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	R16	B	402	16/16	0.81	0.34	97,114,130,135	0
2	R16	A	602	16/16	0.83	0.26	92,123,138,145	0
5	K	A	606	1/1	0.84	0.06	103,103,103,103	0
2	R16	A	601	16/16	0.84	0.21	107,135,143,144	0
5	K	A	609	1/1	0.87	1.12	140,140,140,140	0
5	K	A	607	1/1	0.90	0.06	95,95,95,95	0
3	WUU	A	603	25/25	0.90	0.19	90,122,156,159	0
3	WUU	B	404	25/25	0.90	0.15	99,131,162,168	0
5	K	A	608	1/1	0.93	0.17	102,102,102,102	0
5	K	A	605	1/1	0.96	0.13	88,88,88,88	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.

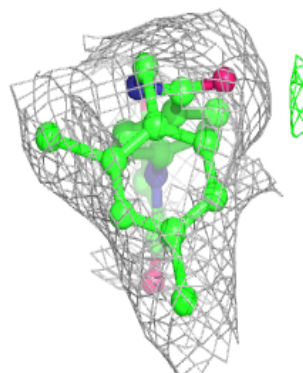
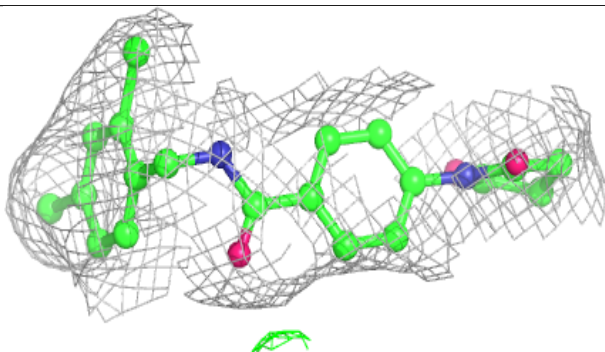
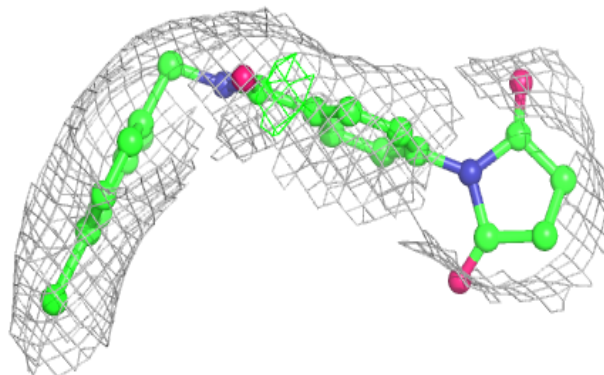


Electron density around WUU A 603:

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

**Electron density around WUU B 404:**

$2mF_o-DF_c$ (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.