



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2023 – 08:15 AM EDT

PDB ID : 6CQ9
Title : K2P2.1(TREK-1):ML402 complex
Authors : Lolicato, M.; Minor, D.L.
Deposited on : 2018-03-14
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

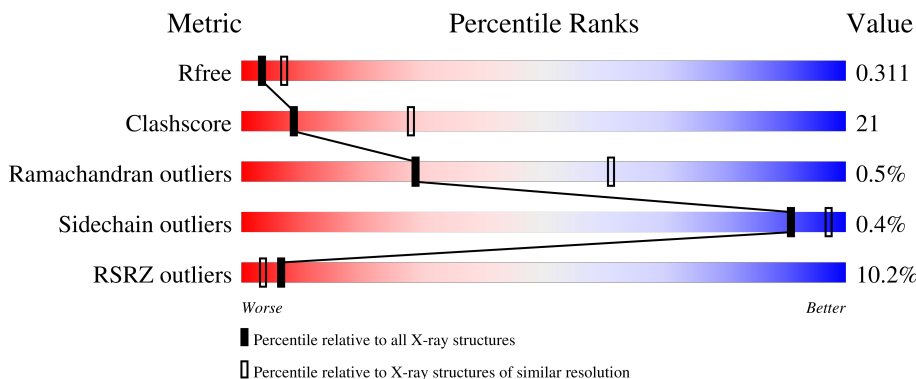
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	312	
1	B	312	

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
4	R16	B	409	-	-	-	X

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 4549 atoms, of which 48 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	276	Total	C	N	O	S	0	0	0
			2155	1436	340	374	5			
1	B	282	Total	C	N	O	S	0	0	0
			2173	1442	346	380	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

Continued on next page...

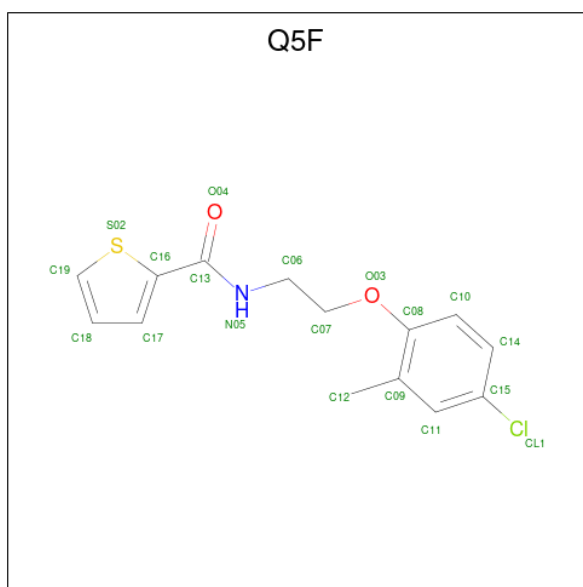
Continued from previous page...

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).

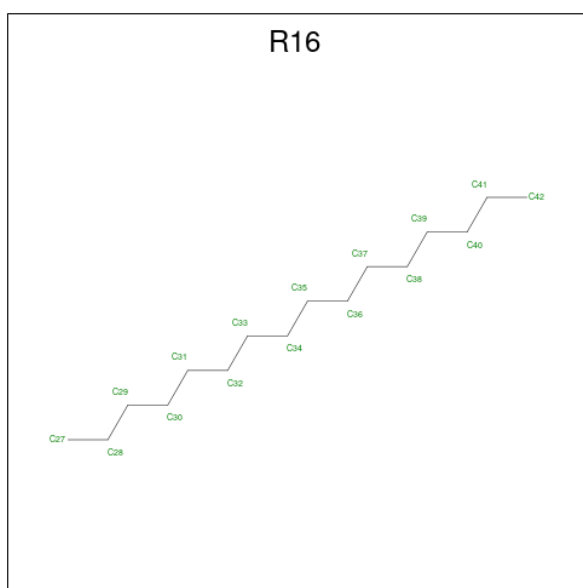
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total K 3 3	0	0
2	B	2	Total K 2 2	0	0

- Molecule 3 is N-[2-(4-chloro-2-methylphenoxy)ethyl]thiophene-2-carboxamide (three-letter code: Q5F) (formula: C₁₄H₁₄ClNO₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
3	A	1	Total	C	Cl	N	O	S	0	0
			19	14	1	1	2	1		
3	B	1	Total	C	Cl	N	O	S	0	0
			19	14	1	1	2	1		

- Molecule 4 is HEXADECANE (three-letter code: R16) (formula: $C_{16}H_{34}$).



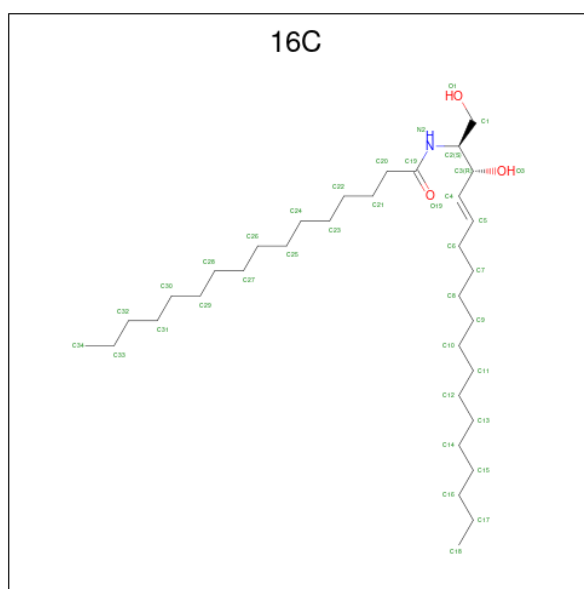
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	C	0	0
			12	12		
4	A	1	Total	C	0	0
			11	11		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H 22 8 14	0	0
4	B	1	Total C 12 12	0	0
4	B	1	Total C 12 12	0	0
4	B	1	Total C 5 5	0	0
4	B	1	Total C H 13 5 8	0	0
4	B	1	Total C H 13 5 8	0	0
4	B	1	Total C 11 11	0	0
4	B	1	Total C H 28 10 18	0	0

- Molecule 5 is N-((E,2S,3R)-1,3-DIHYDROXYOCTADEC-4-EN-2-YL)PALMITAMIDE (three-letter code: 16C) (formula: C₃₄H₆₇NO₃).



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

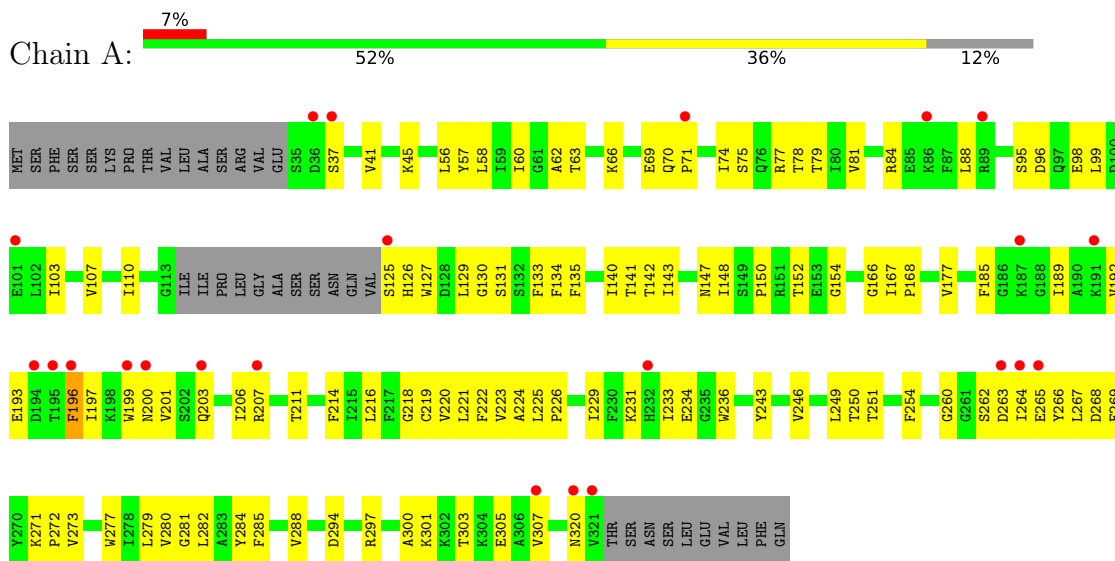
- Molecule 6 is CADMIUM ION (three-letter code: CD) (formula: Cd).

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

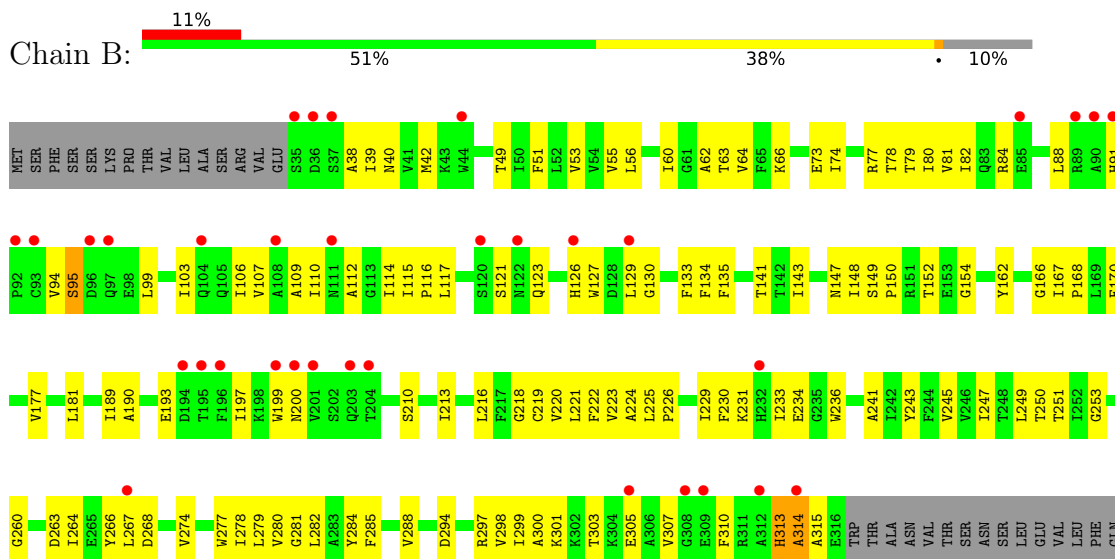
3 Residue-property plots [i](#)

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

- Molecule 1: Potassium channel subfamily K member 2



- Molecule 1: Potassium channel subfamily K member 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.09Å 119.56Å 127.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 14.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.3 (15.00-2.80) 99.8 (14.98-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 2.81Å)	Xtrriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.265 , 0.309 0.268 , 0.311	Depositor DCC
R_{free} test set	1236 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	97.9	Xtrriage
Anisotropy	0.222	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 133.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4549	wwPDB-VP
Average B, all atoms (Å ²)	146.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: Q5F, 16C, K, R16, 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	0.32	0/2208	0.42	0/3003
1	B	0.26	0/2226	0.42	1/3027 (0.0%)
All	All	0.29	0/4434	0.42	1/6030 (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	1
1	B	0	2
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	313	HIS	C-N-CA	5.57	135.63	121.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	199	TRP	Peptide
1	B	263	ASP	Peptide
1	B	95	SER	Peptide

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	2155	0	2201	103	5
1	B	2173	0	2196	99	1
2	A	3	0	0	0	0
2	B	2	0	0	0	0
3	A	19	0	0	1	0
3	B	19	0	0	3	0
4	A	31	14	50	0	0
4	B	60	34	92	0	0
5	A	38	0	67	3	0
6	B	1	0	0	0	0
All	All	4501	48	4606	188	5

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 (188) 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:197:ILE:HG23	1:A:206:ILE:HD13	1.33	1.08
1:A:197:ILE:HD12	1:A:206:ILE:HG21	1.48	0.93
1:A:193:GLU:HA	1:A:197:ILE:HG13	1.53	0.90
1:A:262:SER:O	1:A:266:TYR:OH	1.88	0.90
1:B:229:ILE:HG23	1:B:233:ILE:HD13	1.56	0.88
1:A:203:GLN:HA	1:A:206:ILE:HD12	1.57	0.86
1:A:63:THR:HA	1:A:66:LYS:HE2	1.61	0.83
1:A:229:ILE:HG23	1:A:233:ILE:HD13	1.64	0.80
1:A:263:ASP:OD1	1:A:264:ILE:HG13	1.83	0.79
1:A:197:ILE:HG23	1:A:206:ILE:CD1	2.14	0.77
1:B:126:HIS:HB3	1:B:148:ILE:HD13	1.66	0.76
1:B:221:LEU:HA	1:B:225:LEU:HD12	1.68	0.75
1:B:63:THR:HA	1:B:66:LYS:HE2	1.68	0.74
1:B:91:HIS:HB2	1:B:94:VAL:HG23	1.69	0.74
1:A:84:ARG:NH1	1:B:116:PRO:HA	2.03	0.73
1:A:152:THR:HG22	1:A:154:GLY:H	1.54	0.73
1:B:260:GLY:HA2	1:B:266:TYR:CZ	2.23	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:LEU:HD11	1:A:99:LEU:HD13	1.69	0.72
1:A:193:GLU:HA	1:A:197:ILE:CG1	2.18	0.72
1:A:135:PHE:CZ	1:A:150:PRO:HD3	2.24	0.71
1:A:197:ILE:HD12	1:A:206:ILE:CG2	2.21	0.70
1:B:152:THR:HG22	1:B:154:GLY:H	1.55	0.70
1:A:125:SER:N	1:B:77:ARG:HH12	1.89	0.70
1:B:181:LEU:HD22	1:B:280:VAL:HG13	1.74	0.69
1:B:167:ILE:HB	1:B:168:PRO:HD3	1.76	0.68
1:A:37:SER:O	1:A:41:VAL:HG23	1.95	0.67
1:B:310:PHE:O	1:B:314:ALA:CB	2.43	0.67
1:A:77:ARG:HD3	1:B:123:GLN:OE1	1.95	0.67
1:B:84:ARG:O	1:B:88:LEU:HG	1.96	0.65
1:A:126:HIS:HB2	1:A:148:ILE:CD1	2.26	0.65
1:A:127:TRP:HB2	1:B:73:GLU:OE1	1.97	0.65
1:A:249:LEU:HA	1:A:282:LEU:HD23	1.78	0.65
1:B:229:ILE:CG2	1:B:233:ILE:HD13	2.26	0.64
1:A:229:ILE:CG2	1:A:233:ILE:HD13	2.28	0.62
1:A:95:SER:OG	1:A:98:GLU:OE1	2.17	0.62
1:B:60:ILE:O	1:B:64:VAL:HG23	1.99	0.62
1:B:310:PHE:O	1:B:314:ALA:HB3	1.99	0.61
1:A:264:ILE:HG23	1:A:265:GLU:HG3	1.82	0.61
1:A:74:ILE:O	1:A:78:THR:HG23	2.02	0.59
1:B:91:HIS:HB2	1:B:94:VAL:CG2	2.31	0.59
1:B:106:ILE:O	1:B:110:ILE:HG13	2.03	0.59
1:B:219:CYS:O	1:B:223:VAL:HB	2.03	0.58
1:A:249:LEU:HB2	1:A:285:PHE:CD2	2.39	0.58
1:A:200:ASN:OD1	1:A:201:VAL:N	2.36	0.58
1:A:126:HIS:HB2	1:A:148:ILE:HD13	1.85	0.58
1:B:107:VAL:HA	1:B:110:ILE:HD12	1.86	0.58
1:A:231:LYS:HG3	1:A:236:TRP:O	2.04	0.57
1:B:126:HIS:HB3	1:B:148:ILE:CD1	2.31	0.57
1:A:84:ARG:HH11	1:B:116:PRO:HA	1.67	0.57
1:A:129:LEU:HD12	1:A:130:GLY:N	2.19	0.57
1:A:249:LEU:HB2	1:A:285:PHE:CE2	2.40	0.56
1:B:103:ILE:H	1:B:103:ILE:HD12	1.71	0.56
1:B:129:LEU:HD12	1:B:130:GLY:N	2.21	0.56
1:B:210:SER:O	1:B:213:ILE:HG22	2.05	0.56
1:A:41:VAL:HG12	1:A:45:LYS:HE3	1.87	0.56
1:B:216:LEU:O	1:B:220:VAL:HG23	2.06	0.56
1:A:300:ALA:HA	5:A:406:16C:H202	1.88	0.56
1:B:310:PHE:O	1:B:314:ALA:HB2	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:GLN:HB3	1:A:71:PRO:HD3	1.87	0.56
1:B:234:GLU:HG2	1:B:236:TRP:CE2	2.42	0.56
1:A:218:GLY:HA3	1:A:284:TYR:CZ	2.41	0.55
1:A:294:ASP:HA	1:A:297:ARG:HG2	1.89	0.55
1:B:297:ARG:O	1:B:300:ALA:HB3	2.06	0.55
1:A:189:ILE:O	1:A:193:GLU:HG3	2.07	0.55
1:A:75:SER:O	1:A:79:THR:HG23	2.06	0.54
1:B:250:THR:O	1:B:251:THR:OG1	2.22	0.54
1:B:313:HIS:O	1:B:315:ALA:N	2.28	0.54
1:A:77:ARG:O	1:A:81:VAL:HG23	2.07	0.54
1:B:231:LYS:HG3	1:B:236:TRP:O	2.07	0.54
1:A:264:ILE:CG2	1:A:265:GLU:HG3	2.38	0.54
1:A:218:GLY:HA3	1:A:284:TYR:CE1	2.43	0.54
1:B:249:LEU:HD11	1:B:277:TRP:CZ2	2.43	0.54
1:A:234:GLU:HG2	1:A:236:TRP:CE2	2.43	0.53
1:B:141:THR:HG22	1:B:170:PHE:CE2	2.43	0.53
1:B:218:GLY:HA3	1:B:284:TYR:CZ	2.44	0.53
1:B:221:LEU:O	1:B:226:PRO:HD3	2.07	0.53
1:B:141:THR:HG22	1:B:170:PHE:CZ	2.44	0.53
1:B:260:GLY:HA2	1:B:266:TYR:CE2	2.43	0.53
1:B:56:LEU:HD21	1:B:60:ILE:HD11	1.91	0.52
1:A:222:PHE:CE1	1:A:280:VAL:HG12	2.43	0.52
1:A:192:VAL:HG12	1:A:196:PHE:HE1	1.75	0.52
1:B:149:SER:HB2	1:B:150:PRO:HD2	1.92	0.52
1:A:125:SER:HA	1:B:73:GLU:OE2	2.10	0.51
1:A:131:SER:O	1:A:134:PHE:HB3	2.10	0.51
1:A:267:LEU:HD23	1:A:269:PHE:CE1	2.46	0.51
1:B:278:ILE:HD13	3:B:404:Q5F:C15	2.41	0.51
1:B:77:ARG:O	1:B:81:VAL:HG23	2.10	0.51
1:A:196:PHE:H	1:A:196:PHE:HD1	1.57	0.51
1:A:234:GLU:HG2	1:A:236:TRP:CZ2	2.46	0.51
1:A:250:THR:O	1:A:251:THR:OG1	2.29	0.50
1:B:294:ASP:O	1:B:298:VAL:HG23	2.11	0.50
1:B:299:ILE:O	1:B:303:THR:HG23	2.11	0.50
1:A:126:HIS:HB2	1:A:148:ILE:HD11	1.92	0.50
1:B:39:ILE:HD12	1:B:40:ASN:N	2.26	0.50
1:B:49:THR:O	1:B:53:VAL:HG23	2.11	0.50
1:B:94:VAL:HG11	1:B:99:LEU:HD22	1.94	0.50
1:B:249:LEU:HB2	1:B:285:PHE:CE2	2.47	0.49
1:A:66:LYS:O	1:A:70:GLN:HB2	2.12	0.49
1:B:245:VAL:HG13	1:B:277:TRP:HZ2	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:VAL:CG1	1:A:196:PHE:HE1	2.27	0.48
1:A:277:TRP:O	1:A:281:GLY:N	2.40	0.48
1:A:98:GLU:HG2	1:B:91:HIS:NE2	2.29	0.48
1:A:99:LEU:O	1:A:103:ILE:HG12	2.12	0.48
1:A:177:VAL:HG21	1:A:279:LEU:HD11	1.96	0.48
1:A:192:VAL:CG1	1:A:196:PHE:CE1	2.96	0.48
1:A:58:LEU:HB3	1:B:133:PHE:CE1	2.48	0.48
1:A:260:GLY:HA2	1:A:266:TYR:CE1	2.49	0.47
1:A:62:ALA:HB2	1:B:133:PHE:HA	1.96	0.47
1:B:135:PHE:CZ	1:B:150:PRO:HD3	2.49	0.47
1:B:229:ILE:HG23	1:B:233:ILE:CD1	2.35	0.47
1:B:218:GLY:HA3	1:B:284:TYR:CE1	2.49	0.47
1:B:79:THR:HA	1:B:82:ILE:HD12	1.97	0.47
1:B:177:VAL:HG21	1:B:279:LEU:HD21	1.95	0.47
1:B:274:VAL:O	1:B:278:ILE:HG13	2.14	0.47
1:B:121:SER:O	1:B:123:GLN:HG3	2.15	0.47
1:B:249:LEU:HD22	1:B:281:GLY:C	2.34	0.46
1:A:88:LEU:HD11	1:A:99:LEU:CD1	2.40	0.46
1:B:266:TYR:O	1:B:268:ASP:N	2.48	0.46
1:A:147:ASN:OD1	1:A:148:ILE:N	2.49	0.46
1:A:185:PHE:CZ	1:A:214:PHE:HB2	2.51	0.46
1:A:110:ILE:HD11	1:B:110:ILE:HD13	1.98	0.46
1:A:193:GLU:O	1:A:197:ILE:HB	2.16	0.45
1:B:220:VAL:HA	1:B:224:ALA:HB3	1.98	0.45
1:B:249:LEU:HB2	1:B:285:PHE:CD2	2.51	0.45
1:A:219:CYS:O	1:A:223:VAL:HB	2.15	0.45
1:A:41:VAL:O	1:A:45:LYS:HG3	2.16	0.45
1:B:241:ALA:O	1:B:245:VAL:HG23	2.17	0.45
1:A:134:PHE:HE1	3:A:404:Q5F:C09	2.30	0.45
1:A:269:PHE:O	1:A:273:VAL:HG23	2.16	0.45
1:B:193:GLU:O	1:B:197:ILE:HB	2.16	0.45
1:B:147:ASN:OD1	1:B:148:ILE:N	2.50	0.45
1:A:260:GLY:HA2	1:A:266:TYR:CZ	2.52	0.45
1:B:115:ILE:HG22	1:B:115:ILE:O	2.15	0.45
1:A:167:ILE:HB	1:A:168:PRO:HD3	1.98	0.45
1:A:140:ILE:HG22	1:A:166:GLY:HA3	1.99	0.44
1:B:189:ILE:HD12	1:B:190:ALA:N	2.31	0.44
1:A:135:PHE:HZ	1:A:150:PRO:HD3	1.76	0.44
1:A:303:THR:O	1:A:307:VAL:HG23	2.18	0.44
1:B:222:PHE:CE1	1:B:280:VAL:HG12	2.52	0.44
1:B:189:ILE:O	1:B:193:GLU:HG3	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:PHE:HE1	3:B:404:Q5F:C09	2.31	0.44
5:A:406:16C:H151	5:A:406:16C:H183	1.67	0.44
1:B:303:THR:O	1:B:307:VAL:HG23	2.18	0.44
1:A:69:GLU:HG3	1:B:127:TRP:CH2	2.53	0.44
1:B:94:VAL:HG12	1:B:95:SER:N	2.33	0.43
1:B:181:LEU:HD22	1:B:280:VAL:CG1	2.45	0.43
1:A:192:VAL:HG13	1:A:196:PHE:CE1	2.53	0.43
1:B:143:ILE:O	1:B:253:GLY:HA3	2.18	0.43
1:A:133:PHE:HA	1:B:62:ALA:HB2	1.99	0.43
1:A:196:PHE:N	1:A:196:PHE:CD1	2.87	0.42
1:B:278:ILE:HD13	3:B:404:Q5F:C11	2.49	0.42
1:B:162:TYR:O	1:B:166:GLY:N	2.47	0.42
1:B:284:TYR:CE2	1:B:288:VAL:HG21	2.54	0.42
1:A:41:VAL:CG1	1:A:45:LYS:HE3	2.48	0.42
1:A:56:LEU:HD21	1:A:60:ILE:HD11	2.02	0.42
1:B:249:LEU:HD22	1:B:282:LEU:N	2.35	0.42
1:A:220:VAL:HA	1:A:224:ALA:HB3	2.01	0.42
1:B:38:ALA:O	1:B:42:MET:HG2	2.19	0.42
1:A:221:LEU:HA	1:A:225:LEU:HD12	2.00	0.42
1:A:243:TYR:HH	1:A:254:PHE:HD2	1.67	0.42
1:A:301:LYS:O	1:A:305:GLU:HG2	2.19	0.42
1:B:74:ILE:O	1:B:78:THR:HG23	2.20	0.42
1:B:109:ALA:HB1	1:B:114:ILE:HG21	2.01	0.42
1:A:57:TYR:CE1	5:A:406:16C:H162	2.55	0.42
1:B:301:LYS:O	1:B:305:GLU:HG2	2.20	0.42
1:A:141:THR:O	1:A:142:THR:OG1	2.32	0.42
1:A:143:ILE:HG12	1:A:251:THR:HA	2.02	0.42
1:B:51:PHE:O	1:B:55:VAL:HG23	2.20	0.42
1:A:63:THR:CA	1:A:66:LYS:HE2	2.41	0.41
1:A:225:LEU:N	1:A:226:PRO:HD2	2.35	0.41
1:A:284:TYR:O	1:A:288:VAL:HG23	2.19	0.41
1:A:249:LEU:CB	1:A:285:PHE:CD2	3.03	0.41
1:B:112:ALA:O	1:B:114:ILE:HG23	2.21	0.41
1:B:243:TYR:O	1:B:247:ILE:HG12	2.19	0.41
1:A:216:LEU:O	1:A:220:VAL:HG23	2.20	0.41
1:A:246:VAL:O	1:A:250:THR:HG23	2.21	0.41
1:A:129:LEU:HA	1:B:66:LYS:HD3	2.01	0.41
1:A:264:ILE:HG22	1:A:265:GLU:HB2	2.02	0.41
1:A:103:ILE:HB	1:B:117:LEU:HD21	2.03	0.41
1:A:207:ARG:O	1:A:211:THR:HG23	2.21	0.41
1:A:271:LYS:HB2	1:A:272:PRO:HD3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:PHE:O	1:B:234:GLU:HB3	2.21	0.41
1:A:69:GLU:HG3	1:B:127:TRP:CZ2	2.56	0.40
1:A:249:LEU:HA	1:A:282:LEU:CD2	2.48	0.40
1:A:103:ILE:O	1:A:107:VAL:HG23	2.21	0.40
1:B:77:ARG:HA	1:B:80:ILE:HG22	2.03	0.40
1:B:199:TRP:CE3	1:B:200:ASN:HB2	2.56	0.40
1:B:222:PHE:CE1	1:B:280:VAL:CG1	3.04	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:SER:CA	1:A:268:ASP:OD2[1_455]	1.93	0.27
1:A:37:SER:OG	1:A:268:ASP:CG[1_455]	2.13	0.07
1:A:37:SER:OG	1:A:268:ASP:OD1[1_455]	2.17	0.03
1:A:37:SER:OG	1:A:268:ASP:OD2[1_455]	2.17	0.03
1:A:96:ASP:OD1	1:B:301:LYS:NZ[3_545]	2.19	0.01

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	272/312 (87%)	265 (97%)	7 (3%)	0	100	100
1	B	280/312 (90%)	264 (94%)	13 (5%)	3 (1%)	14	41
All	All	552/624 (88%)	529 (96%)	20 (4%)	3 (0%)	29	61

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	264	ILE
1	B	314	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	226/260 (87%)	224 (99%)	2 (1%)	78	94
1	B	224/260 (86%)	224 (100%)	0	100	100
All	All	450/520 (86%)	448 (100%)	2 (0%)	91	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	196	PHE
1	A	320	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	320	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 6 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
4	R16	B	411	-	9,9,15	0.32	0	8,8,14	0.77	0
5	16C	A	406	-	36,37,37	1.10	2 (5%)	37,39,39	1.08	2 (5%)
4	R16	A	408	-	7,7,15	0.30	0	6,6,14	0.73	0
3	Q5F	A	404	-	19,20,20	2.54	10 (52%)	21,26,26	2.21	5 (23%)
4	R16	B	409	-	4,4,15	0.32	0	3,3,14	0.54	0
4	R16	B	406	-	11,11,15	0.30	0	10,10,14	0.82	0
4	R16	B	410	-	10,10,15	0.30	0	9,9,14	0.82	0
4	R16	A	407	-	10,10,15	0.31	0	9,9,14	0.81	0
4	R16	B	407	-	4,4,15	0.32	0	3,3,14	0.54	0
4	R16	B	408	-	4,4,15	0.32	0	3,3,14	0.56	0
3	Q5F	B	404	-	19,20,20	2.56	10 (52%)	21,26,26	2.11	4 (19%)
4	R16	B	405	-	11,11,15	0.30	0	10,10,14	0.83	0
4	R16	A	405	-	11,11,15	0.30	0	10,10,14	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	R16	B	411	-	-	0/7/7/13	-
5	16C	A	406	-	-	19/40/40/40	-
4	R16	A	408	-	-	0/5/5/13	-
3	Q5F	A	404	-	-	4/9/11/11	0/2/2/2
4	R16	B	409	-	-	0/2/2/13	-
4	R16	B	406	-	-	2/9/9/13	-
4	R16	B	410	-	-	3/8/8/13	-
4	R16	A	407	-	-	2/8/8/13	-
4	R16	B	407	-	-	0/2/2/13	-
4	R16	B	408	-	-	1/2/2/13	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	Q5F	B	404	-	-	2/9/11/11	0/2/2/2
4	R16	B	405	-	-	5/9/9/13	-
4	R16	A	405	-	-	1/9/9/13	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	404	Q5F	C13-N05	5.77	1.46	1.33
3	A	404	Q5F	C13-N05	5.60	1.46	1.33
5	A	406	16C	C19-N2	5.47	1.45	1.34
3	A	404	Q5F	C08-C09	4.34	1.49	1.39
3	B	404	Q5F	C08-C09	3.97	1.48	1.39
3	B	404	Q5F	C06-C07	3.79	1.63	1.50
3	A	404	Q5F	C06-C07	3.63	1.63	1.50
3	A	404	Q5F	C15-CL1	3.36	1.81	1.74
3	B	404	Q5F	C11-C15	3.32	1.43	1.38
3	B	404	Q5F	C15-CL1	3.24	1.81	1.74
3	A	404	Q5F	C11-C15	3.23	1.43	1.38
3	A	404	Q5F	C11-C09	2.83	1.43	1.39
3	B	404	Q5F	C11-C09	2.73	1.43	1.39
3	B	404	Q5F	C14-C15	2.50	1.42	1.38
3	B	404	Q5F	C10-C08	2.38	1.44	1.39
3	B	404	Q5F	C14-C10	2.29	1.42	1.38
3	A	404	Q5F	C10-C08	2.24	1.44	1.39
3	B	404	Q5F	C18-C17	2.23	1.47	1.39
3	A	404	Q5F	C14-C15	2.21	1.42	1.38
5	A	406	16C	O19-C19	-2.20	1.18	1.23
3	A	404	Q5F	C18-C17	2.20	1.46	1.39
3	A	404	Q5F	C14-C10	2.05	1.42	1.38

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	404	Q5F	C16-C13-N05	5.71	123.57	115.59
3	A	404	Q5F	O03-C07-C06	5.45	119.48	107.81
3	A	404	Q5F	C16-C13-N05	5.39	123.13	115.59
3	B	404	Q5F	O03-C07-C06	5.09	118.69	107.81
3	B	404	Q5F	O04-C13-N05	-3.47	115.70	122.61
3	A	404	Q5F	O04-C13-N05	-3.39	115.86	122.61
3	A	404	Q5F	O03-C08-C09	2.85	120.50	115.10
5	A	406	16C	C20-C19-N2	2.57	120.29	115.83
3	B	404	Q5F	O03-C08-C09	2.18	119.23	115.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	404	Q5F	C07-O03-C08	2.14	122.92	117.69
5	A	406	16C	C3-C4-C5	-2.14	120.03	124.79

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	406	16C	O1-C1-C2-C3
5	A	406	16C	C2-C3-C4-C5
5	A	406	16C	O3-C3-C4-C5
3	A	404	Q5F	N05-C06-C07-O03
3	B	404	Q5F	N05-C06-C07-O03
3	A	404	Q5F	C09-C08-O03-C07
4	B	405	R16	C32-C33-C34-C35
4	A	407	R16	C32-C33-C34-C35
4	A	405	R16	C35-C36-C37-C38
5	A	406	16C	C7-C8-C9-C10
5	A	406	16C	C9-C10-C11-C12
3	A	404	Q5F	C10-C08-O03-C07
4	B	405	R16	C29-C30-C31-C32
4	B	406	R16	C29-C30-C31-C32
5	A	406	16C	C13-C14-C15-C16
5	A	406	16C	C5-C6-C7-C8
3	B	404	Q5F	C06-C07-O03-C08
4	A	407	R16	C33-C34-C35-C36
4	B	405	R16	C30-C31-C32-C33
5	A	406	16C	C6-C7-C8-C9
5	A	406	16C	C27-C28-C29-C30
5	A	406	16C	C31-C32-C33-C34
3	A	404	Q5F	C06-C07-O03-C08
4	B	405	R16	C35-C36-C37-C38
4	B	405	R16	C31-C32-C33-C34
4	B	410	R16	C31-C32-C33-C34
4	B	410	R16	C35-C36-C37-C38
4	B	406	R16	C31-C32-C33-C34
5	A	406	16C	C14-C15-C16-C17
5	A	406	16C	C21-C22-C23-C24
5	A	406	16C	O1-C1-C2-N2
5	A	406	16C	C11-C12-C13-C14
5	A	406	16C	C15-C16-C17-C18
5	A	406	16C	C19-C20-C21-C22
5	A	406	16C	C29-C30-C31-C32

Continued on next page...

Continued from previous page...

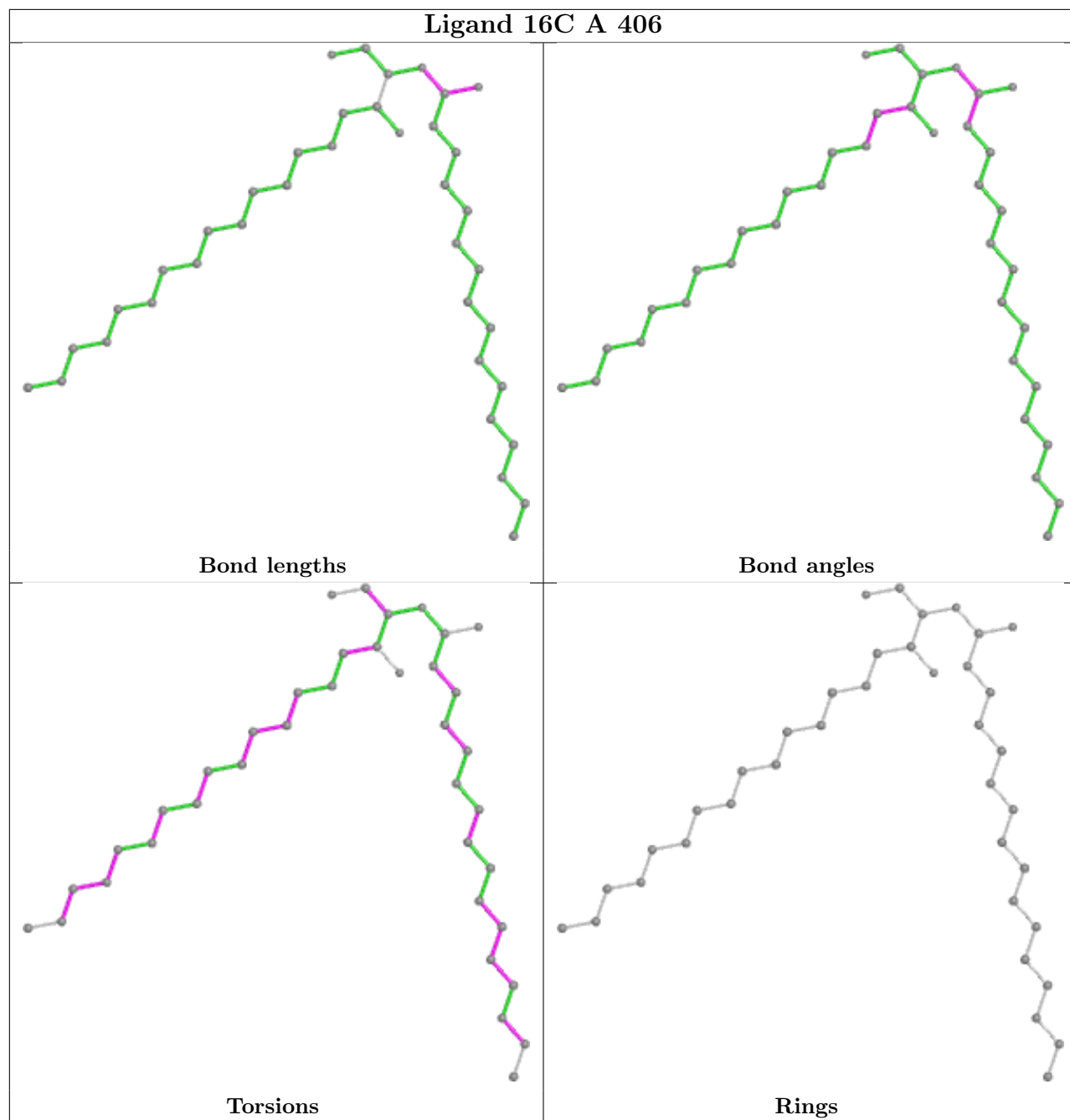
Mol	Chain	Res	Type	Atoms
4	B	408	R16	C31-C32-C33-C34
4	B	410	R16	C36-C37-C38-C39
5	A	406	16C	C28-C29-C30-C31
5	A	406	16C	C24-C25-C26-C27

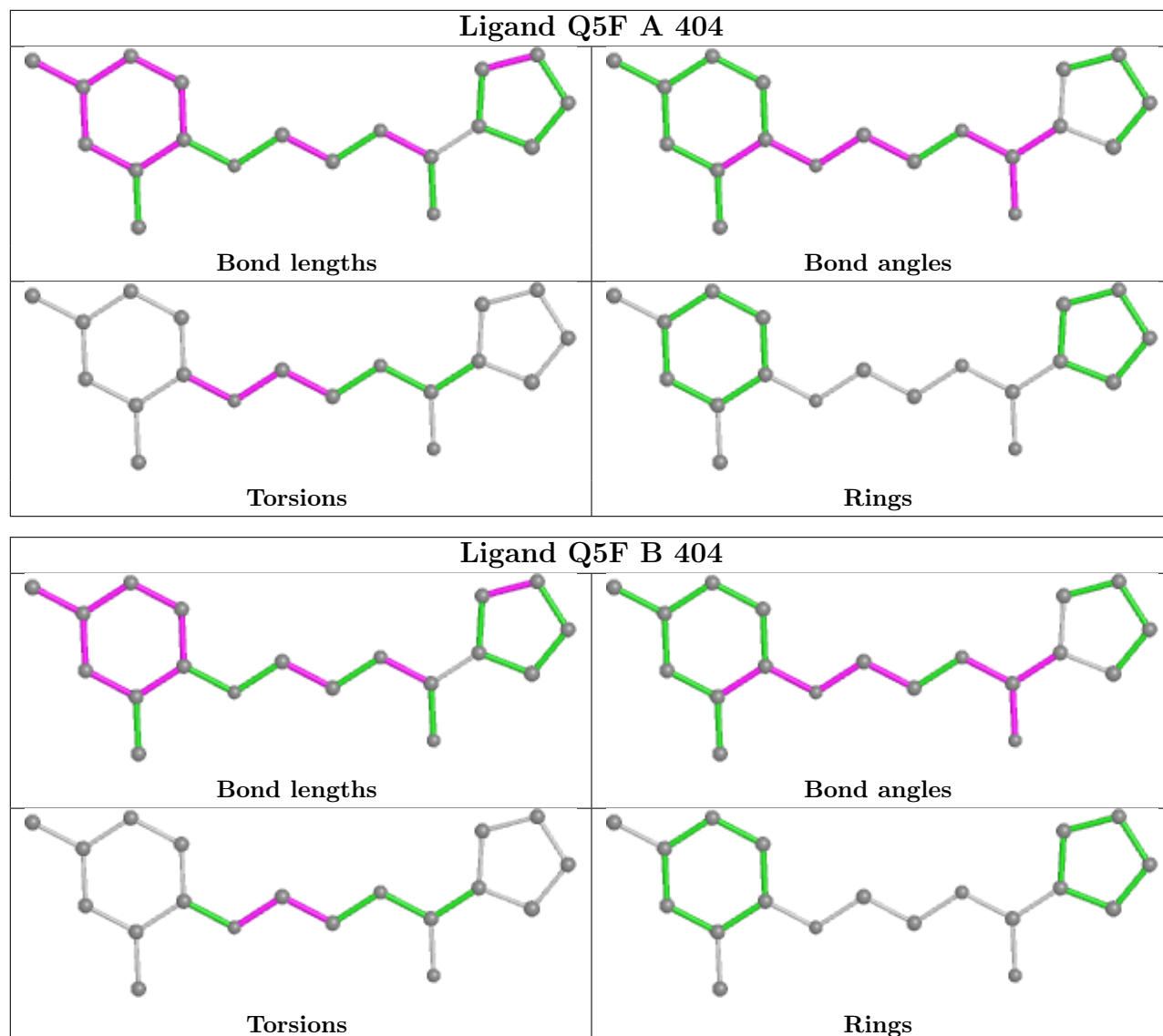
There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	406	16C	3	0
3	A	404	Q5F	1	0
3	B	404	Q5F	3	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	276/312 (88%)	0.12	23 (8%) 11 6	76, 130, 236, 284	0
1	B	282/312 (90%)	0.38	34 (12%) 4 2	72, 135, 240, 324	0
All	All	558/624 (89%)	0.25	57 (10%) 6 3	72, 133, 240, 324	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	92	PRO	27.6
1	B	93	CYS	13.0
1	B	199	TRP	9.3
1	A	36	ASP	8.4
1	A	264	ILE	6.9
1	B	89	ARG	6.6
1	B	200	ASN	6.5
1	A	265	GLU	6.2
1	A	194	ASP	6.1
1	B	309	GLU	6.0
1	B	35	SER	5.9
1	A	195	THR	5.8
1	B	91	HIS	5.6
1	B	97	GLN	5.1
1	B	104	GLN	4.8
1	B	195	THR	4.7
1	A	199	TRP	4.7
1	A	203	GLN	4.4
1	B	232	HIS	3.7
1	B	194	ASP	3.5
1	B	196	PHE	3.5
1	A	207	ARG	3.4
1	A	187	LYS	3.3
1	B	85	GLU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	196	PHE	3.1
1	A	89	ARG	3.1
1	B	36	ASP	3.0
1	B	96	ASP	2.9
1	B	314	ALA	2.9
1	A	263	ASP	2.8
1	A	191	LYS	2.8
1	B	312	ALA	2.8
1	B	204	THR	2.7
1	A	71	PRO	2.7
1	A	232	HIS	2.6
1	B	122	ASN	2.6
1	B	37	SER	2.6
1	B	305	GLU	2.5
1	A	320	ASN	2.5
1	B	44	TRP	2.5
1	B	308	GLY	2.4
1	A	307	VAL	2.4
1	B	267	LEU	2.4
1	A	321	VAL	2.4
1	A	125	SER	2.4
1	B	111	ASN	2.4
1	A	200	ASN	2.3
1	B	203	GLN	2.3
1	B	201	VAL	2.3
1	A	101	GLU	2.2
1	B	108	ALA	2.1
1	B	129	LEU	2.1
1	B	126	HIS	2.1
1	B	90	ALA	2.1
1	A	86	LYS	2.0
1	A	37	SER	2.0
1	B	120	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

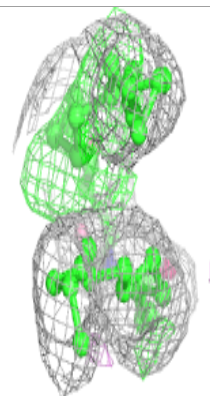
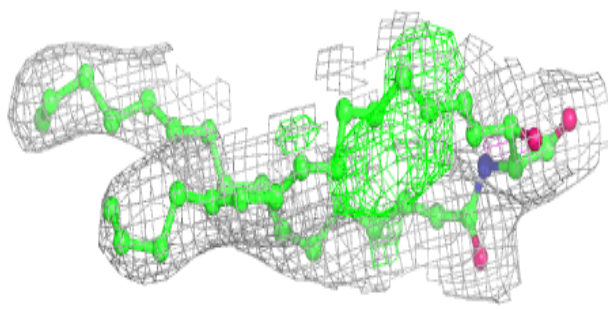
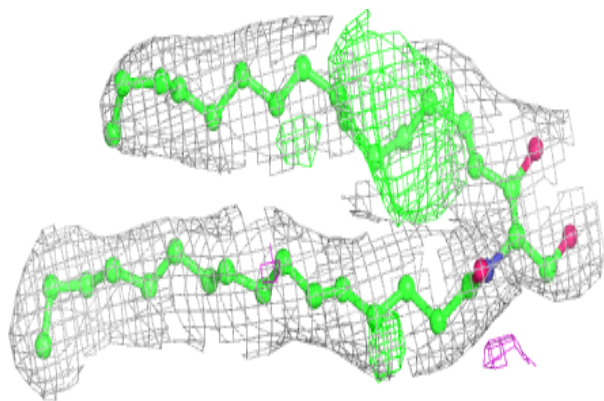
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	16C	A	406	38/38	0.71	0.21	95,114,145,173	0
4	R16	B	411	10/16	0.72	0.23	96,143,172,190	0
4	R16	B	409	5/16	0.72	0.42	118,142,150,164	0
2	K	A	401	1/1	0.83	0.12	150,150,150,150	0
4	R16	B	406	12/16	0.84	0.15	75,102,120,120	0
4	R16	A	407	11/16	0.84	0.16	78,102,129,133	0
4	R16	B	407	5/16	0.87	0.15	93,99,112,123	0
4	R16	A	408	8/16	0.89	0.10	109,154,188,188	0
4	R16	A	405	12/16	0.90	0.12	86,114,133,135	0
4	R16	B	410	11/16	0.90	0.11	99,113,134,139	0
4	R16	B	405	12/16	0.90	0.15	82,106,128,130	0
4	R16	B	408	5/16	0.90	0.16	101,129,146,155	0
3	Q5F	B	404	19/19	0.92	0.19	80,103,153,155	0
3	Q5F	A	404	19/19	0.93	0.17	75,114,130,136	0
2	K	B	401	1/1	0.94	0.08	96,96,96,96	0
2	K	A	402	1/1	0.94	0.15	122,122,122,122	0
2	K	B	402	1/1	0.95	0.20	112,112,112,112	0
2	K	A	403	1/1	0.96	0.04	131,131,131,131	0
6	CD	B	403	1/1	0.97	0.11	165,165,165,165	0

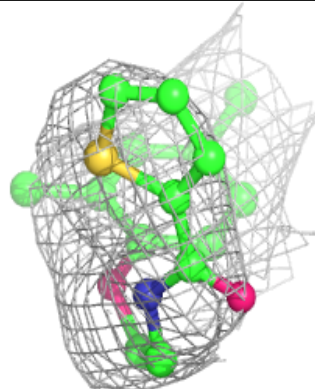
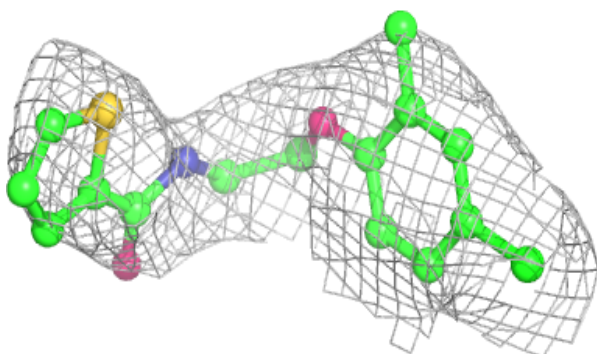
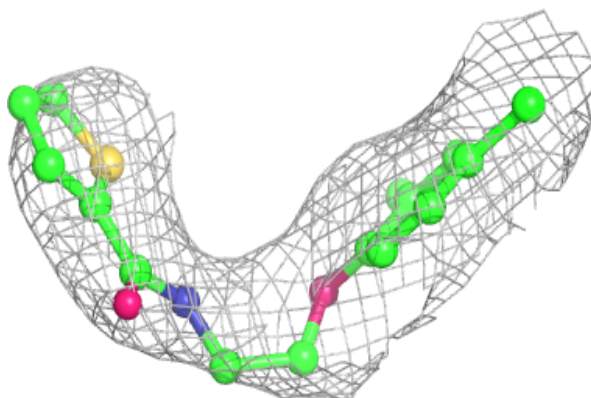
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

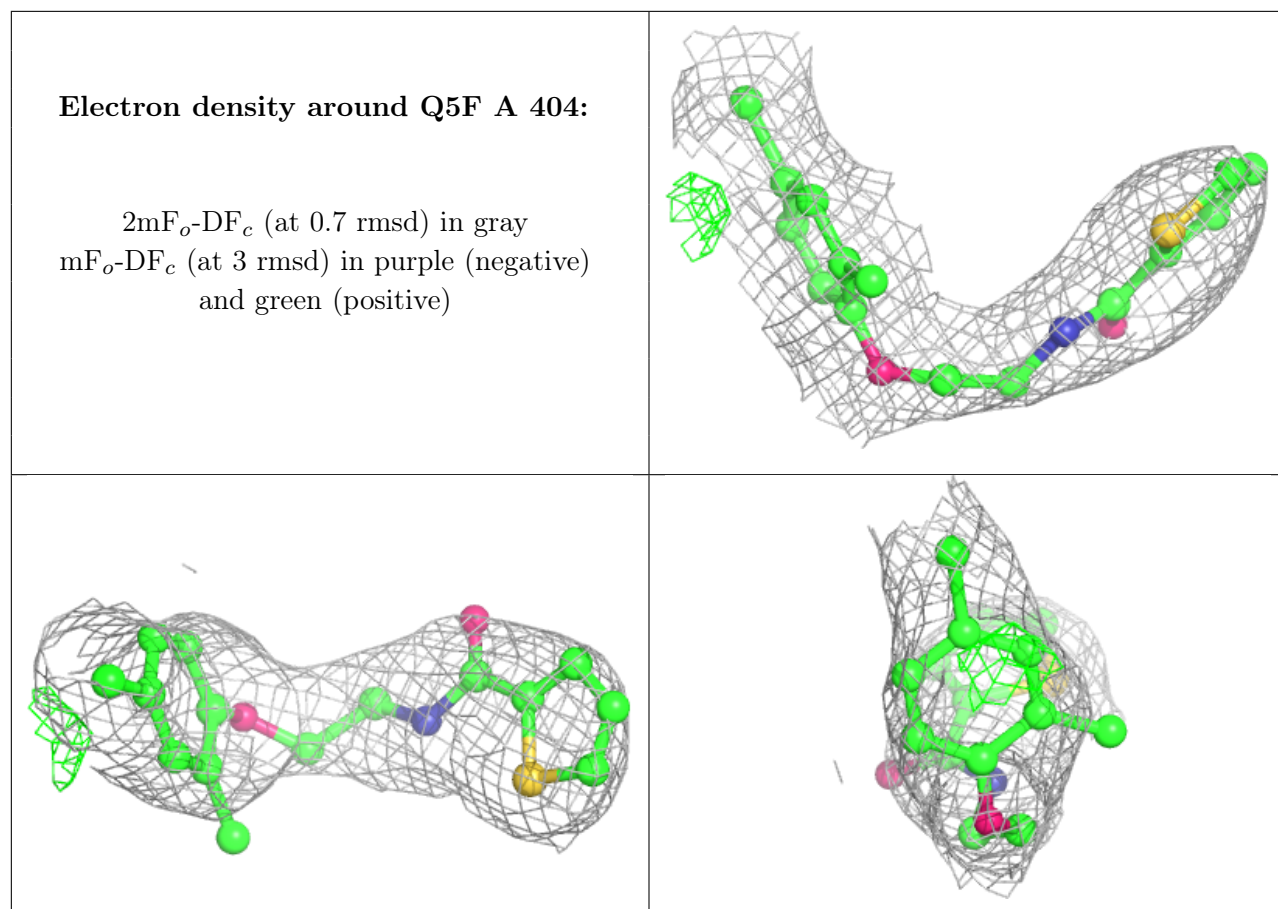
Electron density around 16C A 406:

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

**Electron density around Q5F B 404:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.