



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 03:22 pm BST

PDB ID : 6CQ8  
Title : K2P2.1(TREK-1):ML335 complex  
Authors : Lolicato, M.; Minor, D.L.  
Deposited on : 2018-03-14  
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](mailto: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.

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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 : 2.11  
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) : 2.11

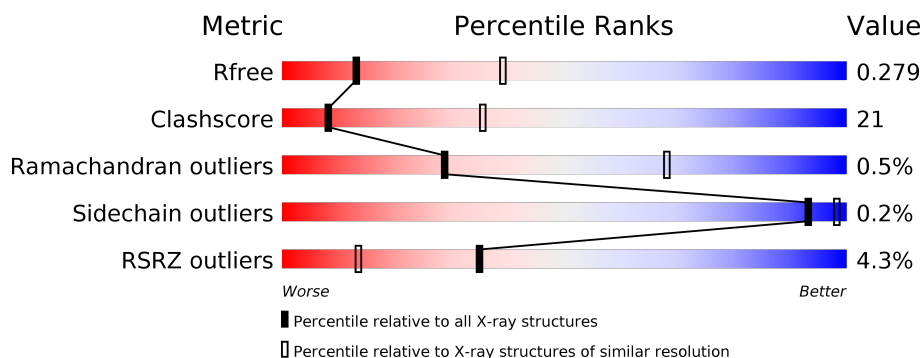
# 1 Overall quality at a glance

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	312	<div> <div>3%</div> <div> <div></div> <div>51%</div> <div>37%</div> <div>12%</div> </div> </div>
1	B	312	<div> <div>4%</div> <div> <div></div> <div>53%</div> <div>37%</div> <div>10%</div> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4645 atoms, of which 88 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	276	Total	C	N	O	S	0	1	0
			2167	1446	341	375	5			
1	B	282	Total	C	N	O	S	0	0	0
			2190	1457	347	381	5			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	LEU	initiating methionine	UNP P97438
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	300	ALA	SER	engineered mutation	UNP P97438
A	306	ALA	GLU	engineered mutation	UNP P97438
A	323	SER	ALA	engineered mutation	UNP P97438
A	324	ASN	GLU	engineered mutation	UNP P97438
A	325	SER	-	expression tag	UNP P97438
A	326	LEU	-	expression tag	UNP P97438
A	327	GLU	-	expression tag	UNP P97438
A	328	VAL	-	expression tag	UNP P97438
A	329	LEU	-	expression tag	UNP P97438
A	330	PHE	-	expression tag	UNP P97438
A	331	GLN	-	expression tag	UNP P97438
B	20	MET	LEU	initiating methionine	UNP P97438
B	84	ARG	LYS	engineered mutation	UNP P97438

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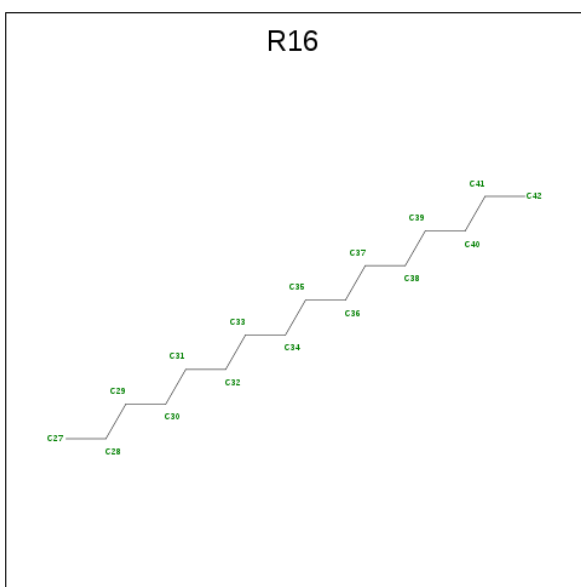
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Chain	Residue	Modelled	Actual	Comment	Reference
B	85	GLU	GLN	engineered mutation	UNP P97438
B	86	LYS	THR	engineered mutation	UNP P97438
B	88	LEU	ILE	engineered mutation	UNP P97438
B	89	ARG	ALA	engineered mutation	UNP P97438
B	90	ALA	GLN	engineered 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
B	300	ALA	SER	engineered mutation	UNP P97438
B	306	ALA	GLU	engineered mutation	UNP P97438
B	323	SER	ALA	engineered mutation	UNP P97438
B	324	ASN	GLU	engineered mutation	UNP P97438
B	325	SER	-	expression tag	UNP P97438
B	326	LEU	-	expression tag	UNP P97438
B	327	GLU	-	expression tag	UNP P97438
B	328	VAL	-	expression tag	UNP P97438
B	329	LEU	-	expression tag	UNP P97438
B	330	PHE	-	expression tag	UNP P97438
B	331	GLN	-	expression tag	UNP P97438

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

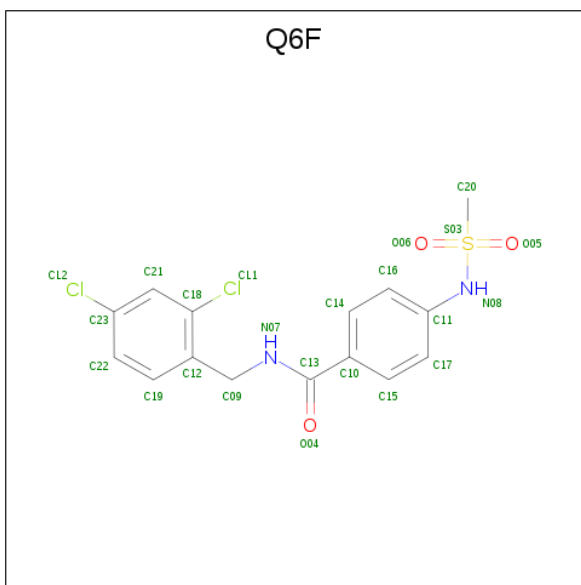
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	3	Total K 3 3	0	0
2	A	3	Total K 3 3	0	0

- Molecule 3 is HEXADECANE (three-letter code: R16) (formula: C<sub>16</sub>H<sub>34</sub>).



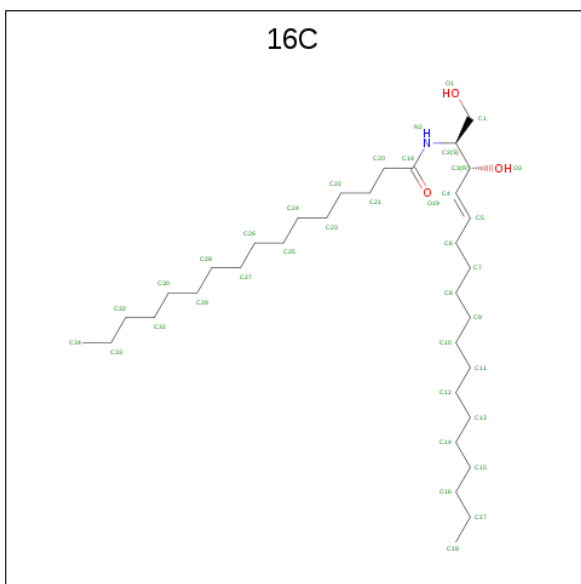
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 8 8	0	0
3	A	1	Total C H 22 8 14	0	0
3	A	1	Total C 11 11	0	0
3	A	1	Total C H 31 11 20	0	0
3	A	1	Total C H 31 11 20	0	0
3	B	1	Total C 12 12	0	0
3	B	1	Total C 16 16	0	0
3	B	1	Total C H 22 8 14	0	0
3	B	1	Total C 11 11	0	0
3	B	1	Total C H 31 11 20	0	0

- Molecule 4 is N-[(2,4-dichlorophenyl)methyl]-4-[(methylsulfonyl)amino]benzamide (three-letter code: Q6F) (formula: C<sub>15</sub>H<sub>14</sub>Cl<sub>2</sub>N<sub>2</sub>O<sub>3</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	S	0	0
			23	15	2	2	3	1		
4	B	1	Total	C	Cl	N	O	S	0	0
			23	15	2	2	3	1		

- Molecule 5 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
5	A	1	Total	C	N	O	0	0
			38	34	1	3		

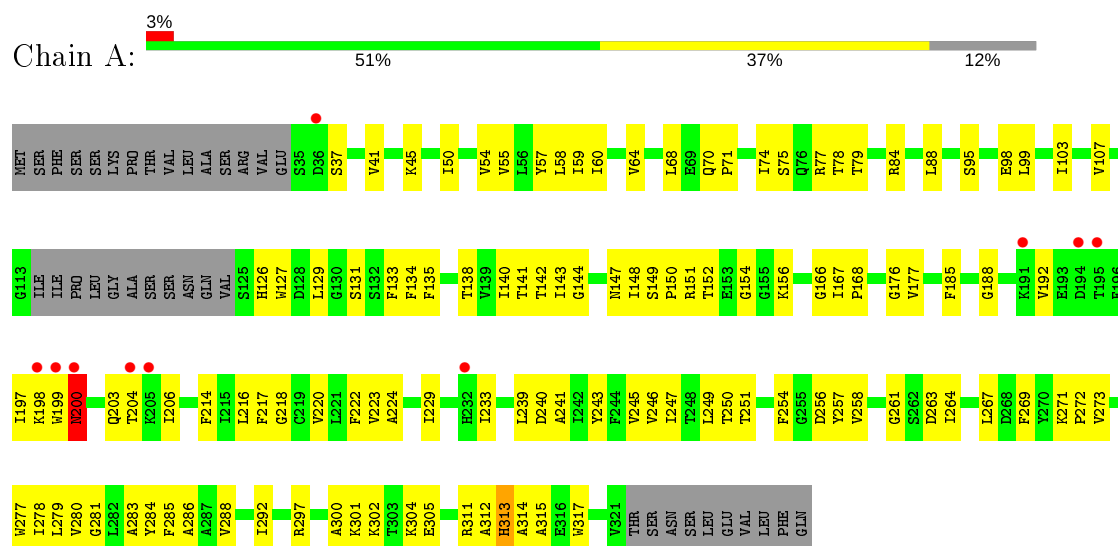
- Molecule 6 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	3	Total	Cd	0	0
			3	3		

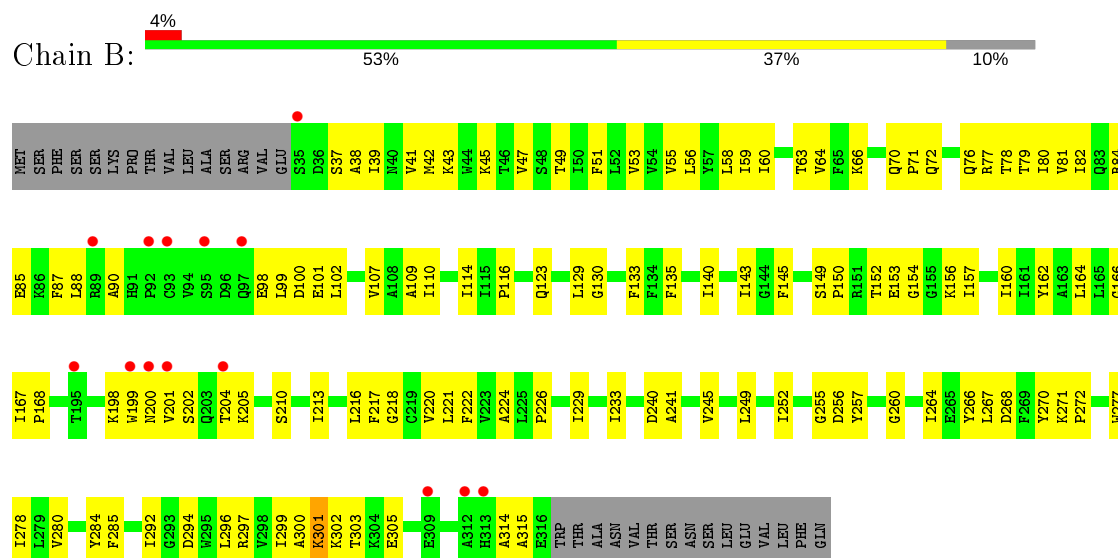
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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, $\alpha$ , $\beta$ , $\gamma$	67.07Å 119.39Å 128.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.95 – 3.00 14.95 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.2 (14.95-3.00) 98.6 (14.95-3.00)	Depositor EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.15 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, $R_{free}$	0.257 , 0.277 0.259 , 0.279	Depositor DCC
$R_{free}$ test set	1008 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	84.7	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 95.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4645	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: R16, Q6F, CD, K, 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	0.33	0/2224	0.48	0/3024
1	B	0.32	0/2243	0.51	1/3051 (0.0%)
All	All	0.32	0/4467	0.50	1/6075 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	301	LYS	CD-CE-NZ	11.33	137.76	111.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	200	ASN	Peptide
1	A	313	HIS	Peptide
1	B	268	ASP	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2167	0	2216	109	0
1	B	2190	0	2248	106	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	49	54	78	2	0
3	B	58	34	102	0	0
4	A	23	0	0	2	0
4	B	23	0	0	4	0
5	A	38	0	67	10	0
6	B	3	0	0	0	0
All	All	4557	88	4711	196	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 21.

All (196) 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:304:LYS:HA	5:A:407:16C:H11	1.41	0.97
1:A:88:LEU:HD11	1:A:99:LEU:HD22	1.46	0.93
1:A:77:ARG:HH12	1:B:123:GLN:HB3	1.38	0.88
1:B:152:THR:HG22	1:B:154:GLY:H	1.45	0.82
1:A:222:PHE:HE1	1:A:280:VAL:HG12	1.45	0.82
1:A:197:ILE:HG13	1:A:206:ILE:HD13	1.62	0.79
1:B:260:GLY:HA2	1:B:266:TYR:CE1	2.18	0.79
1:B:260:GLY:HA2	1:B:266:TYR:CZ	2.19	0.78
1:A:304:LYS:HA	5:A:407:16C:C1	2.13	0.76
1:B:107:VAL:O	1:B:110:ILE:HG22	1.87	0.74
1:B:210:SER:O	1:B:213:ILE:HG22	1.89	0.73
1:A:222:PHE:CE1	1:A:280:VAL:HG12	2.24	0.72
1:B:110:ILE:HA	1:B:114:ILE:HG12	1.72	0.72
1:B:229:ILE:CG2	1:B:233:ILE:HD12	2.21	0.71
1:A:243:TYR:HA	1:B:160:ILE:HD11	1.74	0.70
1:B:198:LYS:O	1:B:201:VAL:HG13	1.92	0.70
1:B:60:ILE:O	1:B:64:VAL:HG23	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:ILE:HG23	1:B:233:ILE:HD12	1.73	0.69
1:A:311:ARG:O	1:A:314:ALA:HB3	1.93	0.69
1:B:98:GLU:HA	1:B:101:GLU:HB2	1.74	0.68
1:A:126:HIS:HB3	1:A:148:ILE:HD12	1.75	0.68
1:B:84:ARG:O	1:B:88:LEU:HG	1.92	0.68
1:A:152:THR:HG22	1:A:154:GLY:H	1.57	0.68
1:A:141:THR:O	1:A:142:THR:OG1	2.10	0.67
1:A:37:SER:O	1:A:41:VAL:HG23	1.95	0.67
1:A:240:ASP:OD1	1:B:156:LYS:NZ	2.27	0.67
1:B:240:ASP:HB3	1:B:257:TYR:CE2	2.29	0.66
1:A:304:LYS:CA	5:A:407:16C:H11	2.22	0.66
1:B:202:SER:OG	1:B:205:LYS:HB2	1.94	0.66
1:A:77:ARG:HH12	1:B:123:GLN:CB	2.08	0.66
1:A:135:PHE:CZ	1:A:150:PRO:HD3	2.32	0.65
1:B:240:ASP:HB3	1:B:257:TYR:HE2	1.60	0.65
1:B:49:THR:O	1:B:53:VAL:HG23	1.96	0.65
1:A:127:TRP:O	1:B:70:GLN:NE2	2.30	0.65
1:B:41:VAL:HG12	1:B:45:LYS:HE3	1.78	0.64
1:A:197:ILE:CG1	1:A:206:ILE:HD13	2.28	0.64
1:B:87:PHE:HA	1:B:90:ALA:HB3	1.80	0.63
1:B:84:ARG:HH22	1:B:100:ASP:HB2	1.64	0.63
1:A:267:LEU:CD1	1:A:269:PHE:HE1	2.12	0.62
1:B:294:ASP:HA	1:B:297:ARG:HD2	1.79	0.62
1:B:222:PHE:CE1	1:B:280:VAL:HG12	2.34	0.61
1:B:77:ARG:HA	1:B:80:ILE:HG22	1.83	0.61
1:A:203:GLN:O	1:A:204:THR:OG1	2.16	0.61
1:A:197:ILE:HD11	1:A:206:ILE:HG21	1.83	0.60
1:A:240:ASP:HB3	1:A:257:TYR:CE2	2.36	0.60
1:B:204:THR:HG23	1:B:205:LYS:HD2	1.83	0.60
1:A:273:VAL:HG12	3:A:405:R16:H292	1.83	0.60
1:A:55:VAL:O	1:A:59:ILE:HG13	2.02	0.59
1:B:240:ASP:CB	1:B:257:TYR:HE2	2.15	0.59
1:A:267:LEU:HD12	1:A:269:PHE:HE1	1.67	0.59
1:B:216:LEU:O	1:B:220:VAL:HG23	2.03	0.58
1:B:98:GLU:O	1:B:102:LEU:N	2.33	0.58
1:A:304:LYS:CB	5:A:407:16C:H12	2.33	0.58
1:A:84:ARG:O	1:A:88:LEU:HD13	2.02	0.58
1:A:304:LYS:HB2	5:A:407:16C:H12	1.86	0.58
1:A:50:ILE:O	1:A:54:VAL:HG23	2.03	0.58
1:A:77:ARG:NH1	1:B:123:GLN:CB	2.67	0.58
1:B:299:ILE:O	1:B:303:THR:HG23	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:ALA:O	1:A:315:ALA:HB3	2.05	0.57
1:A:77:ARG:NH1	1:B:123:GLN:HB3	2.14	0.57
1:A:70:GLN:HB3	1:A:71:PRO:HD3	1.87	0.57
1:A:283:ALA:O	1:A:286:ALA:HB3	2.05	0.56
1:B:167:ILE:HB	1:B:168:PRO:HD3	1.86	0.56
1:A:229:ILE:CG2	1:A:233:ILE:HD12	2.36	0.56
1:B:218:GLY:HA3	1:B:284:TYR:CZ	2.40	0.56
1:B:153:GLU:O	1:B:157:ILE:HG13	2.06	0.56
1:B:84:ARG:HG3	1:B:88:LEU:HD11	1.87	0.55
1:B:245:VAL:HG13	1:B:277:TRP:HZ2	1.72	0.55
1:B:51:PHE:O	1:B:55:VAL:HG23	2.06	0.55
1:A:41:VAL:HG12	1:A:45:LYS:HE3	1.87	0.54
1:B:85:GLU:HA	1:B:88:LEU:HD12	1.88	0.54
1:B:37:SER:O	1:B:41:VAL:HG23	2.07	0.54
1:A:75:SER:O	1:A:79:THR:HG23	2.08	0.54
1:B:39:ILE:O	1:B:43:LYS:HG3	2.08	0.54
1:B:41:VAL:O	1:B:45:LYS:HG3	2.08	0.54
1:B:152:THR:HG22	1:B:154:GLY:N	2.18	0.54
1:B:129:LEU:HD12	1:B:130:GLY:N	2.22	0.53
1:B:38:ALA:O	1:B:42:MET:HG2	2.08	0.53
1:A:103:ILE:O	1:A:107:VAL:HG23	2.08	0.53
1:A:147:ASN:HD22	1:A:258:VAL:HG21	1.73	0.53
1:A:256:ASP:O	1:A:257:TYR:HD1	1.91	0.53
1:B:135:PHE:CZ	1:B:150:PRO:HD3	2.43	0.53
1:B:79:THR:HA	1:B:82:ILE:HD12	1.89	0.53
1:A:222:PHE:HE1	1:A:280:VAL:CG1	2.19	0.52
1:A:95:SER:OG	1:A:98:GLU:HG2	2.10	0.52
1:B:249:LEU:HB2	1:B:285:PHE:CE2	2.45	0.52
1:B:85:GLU:HA	1:B:88:LEU:HB2	1.92	0.52
1:A:167:ILE:HB	1:A:168:PRO:HD3	1.92	0.52
1:B:78:THR:O	1:B:82:ILE:HG13	2.09	0.52
1:A:147:ASN:ND2	1:A:258:VAL:HG21	2.25	0.52
1:A:284:TYR:O	1:A:288:VAL:HG23	2.09	0.52
1:B:199:TRP:CE3	1:B:200:ASN:HB2	2.44	0.52
1:A:269:PHE:O	1:A:273:VAL:HG23	2.10	0.51
1:A:249:LEU:HD22	1:A:281:GLY:C	2.31	0.51
1:A:147:ASN:OD1	1:A:148:ILE:N	2.44	0.51
1:A:304:LYS:CA	5:A:407:16C:C1	2.87	0.51
1:B:229:ILE:HG23	1:B:233:ILE:CD1	2.41	0.51
1:A:271:LYS:N	1:A:272:PRO:HD2	2.27	0.50
1:A:217:PHE:O	1:A:220:VAL:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:THR:HA	1:B:252:ILE:HG12	1.93	0.50
1:A:277:TRP:O	1:A:281:GLY:N	2.39	0.50
1:A:74:ILE:O	1:A:78:THR:HG23	2.11	0.50
1:B:140:ILE:HG22	1:B:166:GLY:HA3	1.93	0.50
1:B:88:LEU:HD23	1:B:99:LEU:CD2	2.41	0.49
1:A:250:THR:O	1:A:251:THR:OG1	2.30	0.49
1:A:297:ARG:O	1:A:301:LYS:HG2	2.12	0.49
1:B:56:LEU:CD2	1:B:60:ILE:HD11	2.42	0.49
1:A:156:LYS:NZ	1:B:240:ASP:OD1	2.44	0.49
1:B:70:GLN:HB3	1:B:71:PRO:HD3	1.94	0.49
1:B:39:ILE:HD13	1:B:43:LYS:HE3	1.95	0.48
1:A:216:LEU:O	1:A:220:VAL:HG23	2.14	0.48
1:B:84:ARG:NH2	1:B:100:ASP:HB2	2.28	0.48
1:A:176:GLY:HA3	1:B:47:VAL:HG22	1.95	0.48
1:B:55:VAL:O	1:B:59:ILE:HG13	2.14	0.48
1:A:129:LEU:HA	1:B:66:LYS:NZ	2.28	0.48
1:B:72:GLN:O	1:B:76:GLN:HG3	2.13	0.48
1:B:149:SER:HB2	1:B:150:PRO:HD2	1.96	0.48
1:A:218:GLY:HA3	1:A:284:TYR:CZ	2.49	0.47
1:B:233:ILE:HD13	1:B:270:TYR:CD1	2.48	0.47
1:B:84:ARG:NE	1:B:88:LEU:HD21	2.30	0.47
1:A:247:ILE:HG21	1:A:254:PHE:CD2	2.50	0.47
1:B:220:VAL:HA	1:B:224:ALA:HB3	1.97	0.47
1:B:271:LYS:N	1:B:272:PRO:HD2	2.30	0.47
1:A:239:LEU:HD13	3:A:404:R16:H332	1.95	0.46
1:B:278:ILE:HD13	4:B:410:Q6F:C21	2.45	0.46
1:B:213:ILE:HG13	1:B:217:PHE:CD2	2.50	0.46
1:A:41:VAL:O	1:A:45:LYS:HG3	2.16	0.46
1:A:263:ASP:O	1:A:264:ILE:HG13	2.15	0.46
1:B:84:ARG:HG3	1:B:88:LEU:CD1	2.46	0.46
1:A:131:SER:O	1:A:134:PHE:HB3	2.16	0.46
1:A:292:ILE:HD13	1:B:164:LEU:O	2.16	0.46
1:B:297:ARG:O	1:B:300:ALA:HB3	2.15	0.45
1:A:152:THR:HG22	1:A:154:GLY:N	2.28	0.45
1:B:84:ARG:HG3	1:B:88:LEU:CG	2.46	0.45
1:A:229:ILE:HG22	1:A:233:ILE:HD12	1.98	0.45
1:A:188:GLY:O	1:A:192:VAL:HG23	2.17	0.45
1:A:198:LYS:HG2	1:A:198:LYS:O	2.17	0.45
1:A:133:PHE:CE1	1:B:58:LEU:HB3	2.50	0.45
1:B:213:ILE:HG13	1:B:217:PHE:HD2	1.82	0.45
1:B:109:ALA:CB	1:B:114:ILE:HD13	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:VAL:HA	1:A:245:VAL:HG11	1.98	0.45
1:B:218:GLY:HA3	1:B:284:TYR:OH	2.17	0.45
1:A:197:ILE:HG21	1:A:203:GLN:HE21	1.82	0.44
1:A:199:TRP:CG	1:A:200:ASN:N	2.85	0.44
1:A:292:ILE:HG21	1:B:164:LEU:O	2.17	0.44
1:A:313:HIS:O	1:A:317:TRP:HB3	2.16	0.44
1:A:247:ILE:HG21	1:A:254:PHE:HD2	1.83	0.44
1:A:278:ILE:CD1	4:A:406:Q6F:C21	2.96	0.44
1:B:278:ILE:CD1	4:B:410:Q6F:C21	2.95	0.44
1:A:41:VAL:CG1	1:A:45:LYS:HE3	2.48	0.44
1:A:60:ILE:CD1	5:A:407:16C:H142	2.47	0.44
1:B:292:ILE:O	1:B:296:LEU:HG	2.18	0.44
1:B:314:ALA:O	1:B:315:ALA:HB3	2.18	0.44
1:B:278:ILE:HD13	4:B:410:Q6F:C23	2.47	0.44
1:A:300:ALA:HA	5:A:407:16C:H202	2.00	0.43
1:A:57:TYR:CE2	1:B:162:TYR:CE1	3.06	0.43
1:B:302:LYS:HD3	1:B:305:GLU:OE2	2.18	0.43
1:B:77:ARG:O	1:B:81:VAL:HG23	2.18	0.43
1:A:103:ILE:HD13	1:B:116:PRO:O	2.18	0.43
1:A:177:VAL:HG21	1:A:279:LEU:HD11	2.00	0.43
1:A:249:LEU:HB2	1:A:285:PHE:CE2	2.53	0.43
1:B:110:ILE:HD12	1:B:114:ILE:HG12	2.01	0.43
1:A:185[A]:PHE:CZ	1:A:214:PHE:HB2	2.54	0.43
1:A:247:ILE:O	1:A:247:ILE:HG22	2.19	0.43
1:A:304:LYS:CB	5:A:407:16C:C1	2.97	0.43
1:A:60:ILE:HD13	5:A:407:16C:H142	2.01	0.42
1:A:58:LEU:HB3	1:B:133:PHE:CE1	2.54	0.42
1:B:294:ASP:HA	1:B:297:ARG:CD	2.46	0.42
1:A:77:ARG:NH1	1:B:123:GLN:HB2	2.34	0.42
1:B:56:LEU:HD23	1:B:60:ILE:CD1	2.49	0.42
1:B:221:LEU:HD12	1:B:221:LEU:N	2.34	0.42
1:B:278:ILE:HD11	4:B:410:Q6F:C18	2.49	0.42
1:A:261:GLY:HA2	4:A:406:Q6F:N08	2.35	0.42
1:A:143:ILE:HG12	1:A:251:THR:HA	2.01	0.42
1:B:85:GLU:HG2	1:B:88:LEU:HD12	2.01	0.42
1:A:138:THR:HB	1:A:144:GLY:HA2	2.02	0.42
1:A:88:LEU:CD1	1:A:99:LEU:HD22	2.33	0.42
1:B:221:LEU:O	1:B:226:PRO:HD3	2.19	0.42
1:B:241:ALA:O	1:B:245:VAL:HG23	2.20	0.42
1:A:229:ILE:HG23	1:A:233:ILE:HD12	2.01	0.42
1:B:256:ASP:O	1:B:257:TYR:HD1	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:ASP:C	1:A:264:ILE:HG13	2.40	0.41
1:A:140:ILE:HG22	1:A:166:GLY:HA3	2.02	0.41
1:B:143:ILE:HG21	1:B:145:PHE:CE2	2.56	0.41
1:B:59:ILE:O	1:B:63:THR:HG23	2.21	0.41
1:A:302:LYS:HD3	1:A:305:GLU:OE2	2.20	0.41
1:A:218:GLY:HA3	1:A:284:TYR:OH	2.21	0.41
1:A:149:SER:HG	1:A:151:ARG:HH12	1.68	0.40
1:A:241:ALA:O	1:A:245:VAL:HG23	2.20	0.40
1:A:64:VAL:O	1:A:68:LEU:HG	2.21	0.40
1:A:240:ASP:HB3	1:A:257:TYR:HE2	1.85	0.40
1:A:246:VAL:HG11	1:B:160:ILE:HG23	2.03	0.40
1:B:204:THR:CG2	1:B:205:LYS:HD2	2.51	0.40
1:A:285:PHE:HA	1:A:288:VAL:HB	2.03	0.40
1:A:220:VAL:HA	1:A:224:ALA:HB3	2.03	0.40
1:B:145:PHE:HD1	1:B:255:GLY:HA2	1.87	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	273/312 (88%)	255 (93%)	17 (6%)	1 (0%)	34	72
1	B	280/312 (90%)	256 (91%)	22 (8%)	2 (1%)	22	60
All	All	553/624 (89%)	511 (92%)	39 (7%)	3 (0%)	29	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	200	ASN
1	B	264	ILE
1	B	267	LEU



### 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	228/260 (88%)	228 (100%)	0	100	100
1	B	231/260 (89%)	230 (100%)	1 (0%)	91	97
All	All	459/520 (88%)	458 (100%)	1 (0%)	93	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	301	LYS

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

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 9 are monoatomic - leaving 13 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$
5	16C	A	407	-	36,37,37	1.16	3 (8%)	37,39,39	1.00	2 (5%)
3	R16	A	404	-	7,7,15	0.33	0	6,6,14	0.70	0
4	Q6F	A	406	-	24,24,24	2.73	6 (25%)	34,34,34	1.44	5 (14%)
3	R16	B	412	-	10,10,15	0.33	0	9,9,14	0.77	0
3	R16	B	408	-	15,15,15	0.36	0	14,14,14	0.83	0
3	R16	A	410	-	10,10,15	0.32	0	9,9,14	0.82	0
3	R16	A	409	-	10,10,15	0.32	0	9,9,14	0.77	0
4	Q6F	B	410	-	24,24,24	2.08	5 (20%)	34,34,34	1.37	5 (14%)
3	R16	B	407	-	11,11,15	0.35	0	10,10,14	0.73	0
3	R16	A	405	-	7,7,15	0.32	0	6,6,14	0.73	0
3	R16	B	411	-	10,10,15	0.33	0	9,9,14	0.76	0
3	R16	A	408	-	10,10,15	0.33	0	9,9,14	0.80	0
3	R16	B	409	-	7,7,15	0.34	0	6,6,14	0.72	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
5	16C	A	407	-	-	18/40/40/40	-
3	R16	A	404	-	-	0/5/5/13	-
4	Q6F	A	406	-	-	2/14/14/14	0/2/2/2
3	R16	B	412	-	-	2/8/8/13	-
3	R16	B	408	-	-	1/13/13/13	-
3	R16	A	410	-	-	0/8/8/13	-
3	R16	A	409	-	-	3/8/8/13	-
4	Q6F	B	410	-	-	1/14/14/14	0/2/2/2
3	R16	B	407	-	-	2/9/9/13	-
3	R16	A	405	-	-	2/5/5/13	-
3	R16	B	411	-	-	3/8/8/13	-
3	R16	A	408	-	-	3/8/8/13	-
3	R16	B	409	-	-	0/5/5/13	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	406	Q6F	O04-C13	-10.16	1.02	1.23
5	A	407	16C	C19-N2	5.73	1.46	1.34
4	B	410	Q6F	C13-N07	5.37	1.45	1.33
4	B	410	Q6F	S03-N08	5.21	1.70	1.63
4	A	406	Q6F	C13-N07	4.72	1.44	1.33
4	A	406	Q6F	S03-N08	3.82	1.68	1.63
4	B	410	Q6F	O04-C13	3.25	1.29	1.23
4	A	406	Q6F	C10-C13	2.90	1.56	1.50
4	B	410	Q6F	C10-C13	2.77	1.56	1.50
4	A	406	Q6F	C18-C12	2.59	1.43	1.39
4	B	410	Q6F	C11-N08	2.13	1.46	1.43
5	A	407	16C	C3-C4	2.10	1.53	1.50
4	A	406	Q6F	C17-C11	2.04	1.42	1.39
5	A	407	16C	O19-C19	-2.02	1.19	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	410	Q6F	O06-S03-O05	-3.33	114.06	118.85
4	A	406	Q6F	C16-C11-C17	-3.31	114.51	119.03
4	B	410	Q6F	C16-C11-C17	-3.22	114.62	119.03
4	A	406	Q6F	O06-S03-O05	-3.19	114.26	118.85
4	B	410	Q6F	C14-C10-C15	-2.74	114.68	118.59
4	A	406	Q6F	C14-C10-C15	-2.68	114.77	118.59
4	A	406	Q6F	C16-C14-C10	2.38	123.55	120.78
5	A	407	16C	C20-C19-N2	2.38	119.96	115.83
4	A	406	Q6F	C14-C16-C11	2.28	122.93	120.30
5	A	407	16C	C3-C4-C5	-2.19	119.91	124.79
4	B	410	Q6F	C15-C17-C11	2.01	122.62	120.30
4	B	410	Q6F	C16-C14-C10	2.00	123.11	120.78

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	407	16C	C11-C10-C9-C8
5	A	407	16C	C12-C13-C14-C15
5	A	407	16C	C24-C25-C26-C27
3	A	409	R16	C34-C35-C36-C37
3	B	407	R16	C32-C33-C34-C35
3	A	409	R16	C33-C34-C35-C36
3	A	408	R16	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
4	A	406	Q6F	C11-N08-S03-C20
5	A	407	16C	C9-C10-C11-C12
5	A	407	16C	C20-C21-C22-C23
5	A	407	16C	C23-C24-C25-C26
5	A	407	16C	C21-C22-C23-C24
5	A	407	16C	C30-C31-C32-C33
5	A	407	16C	C10-C11-C12-C13
5	A	407	16C	C19-C20-C21-C22
5	A	407	16C	C15-C16-C17-C18
5	A	407	16C	C29-C30-C31-C32
5	A	407	16C	C14-C15-C16-C17
3	B	412	R16	C31-C32-C33-C34
5	A	407	16C	C31-C32-C33-C34
3	A	405	R16	C28-C29-C30-C31
5	A	407	16C	C27-C28-C29-C30
5	A	407	16C	C11-C12-C13-C14
3	A	408	R16	C33-C34-C35-C36
3	B	411	R16	C32-C33-C34-C35
3	B	412	R16	C32-C33-C34-C35
3	A	408	R16	C34-C35-C36-C37
3	B	411	R16	C31-C32-C33-C34
4	A	406	Q6F	C11-N08-S03-O05
3	B	408	R16	C37-C38-C39-C40
3	A	405	R16	C31-C32-C33-C34
3	B	411	R16	C33-C34-C35-C36
5	A	407	16C	C7-C8-C9-C10
4	B	410	Q6F	C11-N08-S03-O05
3	A	409	R16	C38-C39-C40-C41
3	B	407	R16	C33-C34-C35-C36
5	A	407	16C	C6-C7-C8-C9

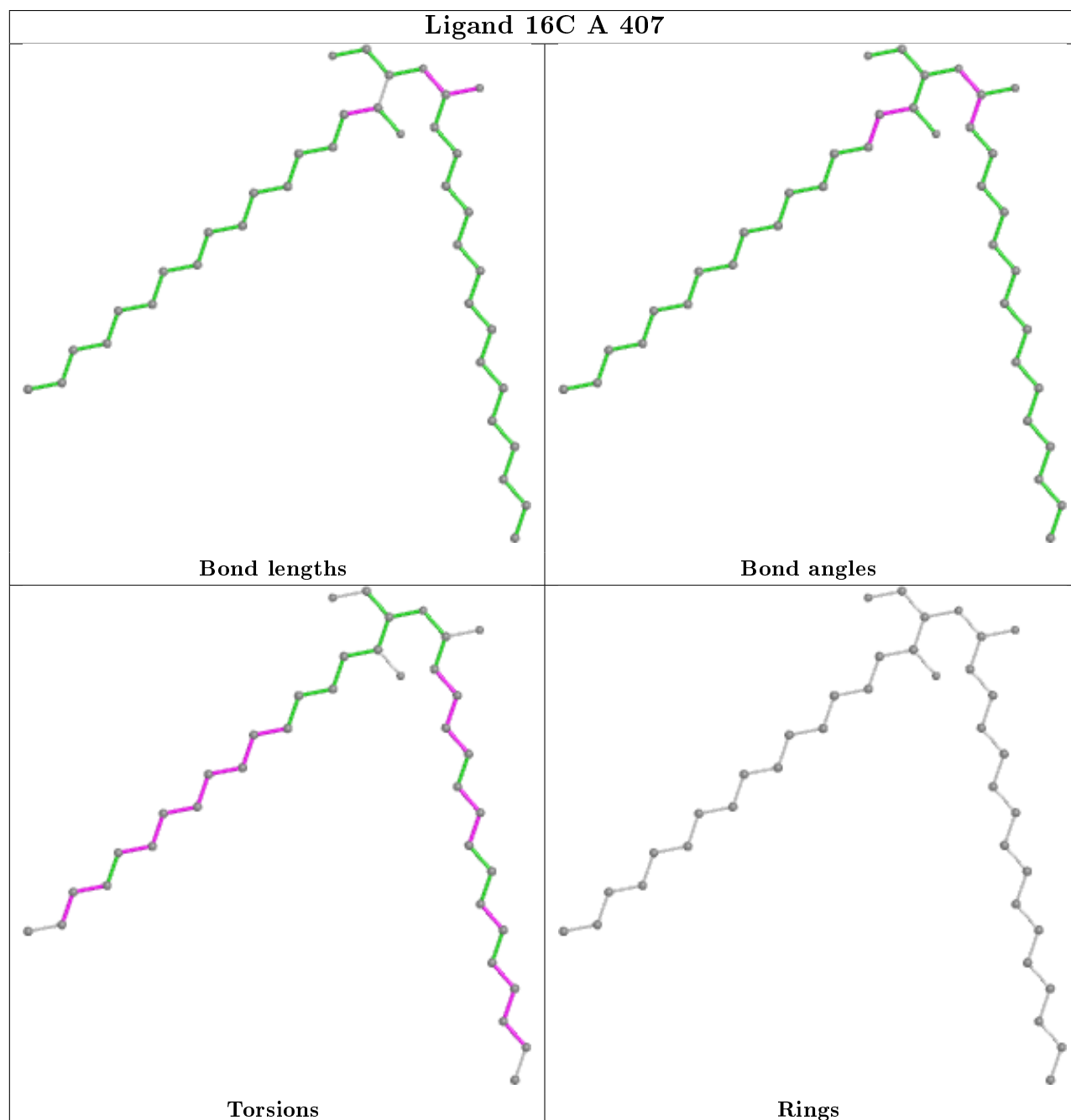
There are no ring outliers.

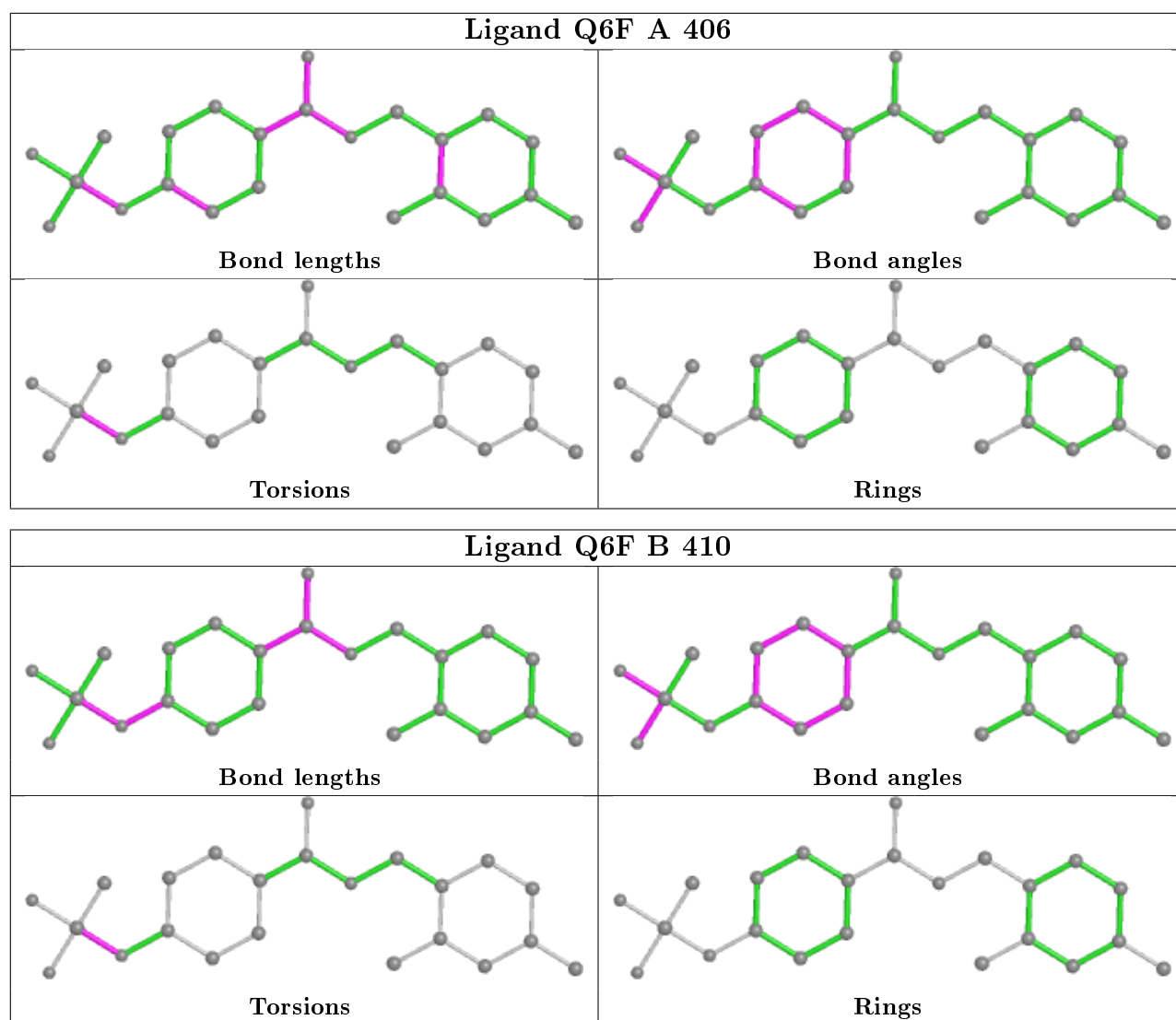
5 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	407	16C	10	0
3	A	404	R16	1	0
4	A	406	Q6F	2	0
4	B	410	Q6F	4	0
3	A	405	R16	1	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	276/312 (88%)	-0.27	10 (3%)	42 17	53, 95, 179, 226	0
1	B	282/312 (90%)	-0.20	14 (4%)	28 10	52, 95, 185, 223	0
All	All	558/624 (89%)	-0.23	24 (4%)	35 13	52, 95, 185, 226	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	199	TRP	6.5
1	A	204	THR	5.6
1	B	199	TRP	5.4
1	B	35	SER	5.4
1	B	93	CYS	5.3
1	B	89	ARG	4.3
1	B	95	SER	3.9
1	A	36	ASP	3.7
1	B	309	GLU	3.5
1	A	198	LYS	3.4
1	B	201	VAL	3.4
1	B	312	ALA	3.1
1	A	232	HIS	3.1
1	B	204	THR	3.0
1	A	200	ASN	2.9
1	A	195	THR	2.6
1	B	92	PRO	2.6
1	A	194	ASP	2.6
1	B	200	ASN	2.4
1	B	313	HIS	2.3
1	A	191	LYS	2.3
1	B	195	THR	2.3
1	B	97	GLN	2.2
1	A	205	LYS	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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<sup>th</sup> 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.

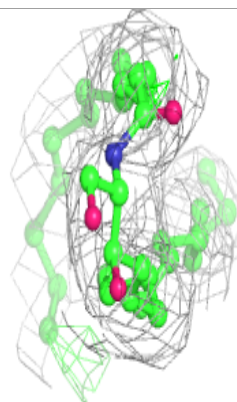
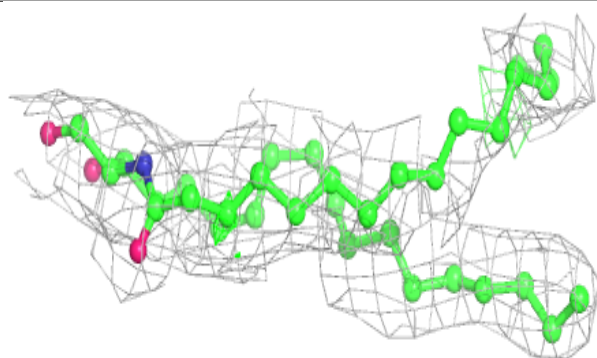
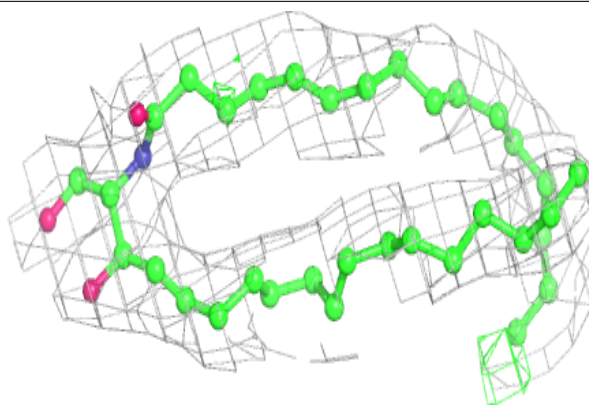
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	16C	A	407	38/38	0.75	0.22	68,104,121,125	0
3	R16	A	409	11/16	0.79	0.32	81,109,127,138	0
2	K	A	401	1/1	0.84	0.10	120,120,120,120	0
3	R16	B	408	16/16	0.87	0.17	67,74,84,87	0
3	R16	A	408	11/16	0.87	0.16	62,85,96,97	0
3	R16	B	412	11/16	0.88	0.15	84,110,133,143	0
3	R16	A	410	11/16	0.88	0.14	92,114,126,131	0
3	R16	B	409	8/16	0.88	0.25	70,120,132,132	0
3	R16	B	407	12/16	0.90	0.19	63,77,84,88	0
6	CD	B	406	1/1	0.91	0.10	132,132,132,132	1
3	R16	B	411	11/16	0.92	0.12	93,101,109,115	0
3	R16	A	404	8/16	0.92	0.22	72,94,100,102	0
4	Q6F	B	410	23/23	0.93	0.17	57,81,103,117	0
2	K	B	402	1/1	0.93	0.08	68,68,68,68	0
6	CD	B	404	1/1	0.94	0.04	179,179,179,179	0
4	Q6F	A	406	23/23	0.94	0.14	60,76,106,119	0
2	K	B	401	1/1	0.96	0.21	84,84,84,84	0
2	K	A	402	1/1	0.96	0.10	69,69,69,69	0
3	R16	A	405	8/16	0.96	0.14	66,101,124,125	0
2	K	B	403	1/1	0.97	0.07	105,105,105,105	0
6	CD	B	405	1/1	0.98	0.04	110,110,110,110	0
2	K	A	403	1/1	0.98	0.12	65,65,65,65	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.

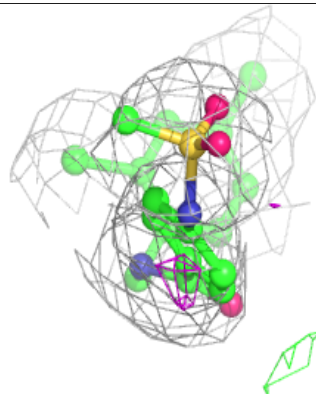
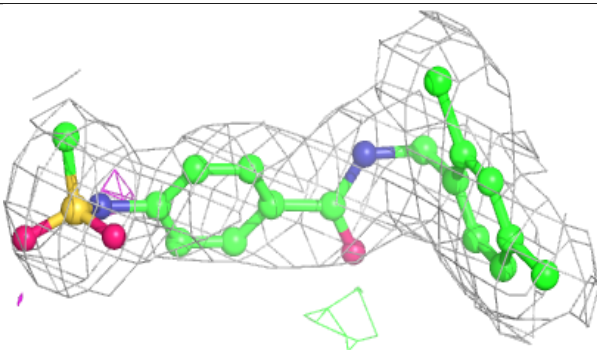
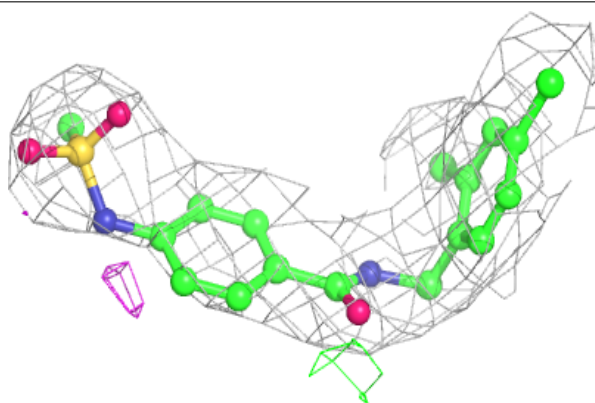


**Electron density around 16C A 407:**

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

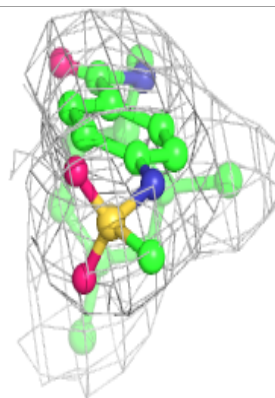
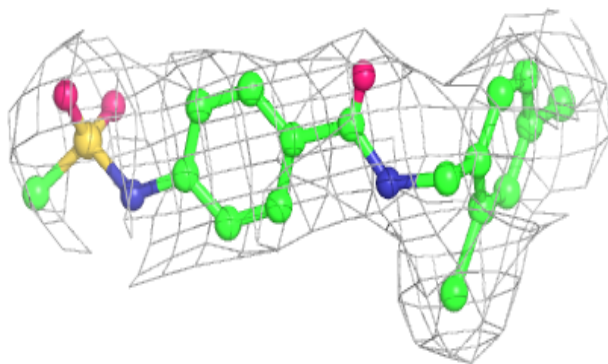
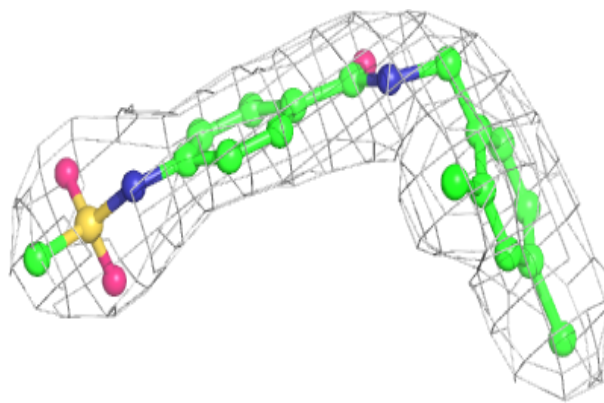
**Electron density around Q6F B 410:**

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



**Electron density around Q6F A 406:**

$2mF_o-DF_c$  (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.