Full wwPDB X-ray Structure Validation Report (i)

Jun 20, 2024 – 12:04 PM EDT

PDB ID	:	8UEC
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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

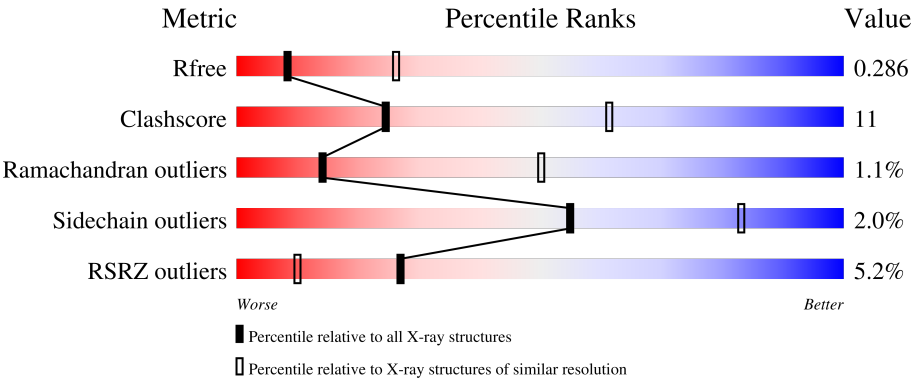
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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 <=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	3% 73% 21% 6%
1	B	287	7% 71% 27%

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
3	D10	A	402	-	-	-	X
3	D10	A	404	-	-	-	X
3	D10	A	413	-	-	-	X
3	D10	A	414	-	-	-	X
5	K	B	407	-	-	-	X
6	R16	A	410	-	-	-	X
6	R16	B	409	-	-	-	X

2 Entry composition (i)

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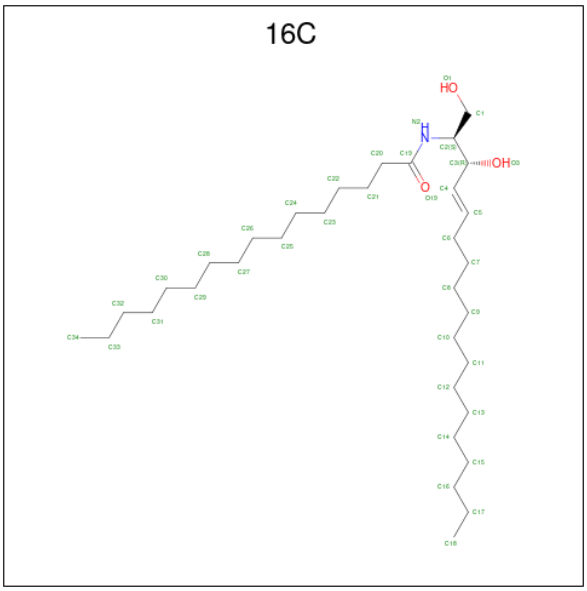
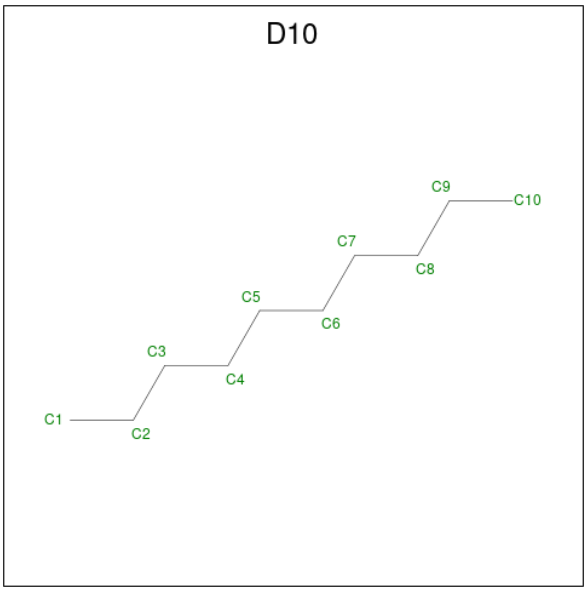
Chain	Residue	Modelled	Actual	Comment	Reference
B	131	CYS	SER	engineered mutation	UNP P97438
B	300	ALA	SER	engineered mutation	UNP P97438
B	306	ALA	GLU	engineered mutation	UNP P97438

- Molecule 2 is N-((E,2S,3R)-1,3-DIHYDROXYOCTADEC-4-EN-2-YL)PALMITAMIDE (three-letter code: 16C) (formula: $C_{34}H_{67}NO_3$).



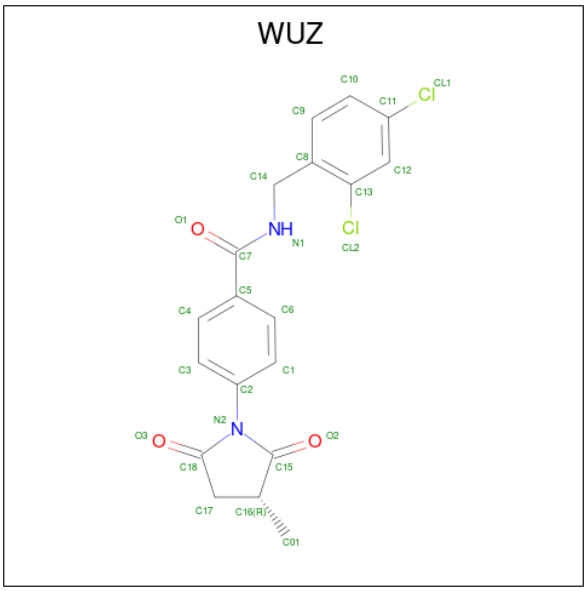
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			38	34	1	3		

- Molecule 3 is DECANE (three-letter code: D10) (formula: $C_{10}H_{22}$).



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 (three-letter code: WUZ) (formula: $C_{19}H_{16}Cl_2N_2O_3$) (labeled as "Ligand of Interest" by depositor).

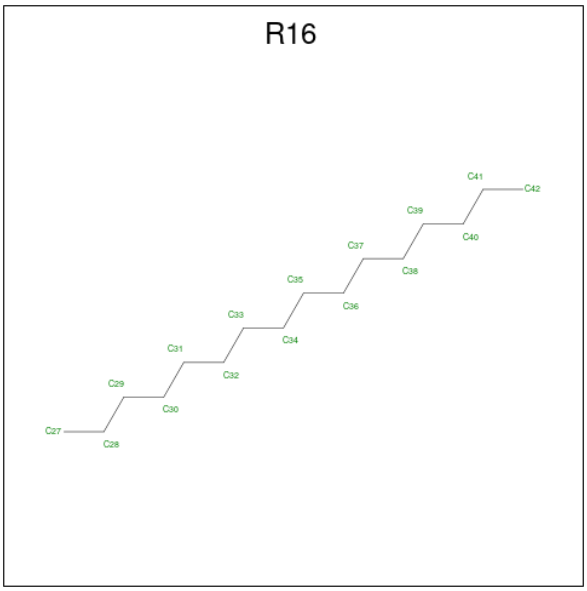


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			26	19	2	2	3		
4	B	1	Total	C	Cl	N	O	0	0
			26	19	2	2	3		

- Molecule 5 is POTASSIUM ION (three-letter code: 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 (three-letter code: R16) (formula: $C_{16}H_{34}$).



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 (three-letter code: CD) (formula: Cd).

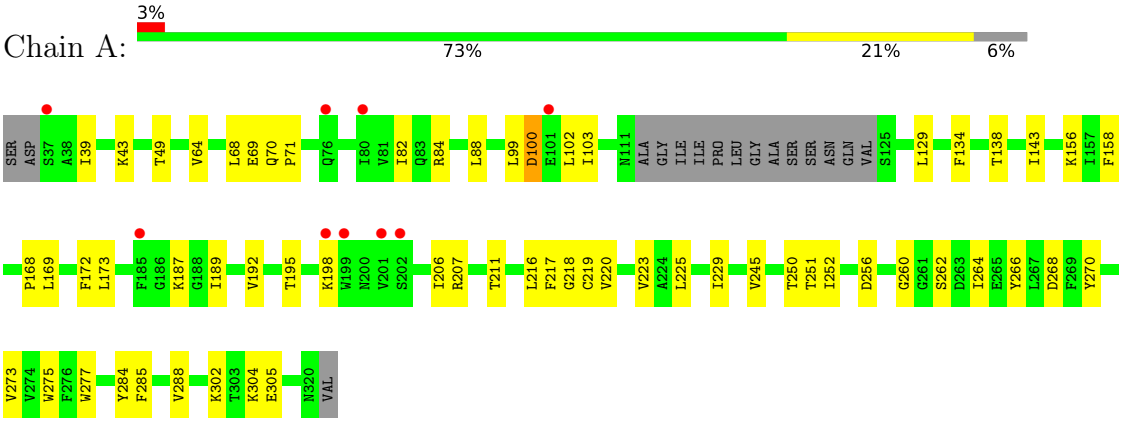
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	2	Total Cd 2 2	0	0
7	B	1	Total Cd 1 1	0	0

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.

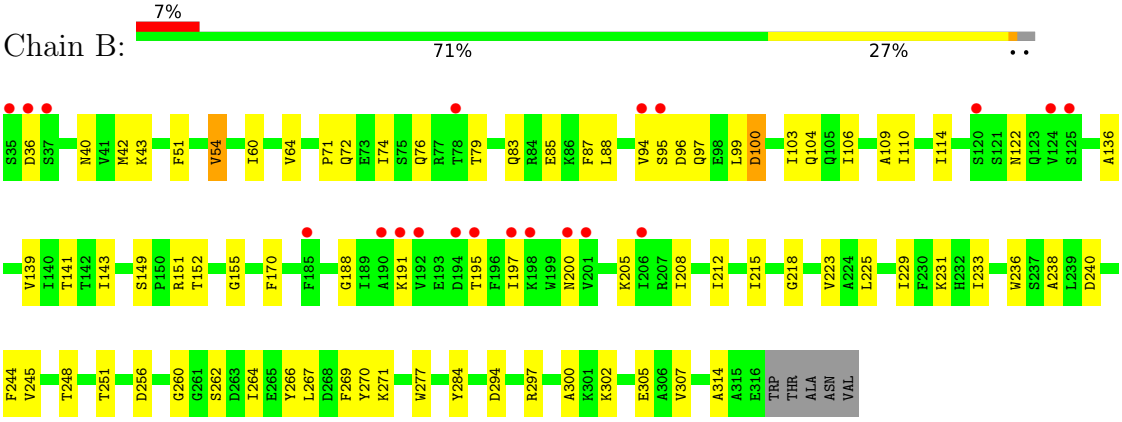
• Molecule 1: Potassium channel subfamily K member 2

Chain A:



• Molecule 1: Potassium channel subfamily K member 2

Chain B:



4 Data and refinement statistics (i)

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 43.36 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.8 (29.35-3.00) 91.7 (43.36-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.273 , 0.293 0.274 , 0.286	Depositor DCC
R_{free} test set	997 reflections (5.04%)	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 , 120.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: D10, CD, K, 16C, R16, WUZ

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	0.30	0/2175	0.49	0/2958
1	B	0.30	0/2208	0.49	0/3005
All	All	0.30	0/4383	0.49	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

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	45	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:A:156:LYS:NZ	1:B:240:ASP:OD1	2.44	0.47
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:PHE:CE1	1:B:248:THR:HG21	2.52	0.43
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: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 (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	267/287 (93%)	251 (94%)	14 (5%)	2 (1%)	22 60
1	B	280/287 (98%)	256 (91%)	20 (7%)	4 (1%)	11 43
All	All	547/574 (95%)	507 (93%)	34 (6%)	6 (1%)	14 50

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 (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	223/236 (94%)	220 (99%)	3 (1%)	69 89
1	B	223/236 (94%)	217 (97%)	6 (3%)	44 77
All	All	446/472 (94%)	437 (98%)	9 (2%)	55 83

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	ASP
1	A	129	LEU
1	A	187	LYS
1	B	42	MET
1	B	54	VAL
1	B	87	PHE
1	B	100	ASP

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Mol	Chain	Res	Type
1	B	122	ASN
1	B	195	THR

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

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 monosaccharides in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
4	WUZ	A	405	1	27,28,28	2.81	4 (14%)	38,40,40	2.12	10 (26%)
2	16C	A	401	-	36,37,37	1.64	5 (13%)	37,39,39	1.29	3 (8%)
3	D10	A	404	-	9,9,9	0.33	0	8,8,8	0.59	0
3	D10	A	414	-	9,9,9	0.33	0	8,8,8	0.76	0
3	D10	B	402	-	9,9,9	0.32	0	8,8,8	0.76	0
6	R16	A	410	-	15,15,15	0.30	0	14,14,14	0.83	0
3	D10	B	403	-	9,9,9	0.31	0	8,8,8	0.76	0
3	D10	A	413	-	9,9,9	0.33	0	8,8,8	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	D10	B	404	-	9,9,9	0.36	0	8,8,8	0.54	0
6	R16	B	409	-	15,15,15	0.31	0	14,14,14	0.84	0
4	WUZ	B	405	1	27,28,28	2.73	6 (22%)	38,40,40	2.10	9 (23%)
3	D10	B	411	-	9,9,9	0.30	0	8,8,8	0.81	0
3	D10	A	403	-	9,9,9	0.32	0	8,8,8	0.76	0
3	D10	B	401	-	9,9,9	0.30	0	8,8,8	0.79	0
6	R16	B	408	-	15,15,15	0.32	0	14,14,14	0.80	0
3	D10	A	402	-	9,9,9	0.31	0	8,8,8	0.76	0
3	D10	A	406	-	9,9,9	0.30	0	8,8,8	0.82	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
4	WUZ	A	405	1	-	0/13/29/29	0/3/3/3
2	16C	A	401	-	-	23/40/40/40	-
3	D10	A	404	-	-	5/7/7/7	-
3	D10	A	414	-	-	4/7/7/7	-
3	D10	B	402	-	-	2/7/7/7	-
6	R16	A	410	-	-	9/13/13/13	-
3	D10	B	403	-	-	4/7/7/7	-
3	D10	A	413	-	-	0/7/7/7	-
3	D10	B	404	-	-	5/7/7/7	-
6	R16	B	409	-	-	6/13/13/13	-
4	WUZ	B	405	1	-	0/13/29/29	0/3/3/3
3	D10	B	411	-	-	3/7/7/7	-
3	D10	A	403	-	-	3/7/7/7	-
3	D10	B	401	-	-	2/7/7/7	-
6	R16	B	408	-	-	6/13/13/13	-
3	D10	A	402	-	-	3/7/7/7	-
3	D10	A	406	-	-	3/7/7/7	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	405	WUZ	C18-N2	9.89	1.52	1.40
4	B	405	WUZ	C18-N2	9.65	1.52	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	405	WUZ	C15-N2	7.39	1.49	1.40
4	B	405	WUZ	C15-N2	7.03	1.49	1.40
2	A	401	16C	C19-N2	6.87	1.48	1.34
4	A	405	WUZ	C7-N1	5.37	1.45	1.33
4	B	405	WUZ	C7-N1	5.24	1.45	1.33
2	A	401	16C	C3-C4	3.93	1.56	1.50
2	A	401	16C	C20-C19	2.67	1.56	1.51
2	A	401	16C	O19-C19	-2.62	1.17	1.23
2	A	401	16C	O3-C3	-2.37	1.39	1.43
4	A	405	WUZ	C13-CL2	2.31	1.79	1.73
4	B	405	WUZ	C13-CL2	2.20	1.78	1.73
4	B	405	WUZ	O1-C7	-2.12	1.19	1.23
4	B	405	WUZ	C11-CL1	2.09	1.79	1.74

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	405	WUZ	C15-N2-C18	-7.21	106.97	112.48
4	B	405	WUZ	C15-N2-C18	-7.13	107.03	112.48
4	B	405	WUZ	C8-C14-N1	-4.43	103.68	113.03
2	A	401	16C	C3-C2-N2	-4.35	102.13	110.01
4	A	405	WUZ	C8-C14-N1	-4.05	104.49	113.03
4	B	405	WUZ	C17-C16-C15	3.99	107.44	103.95
4	A	405	WUZ	O3-C18-N2	3.99	127.57	124.01
4	A	405	WUZ	C17-C16-C15	3.87	107.33	103.95
4	B	405	WUZ	C16-C15-N2	-3.46	106.08	108.26
4	B	405	WUZ	O3-C18-N2	3.31	126.97	124.01
4	B	405	WUZ	C2-N2-C15	3.07	127.06	123.61
4	A	405	WUZ	C16-C15-N2	-3.00	106.37	108.26
4	A	405	WUZ	C17-C18-N2	-2.96	105.57	108.06
4	A	405	WUZ	O2-C15-N2	2.86	127.09	124.30
4	A	405	WUZ	C2-N2-C15	2.81	126.77	123.61
4	A	405	WUZ	C12-C13-C8	-2.72	120.00	122.42
4	B	405	WUZ	C17-C18-N2	-2.71	105.78	108.06
2	A	401	16C	C20-C19-N2	2.39	119.98	115.83
2	A	401	16C	O19-C19-N2	-2.39	118.92	122.95
4	B	405	WUZ	C12-C13-C8	-2.38	120.30	122.42
4	B	405	WUZ	O2-C15-N2	2.37	126.62	124.30
4	A	405	WUZ	C9-C8-C13	2.06	120.30	116.91

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
6	B	408	R16	C35-C36-C37-C38
3	B	403	D10	C4-C5-C6-C7
6	A	410	R16	C38-C39-C40-C41
6	B	409	R16	C35-C36-C37-C38
2	A	401	16C	C20-C21-C22-C23
3	A	402	D10	C2-C3-C4-C5
6	A	410	R16	C34-C35-C36-C37
2	A	401	16C	C10-C11-C12-C13
3	B	402	D10	C2-C3-C4-C5
3	A	414	D10	C4-C5-C6-C7
3	A	403	D10	C3-C4-C5-C6
3	B	403	D10	C3-C4-C5-C6
2	A	401	16C	C12-C13-C14-C15
6	A	410	R16	C28-C29-C30-C31
6	B	409	R16	C28-C29-C30-C31
2	A	401	16C	O1-C1-C2-C3
6	A	410	R16	C30-C31-C32-C33
2	A	401	16C	C13-C14-C15-C16
6	B	408	R16	C28-C29-C30-C31
3	B	411	D10	C6-C7-C8-C9
3	A	403	D10	C5-C6-C7-C8
3	B	404	D10	C5-C6-C7-C8
3	B	404	D10	C1-C2-C3-C4
3	A	404	D10	C1-C2-C3-C4
6	B	408	R16	C34-C35-C36-C37
3	B	403	D10	C5-C6-C7-C8
6	A	410	R16	C31-C32-C33-C34
6	B	409	R16	C32-C33-C34-C35
2	A	401	16C	C31-C32-C33-C34

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

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
3	A	404	D10	2	0

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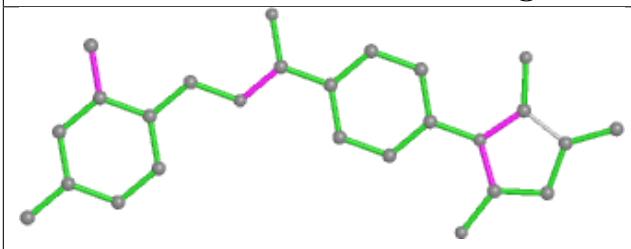
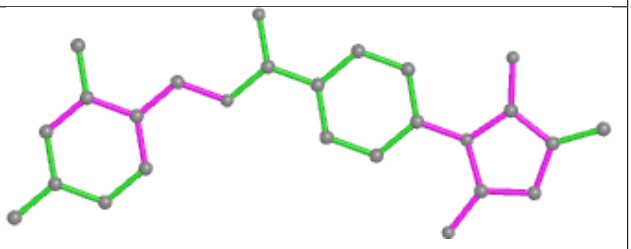
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	414	D10	1	0
6	A	410	R16	7	0
3	B	403	D10	2	0
6	B	409	R16	3	0
6	B	408	R16	3	0
3	A	402	D10	2	0
3	A	406	D10	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

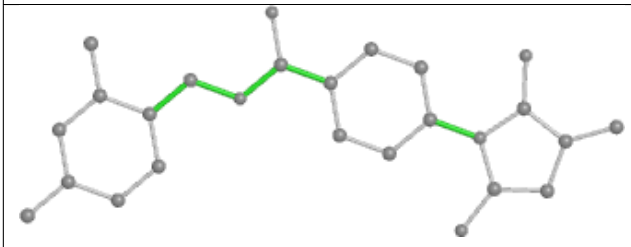
Ligand WUZ A 405



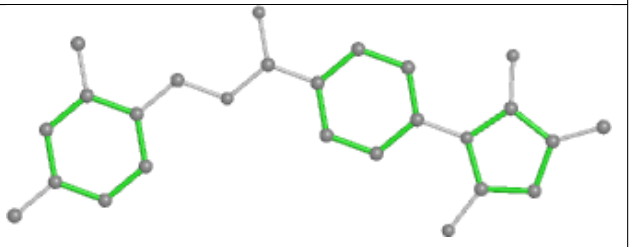
Bond lengths



Bond angles

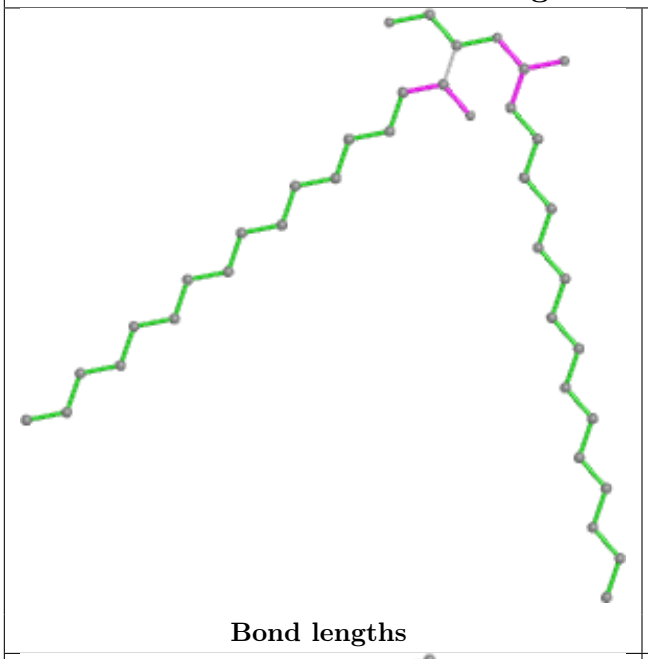


Torsions

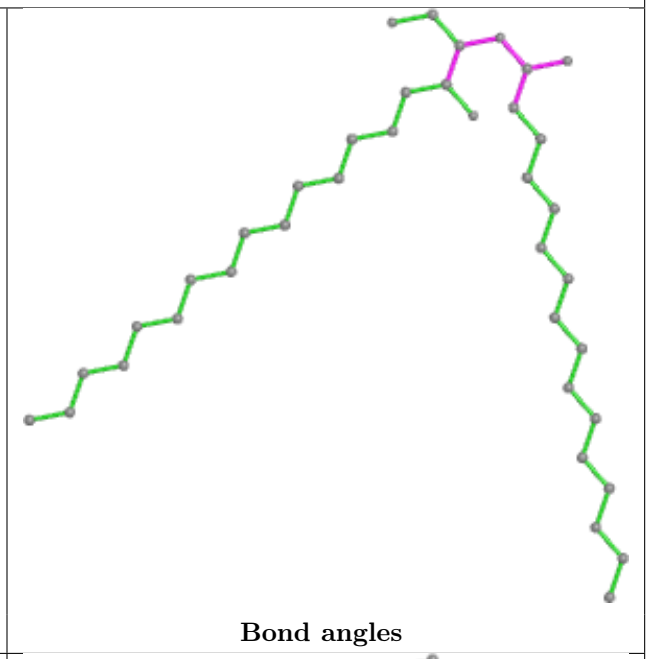


Rings

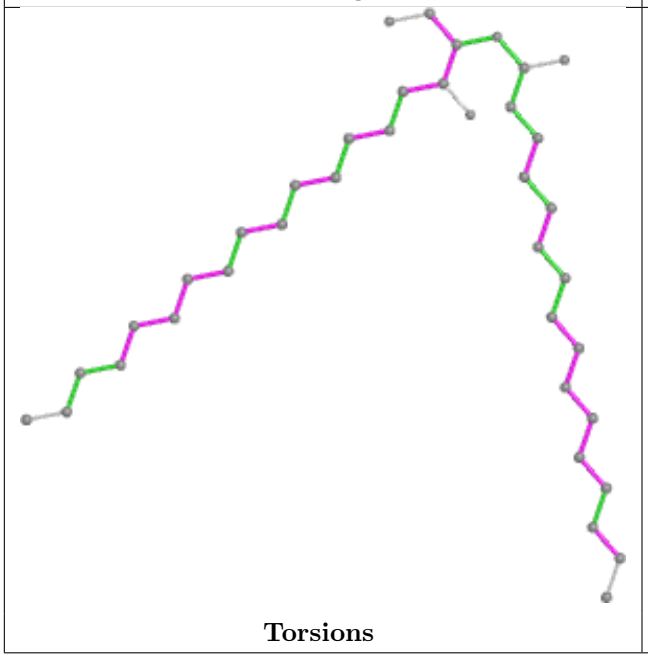
Ligand 16C A 401



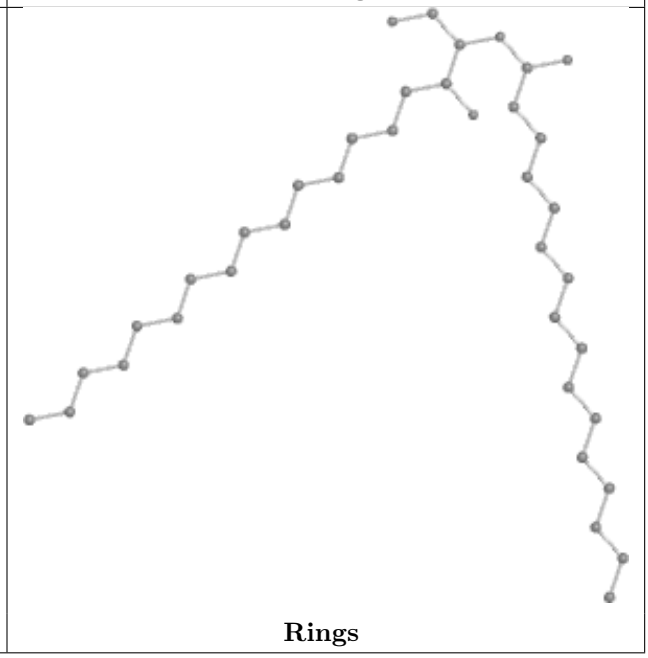
Bond lengths



Bond angles

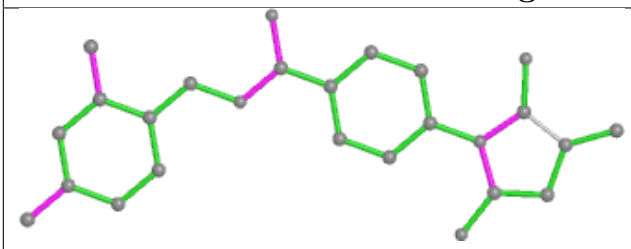


Torsions

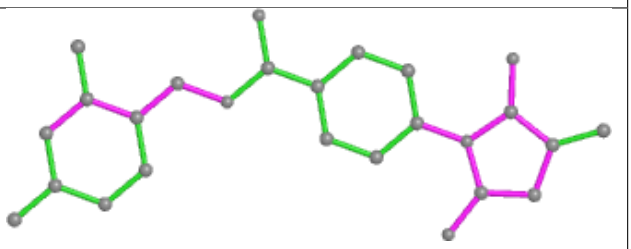


Rings

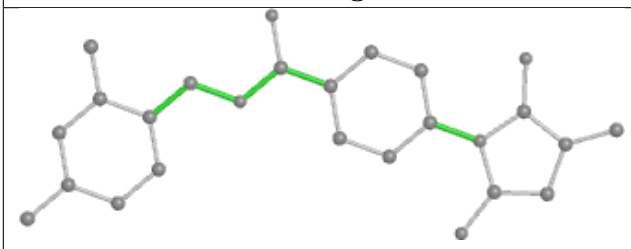
Ligand WUZ B 405



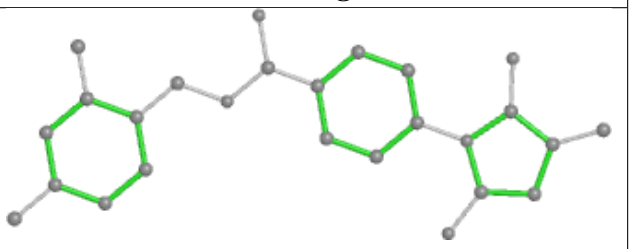
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	271/287 (94%)	0.10	9 (3%) 46 20	71, 119, 236, 259	0
1	B	282/287 (98%)	0.21	20 (7%) 16 5	74, 131, 236, 261	0
All	All	553/574 (96%)	0.16	29 (5%) 27 10	71, 124, 237, 261	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	35	SER	4.9
1	B	190	ALA	4.6
1	A	37	SER	3.7
1	B	120	SER	3.5
1	B	195	THR	3.3
1	A	101	GLU	3.2
1	B	192	VAL	3.1
1	A	202	SER	3.1
1	A	76	GLN	3.0
1	B	200	ASN	2.9
1	A	185	PHE	2.8
1	B	194	ASP	2.8
1	B	191	LYS	2.7
1	A	80	ILE	2.5
1	A	198	LYS	2.5
1	B	37	SER	2.4
1	B	198	LYS	2.4
1	B	197	ILE	2.4
1	B	94	VAL	2.3
1	B	124	VAL	2.3
1	A	201	VAL	2.3
1	B	36	ASP	2.3
1	A	199	TRP	2.2
1	B	201	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	185	PHE	2.1
1	B	206	ILE	2.1
1	B	125	SER	2.1
1	B	78	THR	2.1
1	B	95	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	16C	A	401	38/38	0.47	0.29	108,144,212,229	0
5	K	A	409	1/1	0.59	0.08	98,98,98,98	0
3	D10	A	413	10/10	0.60	0.56	104,135,140,146	0
7	CD	B	410	1/1	0.61	0.25	234,234,234,234	0
3	D10	A	402	10/10	0.66	0.41	129,149,162,170	0
3	D10	B	403	10/10	0.66	0.35	122,135,145,153	0
3	D10	A	403	10/10	0.72	0.40	109,122,136,136	0
3	D10	A	404	10/10	0.72	0.41	100,116,130,135	0
6	R16	A	410	16/16	0.73	0.45	124,134,150,161	0
3	D10	B	402	10/10	0.73	0.30	123,132,136,139	0
5	K	B	407	1/1	0.75	0.88	144,144,144,144	0
3	D10	A	414	10/10	0.76	0.43	87,100,101,114	0
3	D10	B	411	10/10	0.77	0.40	121,139,151,159	0
6	R16	B	409	16/16	0.79	0.44	105,119,136,137	0
3	D10	A	406	10/10	0.81	0.38	103,122,151,159	0
3	D10	B	404	10/10	0.81	1.00	101,105,116,118	0
7	CD	A	411	1/1	0.82	0.09	250,250,250,250	0
6	R16	B	408	16/16	0.82	0.32	91,112,131,133	0

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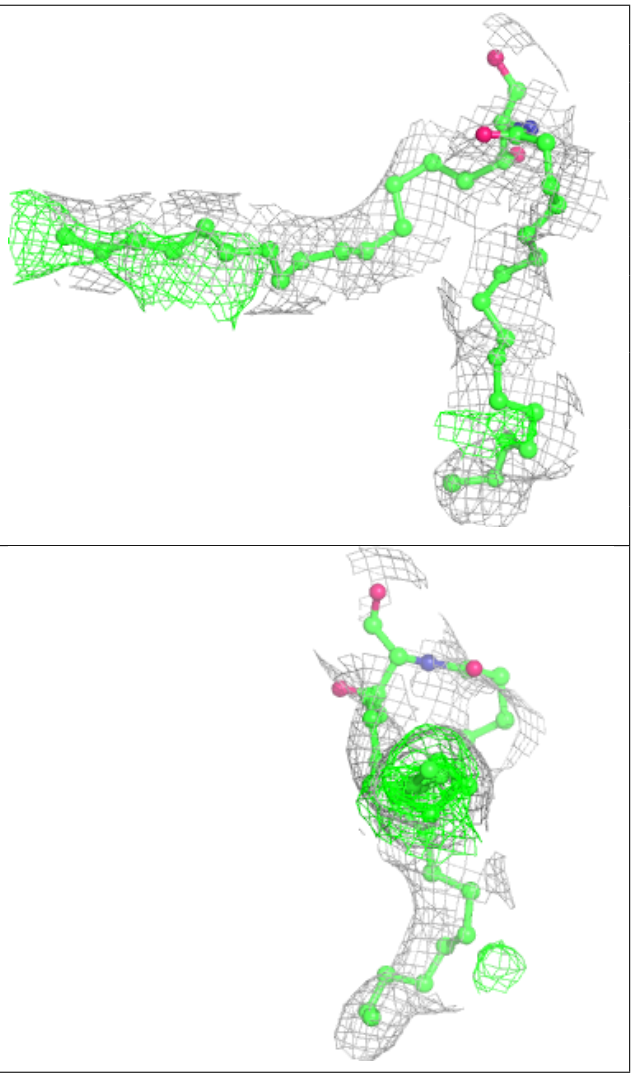
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	D10	B	401	10/10	0.86	0.22	118,137,159,159	0
4	WUZ	B	405	26/26	0.87	0.20	91,118,143,146	0
4	WUZ	A	405	26/26	0.89	0.20	88,109,148,155	0
7	CD	A	412	1/1	0.93	0.20	162,162,162,162	0
5	K	B	406	1/1	0.94	0.30	77,77,77,77	0
5	K	A	408	1/1	0.95	0.11	81,81,81,81	0
5	K	A	407	1/1	0.98	0.07	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.

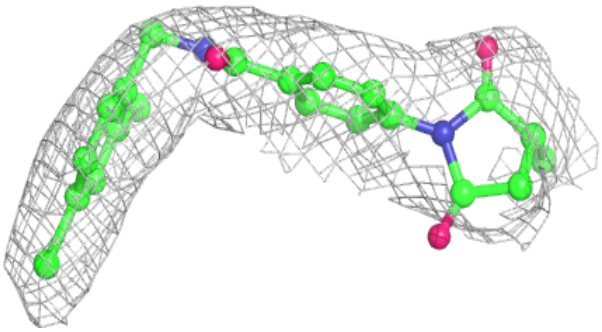
Electron density around 16C A 401:

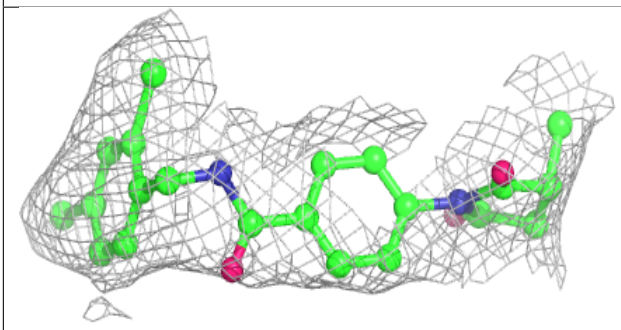
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

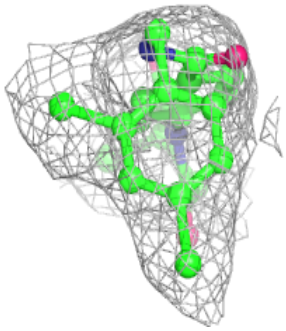


Electron density around WUZ B 405:

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

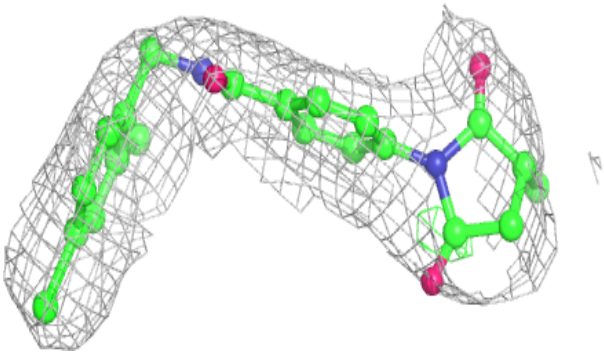


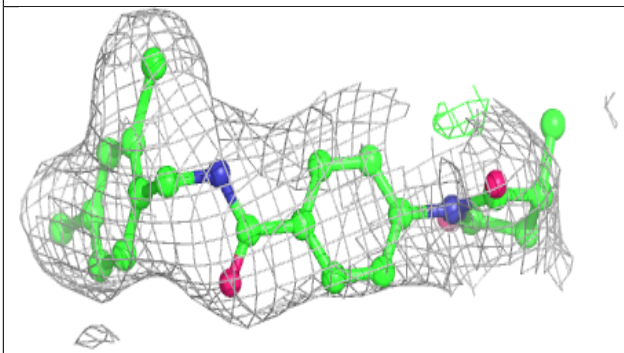


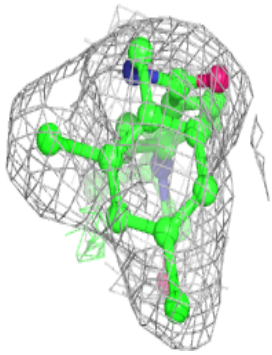


Electron density around WUZ A 405:

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







6.5 Other polymers (i)

There are no such residues in this entry.