



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:44 AM UTC

PDB ID : 8UEC / pdb_00008uec
Title : Structure of TREK-1CG*:CAT335a
Authors : Mondal, A.; Lee, H.; Minor, D.L.
Deposited on : 2023-09-30
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 : 4-5-2 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

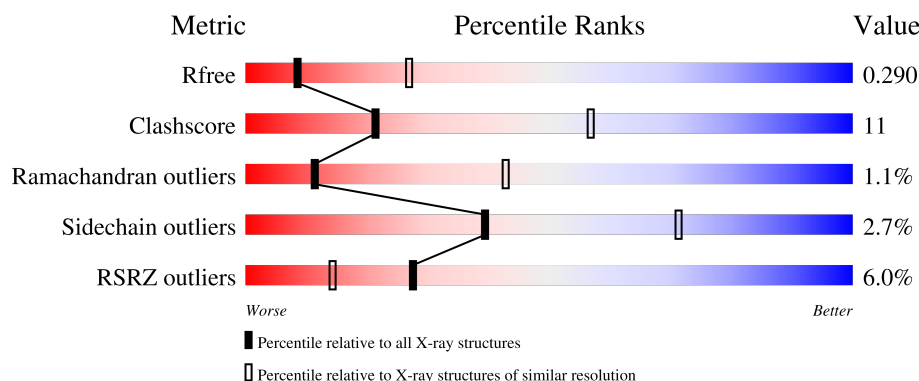
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4536 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
1	A	271	Total	C	N	O	S	0	0	0
			2123	1415	336	366	6			
1	B	282	Total	C	N	O	S	0	0	0
			2157	1436	342	373	6			

There are 28 discrepancies between the modelled and reference sequences:

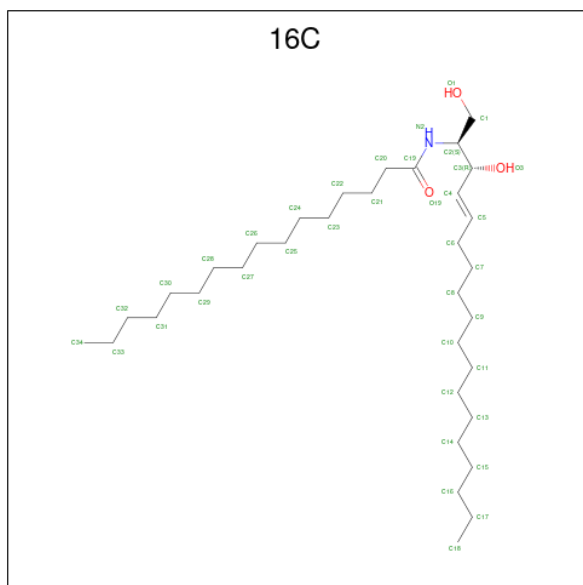
Chain	Residue	Modelled	Actual	Comment	Reference
A	84	ARG	LYS	engineered mutation	UNP P97438
A	85	GLU	GLN	engineered mutation	UNP P97438
A	86	LYS	THR	engineered mutation	UNP P97438
A	88	LEU	ILE	engineered mutation	UNP P97438
A	89	ARG	ALA	engineered mutation	UNP P97438
A	90	ALA	GLN	engineered mutation	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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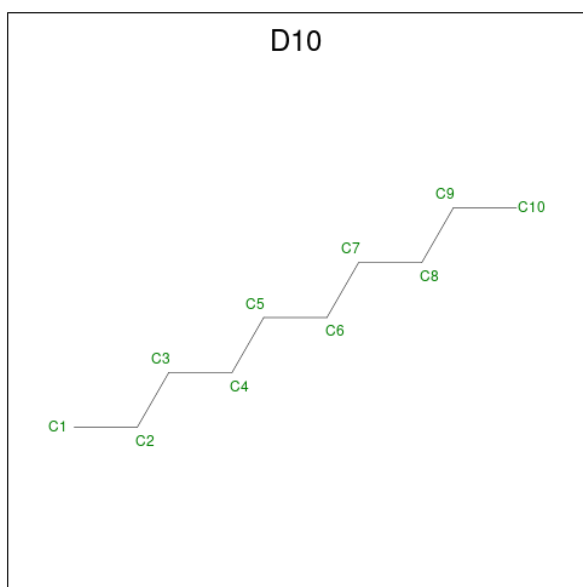
Chain	Residue	Modelled	Actual	Comment	Reference
B	131	CYS	SER	engineered mutation	UNP P97438
B	300	ALA	SER	engineered mutation	UNP P97438
B	306	ALA	GLU	engineered mutation	UNP P97438

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



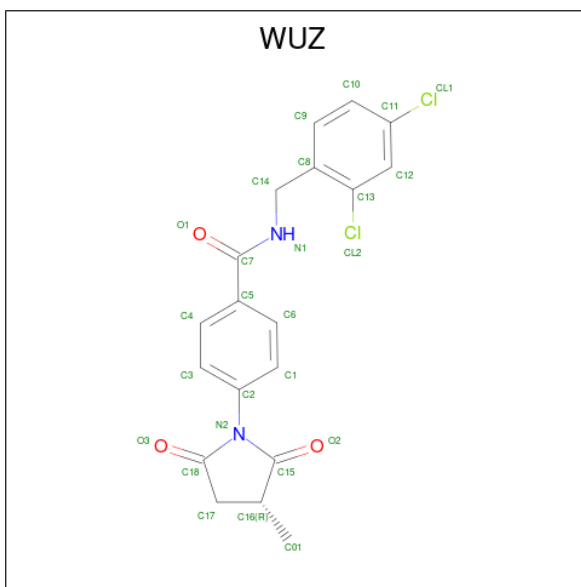
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			38	34	1	3		

- Molecule 3 is DECANE (CCD ID: D10) (formula: C₁₀H₂₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 10 10	0	0
3	A	1	Total C 10 10	0	0
3	A	1	Total C 10 10	0	0
3	A	1	Total C 10 10	0	0
3	A	1	Total C 10 10	0	0
3	A	1	Total C 10 10	0	0
3	B	1	Total C 10 10	0	0
3	B	1	Total C 10 10	0	0
3	B	1	Total C 10 10	0	0
3	B	1	Total C 10 10	0	0
3	B	1	Total C 10 10	0	0

- Molecule 4 is N-[(2,4-dichlorophenyl)methyl]-4-[(3R)-3-methyl-2,5-dioxopyrrolidin-1-yl] benzamide (CCD ID: WUZ) (formula: C₁₉H₁₆Cl₂N₂O₃) (labeled as "Ligand of Interest" by depositor).

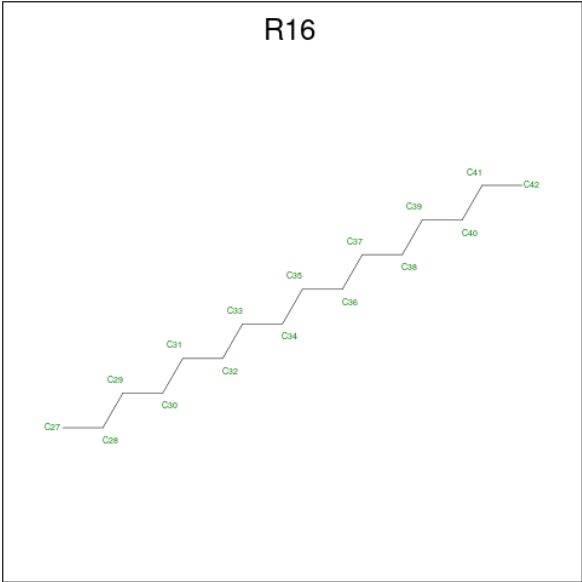


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0
			26	19	2	2	3	
4	B	1	Total	C	Cl	N	O	0
			26	19	2	2	3	

- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	K	0	0
			3	3		
5	B	2	Total	K	0	0
			2	2		

- Molecule 6 is HEXADECANE (CCD ID: R16) (formula: C₁₆H₃₄).



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

- Molecule 7 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	2	Total Cd 2 2	0	0
7	B	1	Total Cd 1 1	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.21Å 120.57Å 128.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.35 – 3.00 29.35 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.8 (29.35-3.00) 91.6 (29.35-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.273 , 0.293 0.278 , 0.290	Depositor DCC
R_{free} test set	1076 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å ²)	107.7	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 117.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4536	wwPDB-VP
Average B, all atoms (Å ²)	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% 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: K, D10, WUZ, R16, 16C, CD

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	0.21	0/2175	0.45	0/2958
1	B	0.20	0/2208	0.46	0/3005
All	All	0.21	0/4383	0.45	0/5963

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2123	0	2175	44	0
1	B	2157	0	2200	50	0
2	A	38	0	67	4	0
3	A	60	0	132	9	0
3	B	50	0	110	2	0
4	A	26	0	0	0	0
4	B	26	0	0	0	0
5	A	3	0	0	0	0
5	B	2	0	0	0	0
6	A	16	0	34	7	0
6	B	32	0	68	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	2	0	0	0	0
7	B	1	0	0	0	0
All	All	4536	0	4786	102	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (102) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ILE:HG21	6:A:410:R16:H412	1.63	0.80
1:B:152:THR:HG23	1:B:155:GLY:H	1.50	0.75
1:A:302:LYS:HA	1:A:305:GLU:HG2	1.70	0.74
1:A:100:ASP:HA	1:A:103:ILE:HD12	1.77	0.66
1:A:285:PHE:HA	1:A:288:VAL:HG22	1.80	0.63
1:A:277:TRP:HB2	6:A:410:R16:H352	1.81	0.62
1:B:100:ASP:OD1	1:B:100:ASP:N	2.31	0.61
2:A:401:16C:H252	2:A:401:16C:H4	1.84	0.60
1:B:307:VAL:HG11	6:B:408:R16:H281	1.83	0.59
1:A:173:LEU:HD22	1:B:54:VAL:HG11	1.84	0.59
3:A:406:D10:H51	6:B:409:R16:H281	1.85	0.58
3:B:403:D10:H82	3:B:403:D10:H31	1.85	0.58
1:B:218:GLY:HA3	1:B:284:TYR:CZ	2.40	0.57
1:B:267:LEU:O	1:B:269:PHE:N	2.34	0.56
1:A:260:GLY:HA2	1:A:266:TYR:CZ	2.41	0.56
1:A:169:LEU:HA	1:A:172:PHE:HD2	1.72	0.55
1:B:302:LYS:O	1:B:305:GLU:HG3	2.06	0.55
1:B:106:ILE:O	1:B:110:ILE:HG13	2.07	0.55
1:A:64:VAL:O	1:A:68:LEU:HD12	2.07	0.55
1:B:109:ALA:HB1	1:B:114:ILE:HG21	1.90	0.54
1:A:275:TRP:HE1	3:A:404:D10:H103	1.73	0.53
1:B:85:GLU:HA	1:B:88:LEU:HB2	1.90	0.53
1:B:71:PRO:O	1:B:74:ILE:HG13	2.09	0.52
1:A:219:CYS:O	1:A:223:VAL:HG22	2.10	0.52
1:B:225:LEU:O	1:B:229:ILE:HG12	2.10	0.52
1:A:304:LYS:HE3	2:A:401:16C:H231	1.92	0.51
1:A:99:LEU:O	1:A:102:LEU:HG	2.10	0.51
1:B:95:SER:O	1:B:97:GLN:N	2.35	0.51
1:B:218:GLY:HA3	1:B:284:TYR:CE1	2.46	0.51
1:A:69:GLU:OE2	1:B:152:THR:HG22	2.12	0.50
1:B:103:ILE:HA	1:B:106:ILE:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:LEU:O	1:A:229:ILE:HG12	2.11	0.50
1:A:218:GLY:HA3	1:A:284:TYR:CE1	2.46	0.50
1:B:40:ASN:HA	1:B:43:LYS:HG2	1.95	0.49
1:A:217:PHE:HA	1:A:220:VAL:HG22	1.94	0.49
1:B:188:GLY:HA2	1:B:191:LYS:HE3	1.93	0.49
1:B:307:VAL:HG21	6:B:408:R16:H281	1.95	0.49
1:A:218:GLY:HA3	1:A:284:TYR:CZ	2.47	0.49
1:A:223:VAL:HA	1:A:245:VAL:HG11	1.94	0.49
1:A:189:ILE:HA	1:A:192:VAL:HG12	1.94	0.49
1:B:60:ILE:O	1:B:64:VAL:HG12	2.13	0.48
1:B:260:GLY:HA2	1:B:266:TYR:CZ	2.49	0.47
1:B:143:ILE:HG12	1:B:251:THR:HA	1.95	0.47
1:B:223:VAL:HA	1:B:245:VAL:HG11	1.97	0.47
1:B:271:LYS:HD2	3:B:403:D10:H71	1.97	0.47
1:B:99:LEU:O	1:B:103:ILE:HG12	2.15	0.47
1:B:245:VAL:HG13	1:B:277:TRP:HZ2	1.80	0.46
1:A:158:PHE:CZ	1:B:64:VAL:HG11	2.50	0.46
3:A:402:D10:H51	3:A:402:D10:H82	1.65	0.46
1:A:252:ILE:HD13	1:B:139:VAL:HG23	1.97	0.46
1:A:270:TYR:CD1	6:A:410:R16:H422	2.51	0.46
1:A:134:PHE:O	1:A:138:THR:HG23	2.16	0.45
1:B:294:ASP:HA	1:B:297:ARG:HE	1.81	0.45
2:A:401:16C:N2	2:A:401:16C:H222	2.31	0.45
3:A:402:D10:H32	3:A:402:D10:H62	1.68	0.45
1:B:205:LYS:O	1:B:208:ILE:HG22	2.16	0.45
1:B:256:ASP:OD1	1:B:256:ASP:N	2.50	0.45
1:A:88:LEU:HD21	1:A:99:LEU:HD22	1.97	0.44
1:A:264:ILE:HB	1:A:266:TYR:CZ	2.52	0.44
1:A:270:TYR:HD1	6:A:410:R16:H422	1.81	0.44
6:A:410:R16:H361	6:A:410:R16:H332	1.53	0.44
1:B:72:GLN:O	1:B:76:GLN:NE2	2.49	0.44
1:A:39:ILE:O	1:A:43:LYS:HG3	2.18	0.44
1:A:102:LEU:HD12	1:A:103:ILE:HG13	2.00	0.44
1:A:262:SER:HB2	1:A:264:ILE:HG12	2.00	0.44
1:B:231:LYS:HE3	1:B:231:LYS:HB3	1.78	0.44
1:A:172:PHE:CG	3:A:406:D10:H82	2.53	0.44
3:A:404:D10:H82	3:A:404:D10:H52	1.55	0.44
6:A:410:R16:H341	6:A:410:R16:H312	1.57	0.44
1:A:250:THR:O	1:A:251:THR:OG1	2.32	0.43
1:B:136:ALA:HA	1:B:139:VAL:HG12	2.00	0.43
1:B:244:PHE:CE1	1:B:248:THR:HG21	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ARG:O	1:A:88:LEU:HD23	2.18	0.43
1:B:262:SER:HB2	1:B:264:ILE:HG13	2.00	0.43
1:A:268:ASP:N	1:A:268:ASP:OD1	2.51	0.43
1:A:192:VAL:HA	1:A:195:THR:HG22	2.01	0.43
1:B:149:SER:HB2	1:B:151:ARG:HH12	1.83	0.43
1:A:49:THR:HG23	2:A:401:16C:H322	2.01	0.43
1:B:51:PHE:O	1:B:54:VAL:HG12	2.19	0.43
1:A:216:LEU:O	1:A:220:VAL:HG13	2.20	0.42
1:B:100:ASP:O	1:B:104:GLN:HG3	2.19	0.42
1:B:233:ILE:HG21	1:B:270:TYR:CE1	2.54	0.42
6:B:408:R16:H362	6:B:408:R16:H392	1.74	0.42
1:B:79:THR:O	1:B:83:GLN:HG2	2.19	0.42
1:B:212:ILE:O	1:B:215:ILE:HG13	2.20	0.42
1:A:256:ASP:OD1	1:A:256:ASP:N	2.52	0.42
1:B:229:ILE:O	1:B:233:ILE:HG22	2.19	0.42
1:A:168:PRO:HA	3:A:414:D10:H31	2.01	0.42
1:A:207:ARG:O	1:A:211:THR:HG23	2.20	0.42
1:A:273:VAL:HG12	6:A:410:R16:H402	2.02	0.41
3:A:406:D10:H102	1:B:300:ALA:HB2	2.03	0.41
1:B:94:VAL:HG12	1:B:96:ASP:H	1.85	0.41
1:B:231:LYS:HD3	1:B:238:ALA:N	2.35	0.41
1:A:70:GLN:N	1:A:71:PRO:HD2	2.35	0.41
1:B:267:LEU:C	1:B:269:PHE:H	2.24	0.41
1:A:82:ILE:HD13	1:A:82:ILE:HA	1.91	0.40
1:A:206:ILE:H	1:A:206:ILE:HG13	1.71	0.40
1:B:233:ILE:HD13	1:B:270:TYR:CE1	2.56	0.40
1:B:141:THR:HG22	1:B:170:PHE:CE2	2.56	0.40
6:B:409:R16:H342	6:B:409:R16:H371	1.69	0.40
3:A:406:D10:H101	6:B:409:R16:H361	2.04	0.40
1:B:231:LYS:HD2	1:B:236:TRP:O	2.21	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	A	267/287 (93%)	251 (94%)	14 (5%)	2 (1%)	18	53
1	B	280/287 (98%)	256 (91%)	20 (7%)	4 (1%)	9	36
All	All	547/574 (95%)	507 (93%)	34 (6%)	6 (1%)	11	43

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	ILE
1	B	314	ALA
1	B	197	ILE
1	B	36	ASP
1	B	200	ASN
1	A	198	LYS

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	A	223/236 (94%)	216 (97%)	7 (3%)	35	68
1	B	223/236 (94%)	218 (98%)	5 (2%)	45	74
All	All	446/472 (94%)	434 (97%)	12 (3%)	39	71

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	ASP
1	A	129	LEU
1	A	201	VAL
1	A	206	ILE
1	A	223	VAL
1	A	279	LEU
1	A	313	HIS

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Mol	Chain	Res	Type
1	B	54	VAL
1	B	56	LEU
1	B	64	VAL
1	B	100	ASP
1	B	195	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	GLN
1	A	72	GLN
1	A	76	GLN
1	A	126	HIS
1	B	76	GLN
1	B	83	GLN
1	B	122	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 8 are monoatomic - leaving 17 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	16C	A	401	-	36,37,37	1.68	5 (13%)	37,39,39	1.30	3 (8%)
6	R16	B	408	-	15,15,15	0.33	0	14,14,14	0.81	0
3	D10	B	403	-	9,9,9	0.32	0	8,8,8	0.78	0
3	D10	B	404	-	9,9,9	0.38	0	8,8,8	0.55	0
3	D10	A	404	-	9,9,9	0.34	0	8,8,8	0.61	0
3	D10	A	413	-	9,9,9	0.34	0	8,8,8	0.75	0
3	D10	A	414	-	9,9,9	0.34	0	8,8,8	0.77	0
3	D10	B	401	-	9,9,9	0.30	0	8,8,8	0.80	0
3	D10	B	402	-	9,9,9	0.33	0	8,8,8	0.77	0
6	R16	B	409	-	15,15,15	0.31	0	14,14,14	0.85	0
4	WUZ	B	405	1	28,28,28	2.63	4 (14%)	40,40,40	1.91	9 (22%)
3	D10	A	406	-	9,9,9	0.30	0	8,8,8	0.83	0
6	R16	A	410	-	15,15,15	0.31	0	14,14,14	0.84	0
3	D10	A	403	-	9,9,9	0.33	0	8,8,8	0.77	0
4	WUZ	A	405	1	28,28,28	2.70	4 (14%)	40,40,40	1.91	10 (25%)
3	D10	B	411	-	9,9,9	0.30	0	8,8,8	0.82	0
3	D10	A	402	-	9,9,9	0.32	0	8,8,8	0.77	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	16C	A	401	-	-	23/40/40/40	-
6	R16	B	408	-	-	6/13/13/13	-
3	D10	B	403	-	-	4/7/7/7	-
3	D10	B	404	-	-	5/7/7/7	-
3	D10	A	404	-	-	5/7/7/7	-
3	D10	A	413	-	-	0/7/7/7	-
3	D10	A	414	-	-	4/7/7/7	-
3	D10	B	401	-	-	2/7/7/7	-
3	D10	B	402	-	-	2/7/7/7	-
6	R16	B	409	-	-	6/13/13/13	-
4	WUZ	B	405	1	-	0/13/29/29	0/3/3/3
3	D10	A	406	-	-	3/7/7/7	-
6	R16	A	410	-	-	9/13/13/13	-
3	D10	A	403	-	-	3/7/7/7	-
4	WUZ	A	405	1	-	0/13/29/29	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	D10	B	411	-	-	3/7/7/7	-
3	D10	A	402	-	-	3/7/7/7	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	405	WUZ	C18-N2	9.92	1.52	1.40
4	B	405	WUZ	C18-N2	9.68	1.52	1.40
2	A	401	16C	C19-N2	6.92	1.48	1.34
4	A	405	WUZ	C15-N2	6.85	1.49	1.40
4	B	405	WUZ	C15-N2	6.51	1.49	1.40
4	A	405	WUZ	C7-N1	5.35	1.45	1.33
4	B	405	WUZ	C7-N1	5.22	1.45	1.33
2	A	401	16C	C3-C4	4.12	1.56	1.50
2	A	401	16C	O19-C19	-2.68	1.17	1.23
2	A	401	16C	C20-C19	2.54	1.56	1.51
2	A	401	16C	O3-C3	-2.50	1.39	1.43
4	A	405	WUZ	C13-CL2	2.33	1.79	1.73
4	B	405	WUZ	C13-CL2	2.22	1.78	1.73

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	405	WUZ	C15-N2-C18	-5.12	106.97	112.46
4	B	405	WUZ	C15-N2-C18	-5.06	107.03	112.46
4	B	405	WUZ	C8-C14-N1	-4.69	103.68	113.15
2	A	401	16C	C3-C2-N2	-4.44	102.13	109.66
4	A	405	WUZ	C8-C14-N1	-4.30	104.49	113.15
4	B	405	WUZ	C17-C16-C15	4.16	107.44	103.94
4	A	405	WUZ	C17-C16-C15	4.03	107.33	103.94
4	B	405	WUZ	C16-C15-N2	-3.57	106.08	108.24
4	A	405	WUZ	O3-C18-N2	3.42	127.57	124.03
4	A	405	WUZ	C17-C18-N2	-3.17	105.57	108.06
4	A	405	WUZ	C16-C15-N2	-3.10	106.37	108.24
4	B	405	WUZ	C17-C18-N2	-2.90	105.78	108.06
4	B	405	WUZ	C2-N2-C15	2.88	127.06	123.59
4	B	405	WUZ	O3-C18-N2	2.84	126.97	124.03
4	A	405	WUZ	C12-C13-C8	-2.76	120.00	122.41
4	A	405	WUZ	C2-N2-C15	2.64	126.77	123.59
4	A	405	WUZ	O2-C15-N2	2.56	127.09	124.30
4	B	405	WUZ	C12-C13-C8	-2.41	120.30	122.41
2	A	401	16C	O19-C19-N2	-2.38	118.92	122.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	16C	C20-C19-N2	2.34	119.98	115.86
4	A	405	WUZ	C9-C8-C13	2.15	120.30	116.91
4	B	405	WUZ	O2-C15-N2	2.12	126.62	124.30

There are no chirality outliers.

All (78) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	16C	O1-C1-C2-N2
2	A	401	16C	N2-C2-C3-C4
2	A	401	16C	N2-C2-C3-O3
2	A	401	16C	C1-C2-C3-C4
2	A	401	16C	C1-C2-C3-O3
2	A	401	16C	C2-C3-C4-C5
2	A	401	16C	O3-C3-C4-C5
3	A	404	D10	C3-C4-C5-C6
3	B	404	D10	C3-C4-C5-C6
3	A	404	D10	C5-C6-C7-C8
6	A	410	R16	C33-C34-C35-C36
6	B	408	R16	C36-C37-C38-C39
3	B	402	D10	C3-C4-C5-C6
3	B	411	D10	C5-C6-C7-C8
3	B	403	D10	C4-C5-C6-C7
6	A	410	R16	C38-C39-C40-C41
6	B	408	R16	C35-C36-C37-C38
3	B	402	D10	C2-C3-C4-C5
3	A	414	D10	C4-C5-C6-C7
3	A	402	D10	C2-C3-C4-C5
3	B	403	D10	C3-C4-C5-C6
6	B	409	R16	C35-C36-C37-C38
3	A	403	D10	C3-C4-C5-C6
2	A	401	16C	C20-C21-C22-C23
6	A	410	R16	C34-C35-C36-C37
2	A	401	16C	O1-C1-C2-C3
2	A	401	16C	C10-C11-C12-C13
6	B	409	R16	C28-C29-C30-C31
2	A	401	16C	C13-C14-C15-C16
3	A	404	D10	C1-C2-C3-C4
3	B	404	D10	C1-C2-C3-C4
2	A	401	16C	C12-C13-C14-C15
6	A	410	R16	C28-C29-C30-C31
3	B	404	D10	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
6	A	410	R16	C30-C31-C32-C33
6	B	408	R16	C28-C29-C30-C31
3	B	411	D10	C6-C7-C8-C9
3	B	403	D10	C5-C6-C7-C8
3	A	403	D10	C5-C6-C7-C8
6	B	408	R16	C34-C35-C36-C37
6	A	410	R16	C31-C32-C33-C34
2	A	401	16C	C31-C32-C33-C34
6	B	409	R16	C32-C33-C34-C35
3	A	414	D10	C3-C4-C5-C6
3	A	406	D10	C5-C6-C7-C8
6	A	410	R16	C36-C37-C38-C39
6	B	409	R16	C29-C30-C31-C32
6	A	410	R16	C32-C33-C34-C35
6	B	409	R16	C34-C35-C36-C37
3	A	414	D10	C7-C8-C9-C10
3	A	402	D10	C3-C4-C5-C6
3	A	414	D10	C5-C6-C7-C8
3	B	401	D10	C1-C2-C3-C4
2	A	401	16C	C26-C27-C28-C29
6	B	408	R16	C33-C34-C35-C36
6	A	410	R16	C35-C36-C37-C38
2	A	401	16C	C11-C12-C13-C14
3	B	411	D10	C4-C5-C6-C7
3	B	404	D10	C6-C7-C8-C9
2	A	401	16C	C27-C28-C29-C30
3	B	404	D10	C7-C8-C9-C10
3	A	404	D10	C7-C8-C9-C10
3	B	401	D10	C5-C6-C7-C8
3	A	404	D10	C6-C7-C8-C9
2	A	401	16C	C6-C7-C8-C9
3	A	406	D10	C3-C4-C5-C6
2	A	401	16C	C28-C29-C30-C31
3	A	406	D10	C4-C5-C6-C7
2	A	401	16C	C11-C10-C9-C8
6	B	409	R16	C39-C40-C41-C42
2	A	401	16C	C25-C26-C27-C28
6	B	408	R16	C29-C30-C31-C32
2	A	401	16C	C22-C23-C24-C25
2	A	401	16C	C29-C30-C31-C32
3	A	403	D10	C1-C2-C3-C4
3	A	402	D10	C5-C6-C7-C8

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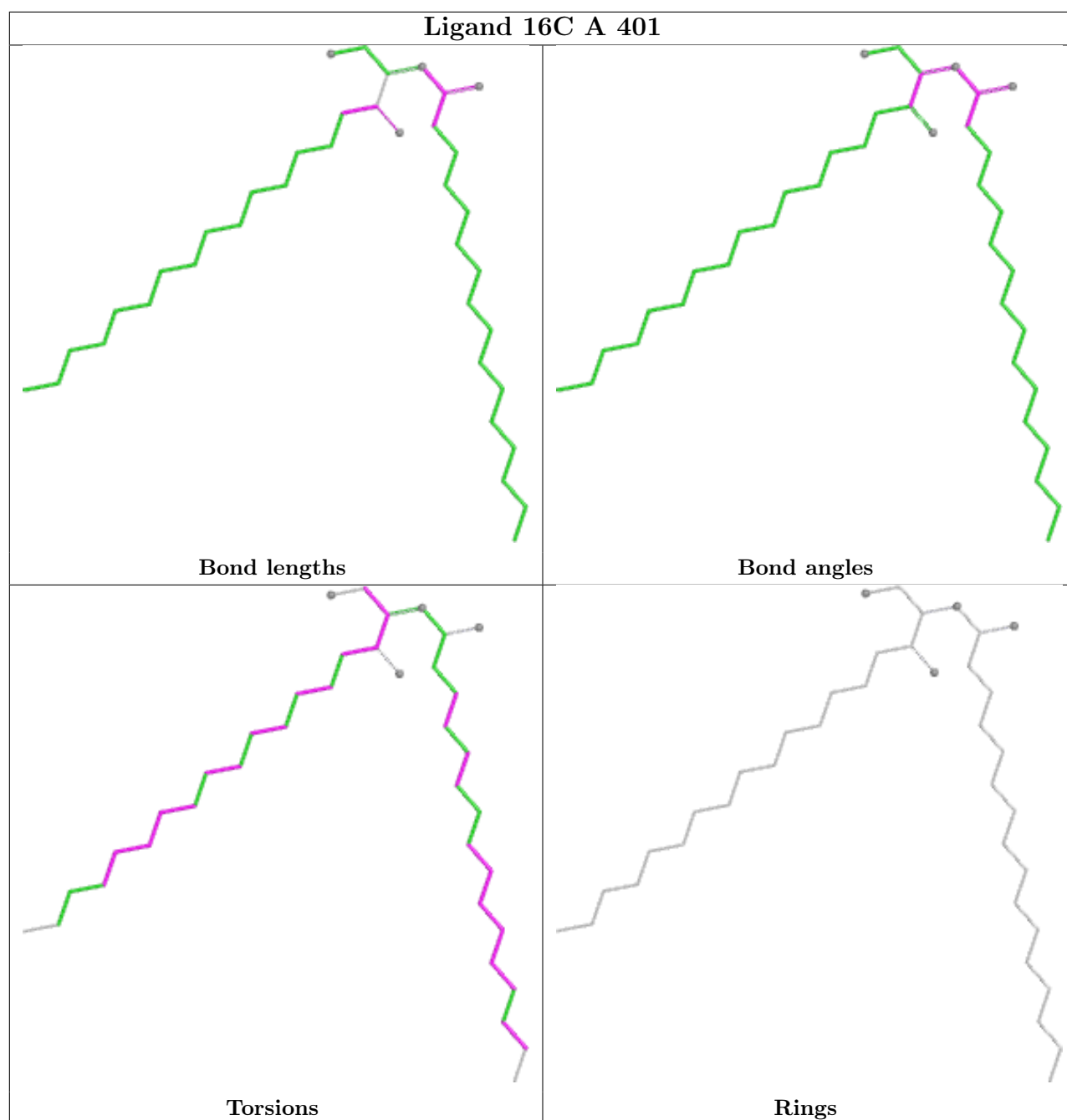
Mol	Chain	Res	Type	Atoms
3	B	403	D10	C7-C8-C9-C10
2	A	401	16C	C4-C5-C6-C7

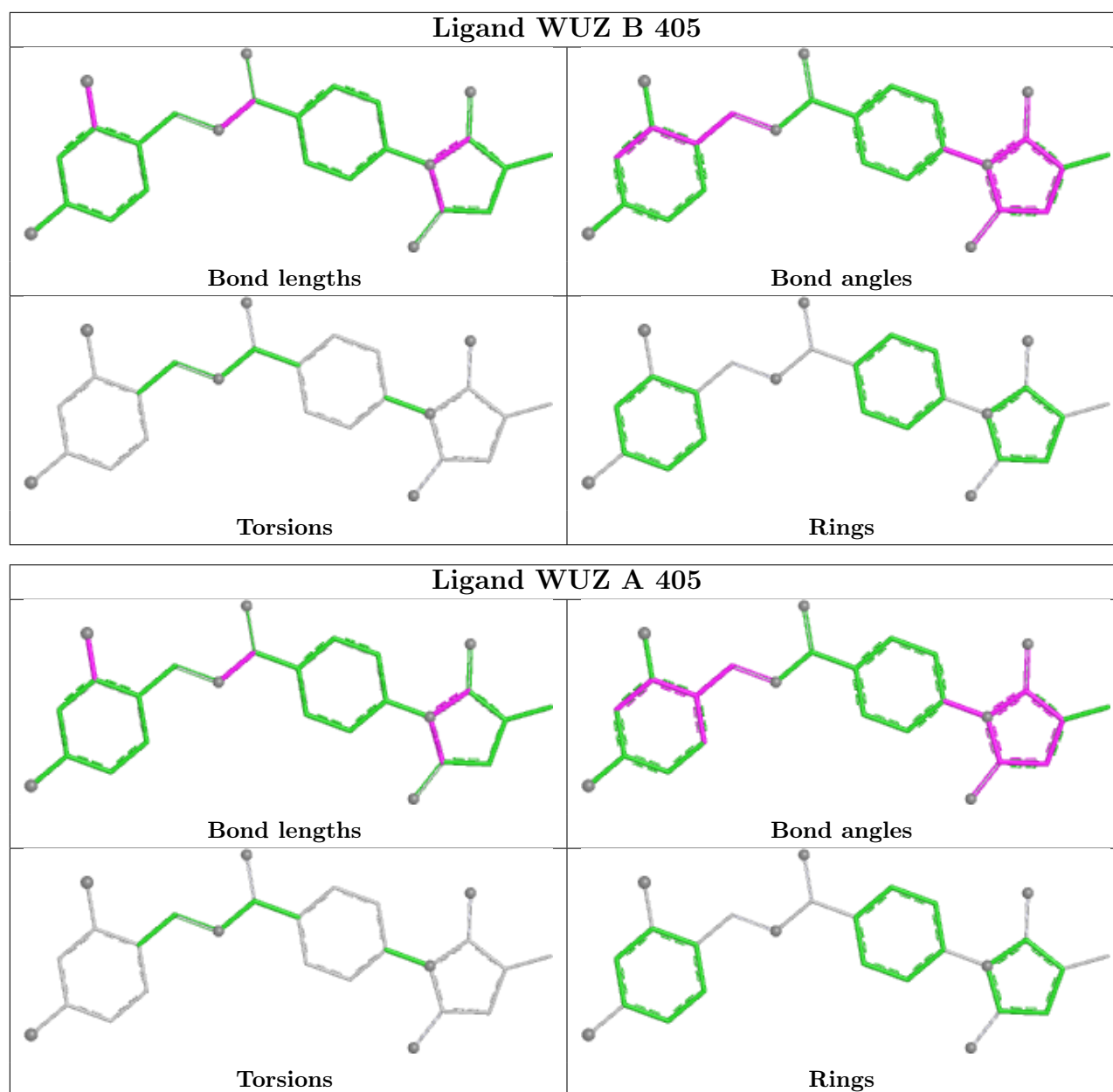
There are no ring outliers.

9 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	16C	4	0
6	B	408	R16	3	0
3	B	403	D10	2	0
3	A	404	D10	2	0
3	A	414	D10	1	0
6	B	409	R16	3	0
3	A	406	D10	4	0
6	A	410	R16	7	0
3	A	402	D10	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	271/287 (94%)	0.39	9 (3%)	49 28	71, 119, 236, 259	0
1	B	282/287 (98%)	0.45	24 (8%)	16 8	74, 131, 236, 261	0
All	All	553/574 (96%)	0.42	33 (5%)	27 14	71, 124, 237, 261	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	255	GLY	5.4
1	A	147	ASN	5.3
1	B	276	PHE	5.0
1	B	36	ASP	4.3
1	B	265	GLU	3.4
1	A	41	VAL	3.4
1	B	158	PHE	3.3
1	A	37	SER	3.1
1	B	254	PHE	3.1
1	A	149	SER	3.0
1	B	124	VAL	3.0
1	B	256	ASP	2.9
1	B	116	PRO	2.8
1	A	146	GLY	2.8
1	A	78	THR	2.8
1	A	96	ASP	2.7
1	B	119	ALA	2.7
1	B	148	ILE	2.6
1	B	37	SER	2.6
1	B	115	ILE	2.6
1	B	147	ASN	2.5
1	B	100	ASP	2.5
1	B	263	ASP	2.4
1	B	38	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	132	SER	2.4
1	B	120	SER	2.4
1	B	63	THR	2.3
1	B	200	ASN	2.3
1	B	255	GLY	2.2
1	B	118	GLY	2.2
1	B	106	ILE	2.1
1	A	256	ASP	2.0
1	B	272	PRO	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
2	16C	A	401	38/38	0.60	0.23	108,144,212,229	0
3	D10	A	402	10/10	0.66	0.23	129,149,162,170	0
3	D10	A	413	10/10	0.76	0.36	104,135,140,146	0
3	D10	B	401	10/10	0.78	0.23	118,137,159,159	0
3	D10	A	403	10/10	0.79	0.27	109,122,136,136	0
3	D10	A	404	10/10	0.81	0.26	100,116,130,135	0
3	D10	A	414	10/10	0.85	0.20	87,100,101,114	0
3	D10	A	406	10/10	0.85	0.23	103,122,151,159	0
3	D10	B	403	10/10	0.86	0.33	122,135,145,153	0
3	D10	B	411	10/10	0.86	0.21	121,139,151,159	0
6	R16	A	410	16/16	0.86	0.33	124,134,150,161	0
4	WUZ	A	405	26/26	0.87	0.13	88,109,148,155	0
6	R16	B	408	16/16	0.87	0.21	91,112,131,133	0
6	R16	B	409	16/16	0.87	0.26	105,119,136,137	0

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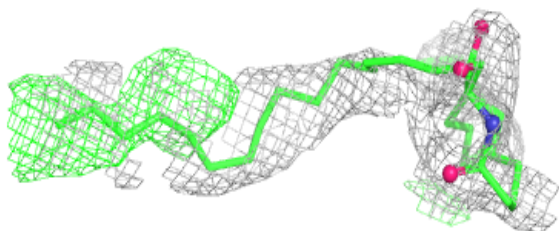
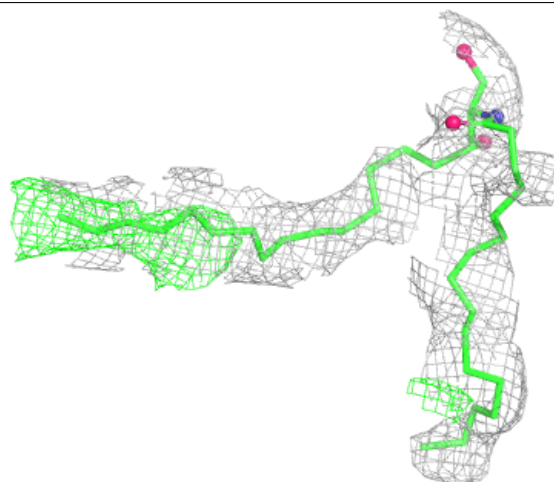
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	CD	B	410	1/1	0.87	0.10	234,234,234,234	0
3	D10	B	402	10/10	0.88	0.22	123,132,136,139	0
4	WUZ	B	405	26/26	0.89	0.14	91,118,143,146	0
5	K	B	407	1/1	0.89	0.13	144,144,144,144	0
5	K	B	406	1/1	0.91	0.06	77,77,77,77	0
3	D10	B	404	10/10	0.91	0.24	101,105,116,118	0
7	CD	A	412	1/1	0.95	0.09	162,162,162,162	0
7	CD	A	411	1/1	0.96	0.10	250,250,250,250	0
5	K	A	409	1/1	0.97	0.13	98,98,98,98	0
5	K	A	408	1/1	0.98	0.05	81,81,81,81	0
5	K	A	407	1/1	0.98	0.10	84,84,84,84	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.

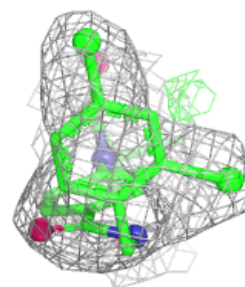
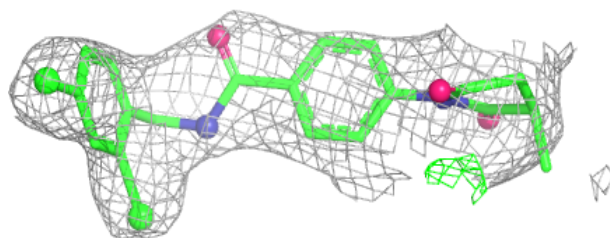
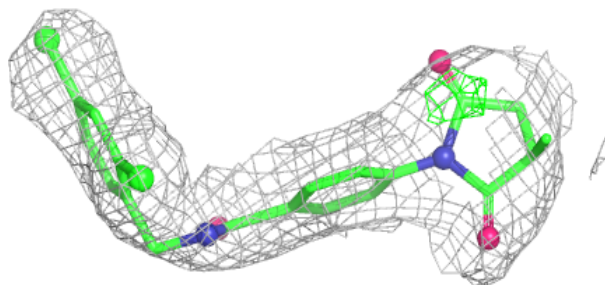
Electron density around 16C A 401:

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

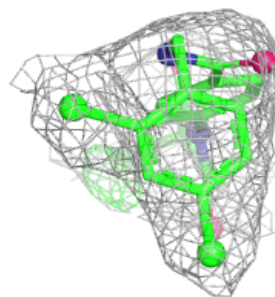
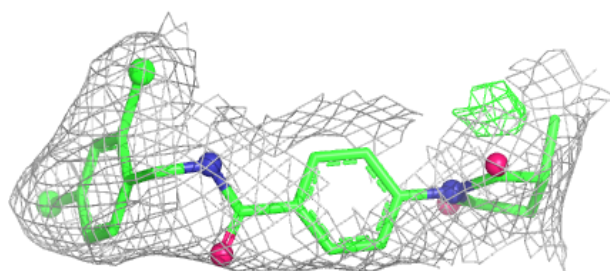
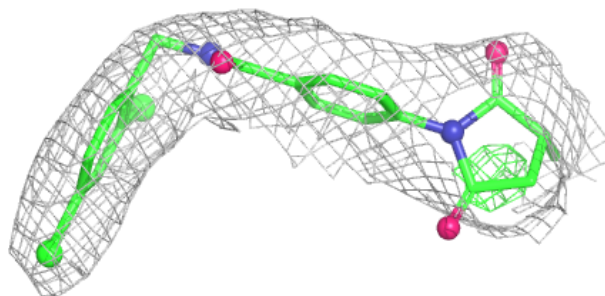


Electron density around WUZ A 405:

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

**Electron density around WUZ B 405:**

$2mF_o-DF_c$ (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.