Full wwPDB X-ray Structure Validation Report (i)

Oct 27, 2021 – 09:09 pm BST

PDB ID	:	7OAJ
Title	:	Crystal structure of pseudokinase CASK in complex with compound 7
Authors	:	Chaikuad, A.; Russ, N.; Knapp, S.; Structural Genomics Consortium (SGC)
Deposited on	:	2021-04-19
Resolution	:	1.93 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 following versions of software and data (see references (i)) were used in the production of this report:

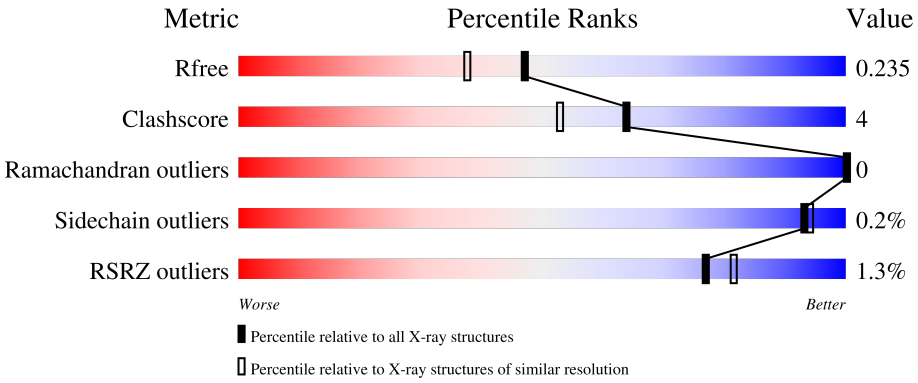
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 1.93 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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	353	74% 10% 16%
1	B	353	76% 8% 16%
1	C	353	76% 8% 16%
1	D	353	76% 8% 16%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10317 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 Peripheral plasma membrane protein CASK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	0	3	0
			2398	1538	418	425	17			
1	B	297	Total	C	N	O	S	0	3	0
			2389	1535	414	422	18			
1	C	297	Total	C	N	O	S	0	0	0
			2373	1522	414	420	17			
1	D	297	Total	C	N	O	S	0	2	0
			2384	1531	414	422	17			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	SER	-	expression tag	UNP O14936
A	-14	MET	-	expression tag	UNP O14936
A	-13	GLY	-	expression tag	UNP O14936
A	-12	SER	-	expression tag	UNP O14936
A	-11	PRO	-	expression tag	UNP O14936
A	-10	GLY	-	expression tag	UNP O14936
A	-9	ILE	-	expression tag	UNP O14936
A	-8	SER	-	expression tag	UNP O14936
A	-7	GLY	-	expression tag	UNP O14936
A	-6	GLY	-	expression tag	UNP O14936
A	-5	GLY	-	expression tag	UNP O14936
A	-4	GLY	-	expression tag	UNP O14936
A	-3	GLY	-	expression tag	UNP O14936
A	-2	ILE	-	expression tag	UNP O14936
A	-1	ARG	-	expression tag	UNP O14936
A	0	THR	-	expression tag	UNP O14936
B	-15	SER	-	expression tag	UNP O14936
B	-14	MET	-	expression tag	UNP O14936
B	-13	GLY	-	expression tag	UNP O14936
B	-12	SER	-	expression tag	UNP O14936
B	-11	PRO	-	expression tag	UNP O14936

Continued on next page...

Continued from previous page...

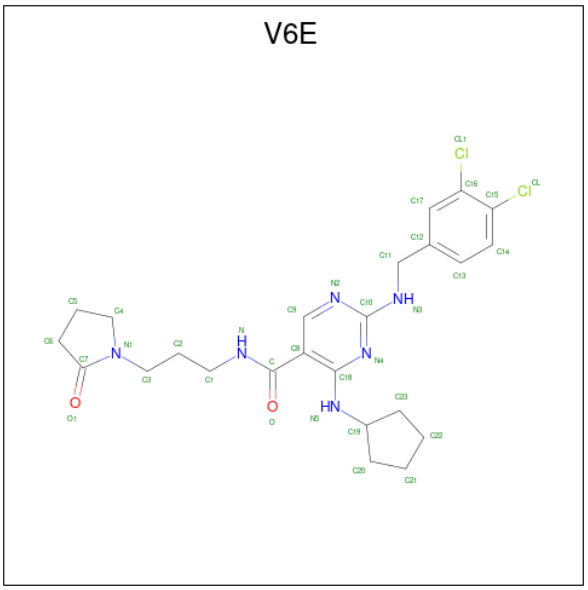
Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	GLY	-	expression tag	UNP O14936
B	-9	ILE	-	expression tag	UNP O14936
B	-8	SER	-	expression tag	UNP O14936
B	-7	GLY	-	expression tag	UNP O14936
B	-6	GLY	-	expression tag	UNP O14936
B	-5	GLY	-	expression tag	UNP O14936
B	-4	GLY	-	expression tag	UNP O14936
B	-3	GLY	-	expression tag	UNP O14936
B	-2	ILE	-	expression tag	UNP O14936
B	-1	ARG	-	expression tag	UNP O14936
B	0	THR	-	expression tag	UNP O14936
C	-15	SER	-	expression tag	UNP O14936
C	-14	MET	-	expression tag	UNP O14936
C	-13	GLY	-	expression tag	UNP O14936
C	-12	SER	-	expression tag	UNP O14936
C	-11	PRO	-	expression tag	UNP O14936
C	-10	GLY	-	expression tag	UNP O14936
C	-9	ILE	-	expression tag	UNP O14936
C	-8	SER	-	expression tag	UNP O14936
C	-7	GLY	-	expression tag	UNP O14936
C	-6	GLY	-	expression tag	UNP O14936
C	-5	GLY	-	expression tag	UNP O14936
C	-4	GLY	-	expression tag	UNP O14936
C	-3	GLY	-	expression tag	UNP O14936
C	-2	ILE	-	expression tag	UNP O14936
C	-1	ARG	-	expression tag	UNP O14936
C	0	THR	-	expression tag	UNP O14936
D	-15	SER	-	expression tag	UNP O14936
D	-14	MET	-	expression tag	UNP O14936
D	-13	GLY	-	expression tag	UNP O14936
D	-12	SER	-	expression tag	UNP O14936
D	-11	PRO	-	expression tag	UNP O14936
D	-10	GLY	-	expression tag	UNP O14936
D	-9	ILE	-	expression tag	UNP O14936
D	-8	SER	-	expression tag	UNP O14936
D	-7	GLY	-	expression tag	UNP O14936
D	-6	GLY	-	expression tag	UNP O14936
D	-5	GLY	-	expression tag	UNP O14936
D	-4	GLY	-	expression tag	UNP O14936
D	-3	GLY	-	expression tag	UNP O14936
D	-2	ILE	-	expression tag	UNP O14936
D	-1	ARG	-	expression tag	UNP O14936

Continued on next page...

Continued from previous page...

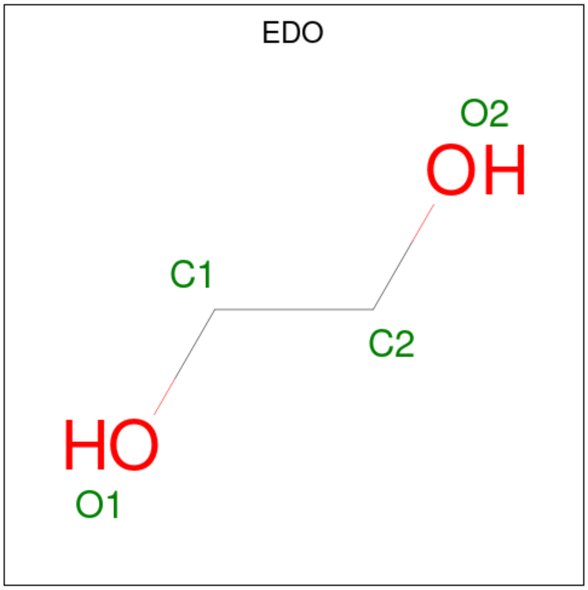
Chain	Residue	Modelled	Actual	Comment	Reference
D	0	THR	-	expression tag	UNP O14936

- Molecule 2 is 4-(cyclopentylamino)-2-[(3,4-dichlorophenyl)methylamino]-N-[3-(2-oxidanylidenepyrrolidin-1-yl)propyl]pyrimidine-5-carboxamide (three-letter code: V6E) (formula: $C_{24}H_{30}Cl_2N_6O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			34	24	2	6	2		
2	B	1	Total	C	Cl	N	O	0	0
			34	24	2	6	2		
2	C	1	Total	C	Cl	N	O	0	0
			34	24	2	6	2		
2	D	1	Total	C	Cl	N	O	0	0
			34	24	2	6	2		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0

- Molecule 4 is water.

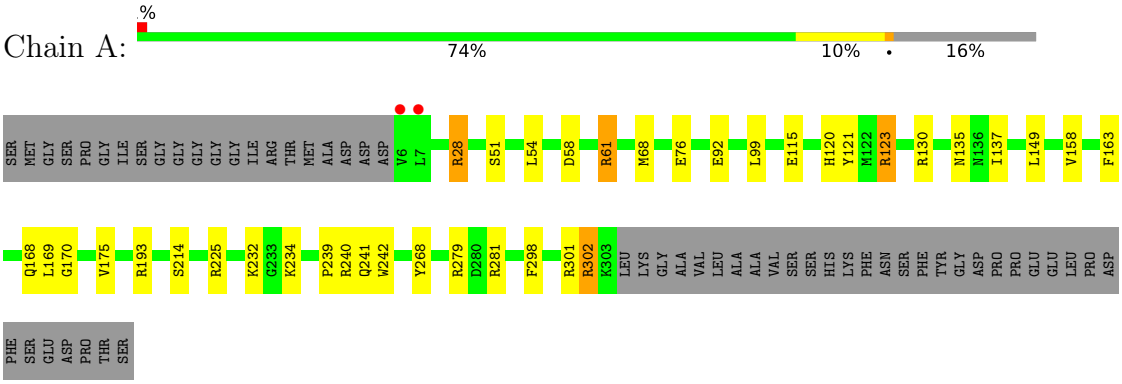
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	139	Total O 139 139	0	0
4	B	151	Total O 151 151	0	0
4	C	139	Total O 139 139	0	0
4	D	120	Total O 120 120	0	0

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.

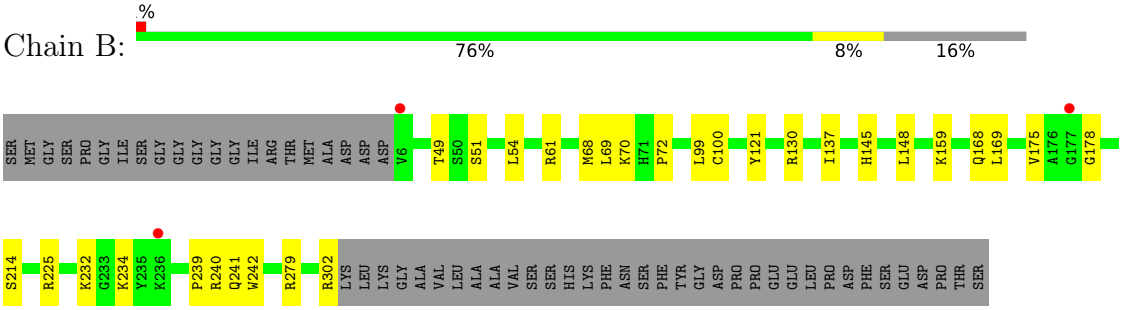
• Molecule 1: Peripheral plasma membrane protein CASK

Chain A:



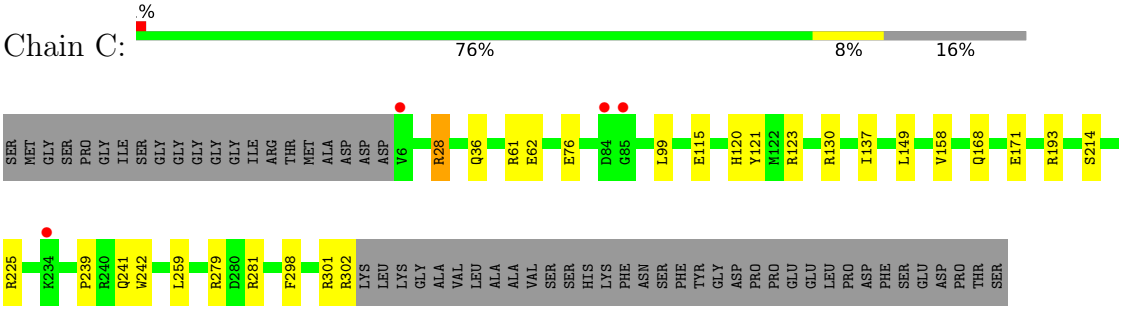
• Molecule 1: Peripheral plasma membrane protein CASK

Chain B:



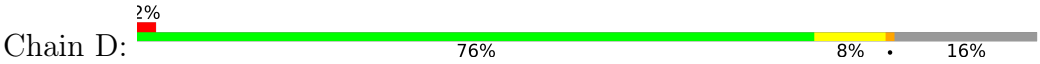
• Molecule 1: Peripheral plasma membrane protein CASK

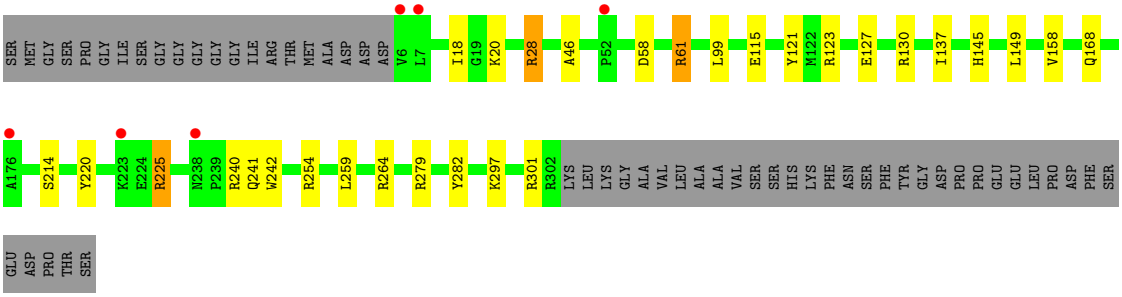
Chain C:



• Molecule 1: Peripheral plasma membrane protein CASK

Chain D:




SER MET GLY SER PRO GLY ILE SER GLY GLY GLY GLY ILE ARG THR MET ALA ASP ASP ASP
V6 L7 I18 G19 K20 R28 A46 P52 D58 R61 L99 E115 Y121 M122 R123 E127 R130 I137 H145 L149 V158 Q168
A176 S214 Y220 K223 E224 R225 N238 P239 R240 Q241 W242 R254 L259 R264 R279 Y282 K297 R301 H302
LYS LEU LYS GLY ALA VAL LEU ALA ALA VAL SER SER HIS LYS PHE ASN SER PHE TYR GLY ASP PRO PRO GLU GLU LEU PRO ASP PHE SER
GLU ASP PRO THR SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	41.35Å 66.84Å 130.20Å 76.20° 89.99° 90.00°	Depositor
Resolution (Å)	42.15 – 1.93 42.15 – 1.93	Depositor EDS
% Data completeness (in resolution range)	91.6 (42.15-1.93) 99.0 (42.15-1.93)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.195 , 0.224 0.209 , 0.235	Depositor DCC
R_{free} test set	4842 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å^2)	31.8	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.306 for h,-k,-l 0.128 for -h,k,k-l 0.138 for -h,-k,-k+l	Xtriage
Reported twinning fraction	0.542 for H, K, L 0.458 for h,-k,-l	Depositor
Outliers	0 of 100968 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10317	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.55% 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: EDO, V6E

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	0.72	1/2463 (0.0%)	0.71	0/3323
1	B	0.71	0/2454	0.69	0/3311
1	C	0.71	2/2429 (0.1%)	0.68	0/3278
1	D	0.69	1/2446 (0.0%)	0.68	0/3301
All	All	0.71	4/9792 (0.0%)	0.69	0/13213

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	10
1	B	0	5
1	C	0	8
1	D	0	8
All	All	0	31

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	115	GLU	CD-OE1	-5.46	1.19	1.25
1	C	62	GLU	CD-OE2	-5.32	1.19	1.25
1	D	115	GLU	CD-OE2	-5.04	1.20	1.25
1	A	115	GLU	CD-OE2	-5.00	1.20	1.25

There are no bond angle outliers.

There are no chirality outliers.

All (31) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	123[A]	ARG	Sidechain
1	A	123[B]	ARG	Sidechain
1	A	130	ARG	Sidechain
1	A	193	ARG	Sidechain
1	A	240	ARG	Sidechain
1	A	279	ARG	Sidechain
1	A	28	ARG	Sidechain
1	A	281	ARG	Sidechain
1	A	302	ARG	Sidechain
1	A	61	ARG	Sidechain
1	B	130	ARG	Sidechain
1	B	225	ARG	Sidechain
1	B	240	ARG	Sidechain
1	B	279	ARG	Sidechain
1	B	61	ARG	Sidechain
1	C	123	ARG	Sidechain
1	C	130	ARG	Sidechain
1	C	193	ARG	Sidechain
1	C	225	ARG	Sidechain
1	C	279	ARG	Sidechain
1	C	28	ARG	Sidechain
1	C	281	ARG	Sidechain
1	C	61	ARG	Sidechain
1	D	123	ARG	Sidechain
1	D	130	ARG	Sidechain
1	D	225	ARG	Sidechain
1	D	240	ARG	Sidechain
1	D	264	ARG	Sidechain
1	D	279	ARG	Sidechain
1	D	28	ARG	Sidechain
1	D	61	ARG	Sidechain

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	2398	0	2414	28	0
1	B	2389	0	2413	20	0
1	C	2373	0	2387	16	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2384	0	2404	21	0
2	A	34	0	0	0	0
2	B	34	0	0	1	0
2	C	34	0	0	0	0
2	D	34	0	0	1	0
3	A	24	0	36	3	0
3	B	32	0	48	1	0
3	C	20	0	30	3	0
3	D	12	0	18	2	0
4	A	139	0	0	5	0
4	B	151	0	0	3	0
4	C	139	0	0	4	0
4	D	120	0	0	5	0
All	All	10317	0	9750	82	1

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 4.

All (82) 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:298:PHE:O	1:A:302:ARG:HG3	1.80	0.81
1:C:239:PRO:HG3	4:C:563:HOH:O	1.87	0.74
1:C:36:GLN:OE1	4:C:501:HOH:O	2.11	0.68
1:A:76:GLU:HB3	1:A:92[B]:GLU:HG3	1.76	0.68
1:B:178:GLY:HA3	1:D:46:ALA:HB1	1.74	0.68
1:A:163:PHE:CD1	3:A:404:EDO:H22	2.31	0.66
1:C:298:PHE:O	1:C:302:ARG:HG3	1.96	0.65
1:C:99:LEU:HD11	1:C:121:TYR:CD2	2.32	0.65
1:A:239:PRO:HG3	4:A:566:HOH:O	1.97	0.64
1:B:54:LEU:O	1:D:20:LYS:NZ	2.22	0.63
1:D:99:LEU:HD11	1:D:121:TYR:CD2	2.34	0.63
1:C:239:PRO:CG	4:C:563:HOH:O	2.43	0.62
1:A:99:LEU:HD11	1:A:121:TYR:CD2	2.35	0.62
1:B:99:LEU:HD11	1:B:121:TYR:CD2	2.35	0.61
1:D:225:ARG:HH11	1:D:225:ARG:HG3	1.67	0.60
1:A:225:ARG:HH11	1:A:225:ARG:HG3	1.66	0.59
1:A:268:TYR:HB2	3:A:405:EDO:O1	2.04	0.57
1:C:171:GLU:HG2	1:D:282:TYR:CD1	2.40	0.55
1:D:28:ARG:HH22	3:D:402:EDO:C1	2.19	0.55
1:A:214:SER:O	1:A:241:GLN:HG2	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:PRO:CG	4:A:566:HOH:O	2.53	0.53
1:D:214:SER:O	1:D:241:GLN:HG2	2.09	0.53
1:B:214:SER:O	1:B:241:GLN:HG2	2.09	0.52
1:C:214:SER:O	1:C:241:GLN:HG2	2.10	0.52
1:B:68:MET:HE1	4:B:543:HOH:O	2.09	0.51
1:C:120:HIS:ND1	3:C:404:EDO:O2	2.39	0.50
1:A:76:GLU:HB3	1:A:92[B]:GLU:CG	2.39	0.50
1:A:120:HIS:CE1	1:A:123[B]:ARG:NH2	2.80	0.50
2:D:401:V6E:C12	2:D:401:V6E:N4	2.76	0.49
1:A:120:HIS:CE1	1:A:123[B]:ARG:HH21	2.31	0.48
1:B:232:LYS:HE2	1:B:234:LYS:HB2	1.94	0.48
1:B:68:MET:CE	4:B:543:HOH:O	2.62	0.48
1:D:254:ARG:NE	4:D:515:HOH:O	2.45	0.48
1:D:18:ILE:HG22	4:D:502:HOH:O	2.13	0.48
1:B:214:SER:HB3	1:B:242:TRP:CE2	2.50	0.47
1:C:301:ARG:NH1	4:C:511:HOH:O	2.47	0.47
1:A:169:LEU:HD23	1:A:175:VAL:HG23	1.97	0.47
1:D:127[B]:GLU:HG2	4:D:540:HOH:O	2.14	0.47
1:C:28:ARG:HH22	3:C:402:EDO:C1	2.28	0.47
1:D:99:LEU:HD11	1:D:121:TYR:CE2	2.50	0.46
1:C:99:LEU:HD11	1:C:121:TYR:CE2	2.51	0.46
1:B:137[A]:ILE:HD13	1:B:168:GLN:HA	1.97	0.46
1:A:68:MET:HE1	1:A:135:ASN:HB3	1.96	0.45
1:D:28:ARG:HH22	3:D:402:EDO:H12	1.82	0.45
1:B:72:PRO:O	1:B:159:LYS:HE2	2.17	0.45
1:B:239:PRO:HG3	4:B:631:HOH:O	2.17	0.45
1:C:137:ILE:HD13	1:C:168:GLN:HA	1.99	0.45
1:B:169:LEU:CD2	1:B:175:VAL:HG23	2.47	0.45
1:D:58:ASP:OD1	1:D:61:ARG:NH2	2.49	0.45
1:B:70:LYS:HB3	3:B:405:EDO:H22	1.98	0.45
1:C:214:SER:HB3	1:C:242:TRP:CE2	2.52	0.45
1:B:49:THR:O	1:D:20:LYS:NZ	2.48	0.44
1:D:214:SER:HB3	1:D:242:TRP:CE2	2.52	0.44
1:D:149:LEU:HD22	1:D:158:VAL:HG12	1.99	0.44
1:A:232:LYS:HE2	1:A:234:LYS:HB2	1.98	0.44
1:A:298:PHE:CZ	1:A:302:ARG:HD3	2.53	0.44
1:B:69:LEU:HD21	1:B:137[B]:ILE:HD13	1.98	0.44
1:B:148:LEU:HD22	2:B:401:V6E:CL1	2.54	0.44
1:A:51:SER:HB3	1:A:54:LEU:HD12	1.99	0.44
1:D:18:ILE:HA	4:D:502:HOH:O	2.16	0.44
1:D:137[A]:ILE:HD13	1:D:168:GLN:HA	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:220:TYR:HB2	4:D:559:HOH:O	2.17	0.43
1:A:225:ARG:HG3	1:A:225:ARG:NH1	2.33	0.43
1:B:99:LEU:HD11	1:B:121:TYR:CE2	2.53	0.43
1:C:28:ARG:HH22	3:C:402:EDO:H12	1.83	0.43
1:A:99:LEU:HD11	1:A:121:TYR:CE2	2.53	0.43
1:A:137:ILE:HD13	1:A:168:GLN:HA	2.00	0.43
1:C:149:LEU:HD22	1:C:158:VAL:HG12	2.00	0.42
1:A:58:ASP:O	1:A:61:ARG:NH1	2.53	0.42
1:A:214:SER:HB3	1:A:242:TRP:CE2	2.55	0.42
1:B:51:SER:HB3	1:B:54:LEU:HD12	2.01	0.42
1:A:301:ARG:O	1:A:302:ARG:C	2.58	0.41
1:B:100:CYS:HB2	1:B:302:ARG:NH2	2.35	0.41
1:A:28:ARG:NH1	3:A:402:EDO:O1	2.37	0.41
1:A:68:MET:HE1	4:A:590:HOH:O	2.19	0.41
1:A:149:LEU:HD22	1:A:158:VAL:HG12	2.01	0.41
1:A:239:PRO:CD	4:A:566:HOH:O	2.69	0.41
1:D:259:LEU:HD23	1:D:259:LEU:HA	1.89	0.41
1:B:169:LEU:HD23	1:B:175:VAL:HG23	2.02	0.41
1:C:259:LEU:HD23	1:C:259:LEU:HA	1.92	0.41
1:D:297:LYS:O	1:D:301:ARG:HG3	2.21	0.41
1:A:170:GLY:HA3	4:A:552:HOH:O	2.20	0.40

All (1) 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:C:76:GLU:OE2	1:C:301:ARG:NH2[1_455]	2.05	0.15

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	299/353 (85%)	293 (98%)	6 (2%)	0	100	100
1	B	298/353 (84%)	293 (98%)	5 (2%)	0	100	100
1	C	295/353 (84%)	289 (98%)	6 (2%)	0	100	100
1	D	297/353 (84%)	290 (98%)	7 (2%)	0	100	100
All	All	1189/1412 (84%)	1165 (98%)	24 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	259/299 (87%)	259 (100%)	0	100	100
1	B	259/299 (87%)	258 (100%)	1 (0%)	91	91
1	C	256/299 (86%)	256 (100%)	0	100	100
1	D	258/299 (86%)	257 (100%)	1 (0%)	91	91
All	All	1032/1196 (86%)	1030 (100%)	2 (0%)	93	94

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

Mol	Chain	Res	Type
1	B	145	HIS
1	D	145	HIS

Sometimes 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 monosaccharides in this entry.

5.6 Ligand geometry (i)

26 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
3	EDO	D	403	-	3,3,3	0.28	0	2,2,2	0.44	0
3	EDO	C	404	-	3,3,3	0.30	0	2,2,2	0.46	0
3	EDO	A	402	-	3,3,3	0.23	0	2,2,2	1.04	0
3	EDO	C	402	-	3,3,3	0.36	0	2,2,2	0.23	0
3	EDO	C	403	-	3,3,3	0.59	0	2,2,2	0.40	0
3	EDO	B	406	-	3,3,3	0.62	0	2,2,2	0.33	0
3	EDO	A	407	-	3,3,3	0.33	0	2,2,2	0.55	0
2	V6E	A	401	-	37,37,37	0.39	0	48,50,50	0.70	1 (2%)
2	V6E	D	401	-	37,37,37	0.32	0	48,50,50	1.03	1 (2%)
3	EDO	A	405	-	3,3,3	0.36	0	2,2,2	0.59	0
2	V6E	C	401	-	37,37,37	0.30	0	48,50,50	1.51	1 (2%)
3	EDO	B	403	-	3,3,3	0.26	0	2,2,2	0.77	0
3	EDO	B	402	-	3,3,3	0.52	0	2,2,2	0.37	0
3	EDO	A	403	-	3,3,3	0.28	0	2,2,2	0.87	0
3	EDO	B	407	-	3,3,3	0.30	0	2,2,2	0.73	0
3	EDO	C	406	-	3,3,3	0.60	0	2,2,2	0.31	0
3	EDO	D	404	-	3,3,3	0.32	0	2,2,2	0.53	0
3	EDO	A	404	-	3,3,3	0.61	0	2,2,2	0.22	0
3	EDO	B	405	-	3,3,3	0.40	0	2,2,2	0.74	0
2	V6E	B	401	-	37,37,37	0.25	0	48,50,50	1.70	1 (2%)
3	EDO	B	404	-	3,3,3	0.54	0	2,2,2	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	EDO	D	402	-	3,3,3	0.41	0	2,2,2	0.25	0
3	EDO	A	406	-	3,3,3	0.29	0	2,2,2	0.91	0
3	EDO	C	405	-	3,3,3	0.38	0	2,2,2	0.78	0
3	EDO	B	409	-	3,3,3	0.77	0	2,2,2	0.09	0
3	EDO	B	408	-	3,3,3	0.44	0	2,2,2	0.47	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
3	EDO	D	403	-	-	1/1/1/1	-
3	EDO	C	404	-	-	0/1/1/1	-
3	EDO	A	402	-	-	0/1/1/1	-
3	EDO	C	402	-	-	1/1/1/1	-
3	EDO	C	403	-	-	1/1/1/1	-
3	EDO	B	406	-	-	0/1/1/1	-
3	EDO	A	407	-	-	1/1/1/1	-
2	V6E	A	401	-	-	3/20/37/37	0/4/4/4
2	V6E	D	401	-	-	3/20/37/37	0/4/4/4
3	EDO	A	405	-	-	1/1/1/1	-
2	V6E	C	401	-	-	1/20/37/37	0/4/4/4
3	EDO	B	403	-	-	1/1/1/1	-
3	EDO	B	402	-	-	1/1/1/1	-
3	EDO	A	403	-	-	0/1/1/1	-
3	EDO	B	407	-	-	0/1/1/1	-
3	EDO	C	406	-	-	1/1/1/1	-
3	EDO	D	404	-	-	0/1/1/1	-
3	EDO	A	404	-	-	0/1/1/1	-
3	EDO	B	405	-	-	1/1/1/1	-
2	V6E	B	401	-	-	1/20/37/37	0/4/4/4
3	EDO	B	404	-	-	1/1/1/1	-
3	EDO	D	402	-	-	1/1/1/1	-
3	EDO	A	406	-	-	0/1/1/1	-
3	EDO	C	405	-	-	0/1/1/1	-
3	EDO	B	409	-	-	1/1/1/1	-
3	EDO	B	408	-	-	1/1/1/1	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	V6E	C18-C8-C	11.51	124.54	120.69
2	C	401	V6E	C18-C8-C	10.05	124.05	120.69
2	D	401	V6E	C18-C8-C	6.55	122.88	120.69
2	A	401	V6E	C18-C8-C	3.53	121.87	120.69

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	V6E	C12-C11-N3-C10
2	D	401	V6E	O-C-C8-C9
3	A	405	EDO	O1-C1-C2-O2
3	B	405	EDO	O1-C1-C2-O2
3	C	403	EDO	O1-C1-C2-O2
3	C	406	EDO	O1-C1-C2-O2
3	D	402	EDO	O1-C1-C2-O2
2	A	401	V6E	O-C-C8-C9
2	A	401	V6E	N-C-C8-C9
3	A	407	EDO	O1-C1-C2-O2
3	B	404	EDO	O1-C1-C2-O2
3	B	409	EDO	O1-C1-C2-O2
2	D	401	V6E	N-C-C8-C9
2	C	401	V6E	O-C-C8-C9
3	B	402	EDO	O1-C1-C2-O2
3	B	403	EDO	O1-C1-C2-O2
2	A	401	V6E	C12-C11-N3-C10
3	C	402	EDO	O1-C1-C2-O2
3	B	408	EDO	O1-C1-C2-O2
2	B	401	V6E	C12-C11-N3-C10
3	D	403	EDO	O1-C1-C2-O2

There are no ring outliers.

9 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	404	EDO	1	0
3	A	402	EDO	1	0
3	C	402	EDO	2	0
2	D	401	V6E	1	0
3	A	405	EDO	1	0
3	A	404	EDO	1	0
3	B	405	EDO	1	0

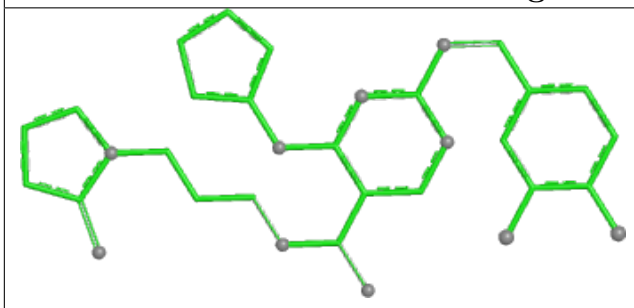
Continued on next page...

Continued from previous page...

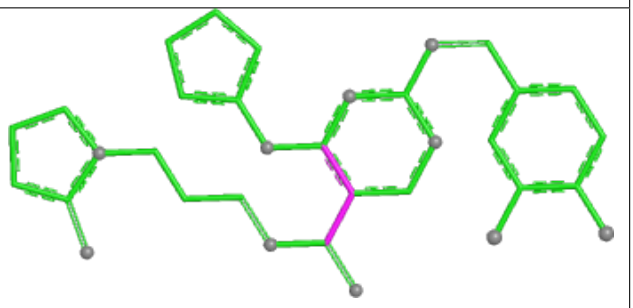
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	V6E	1	0
3	D	402	EDO	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

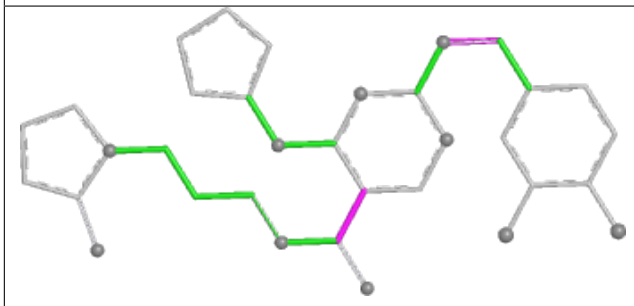
Ligand V6E A 401



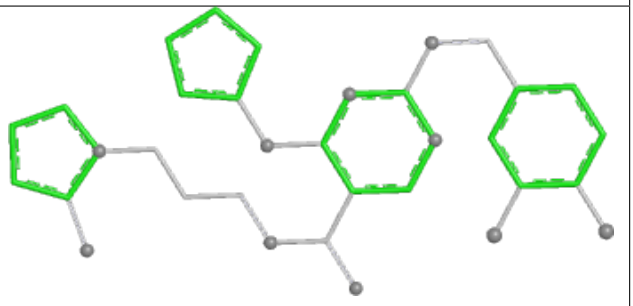
Bond lengths



Bond angles

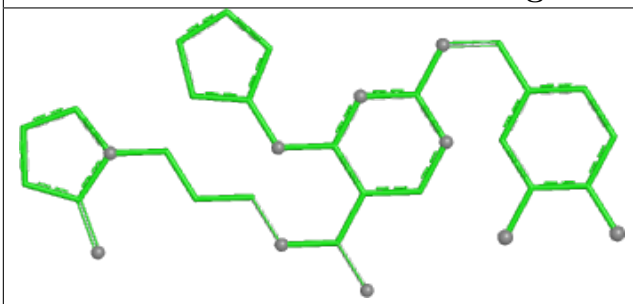


Torsions

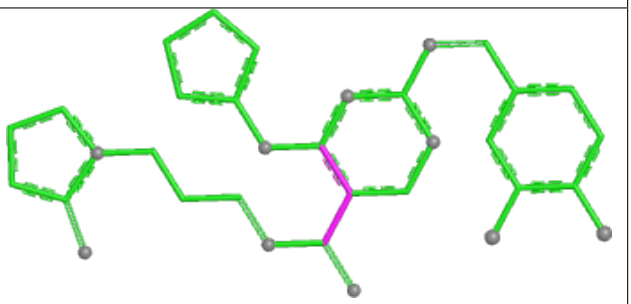


Rings

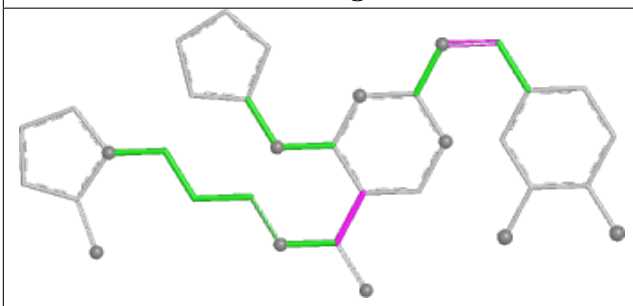
Ligand V6E D 401



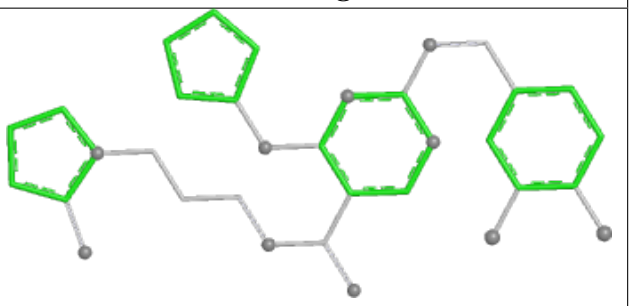
Bond lengths



Bond angles

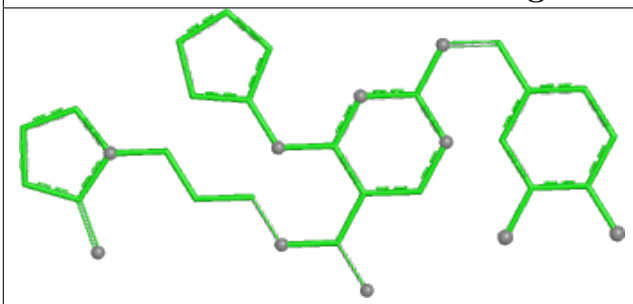


Torsions

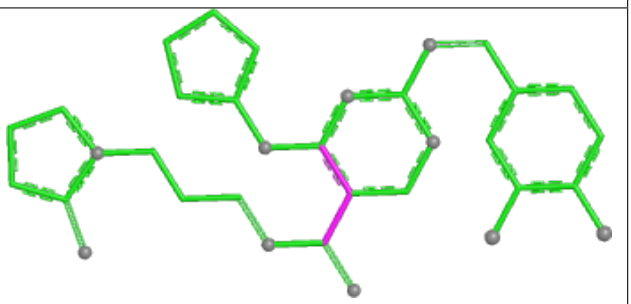


Rings

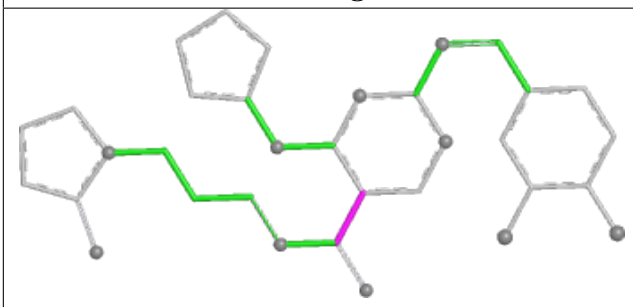
Ligand V6E C 401



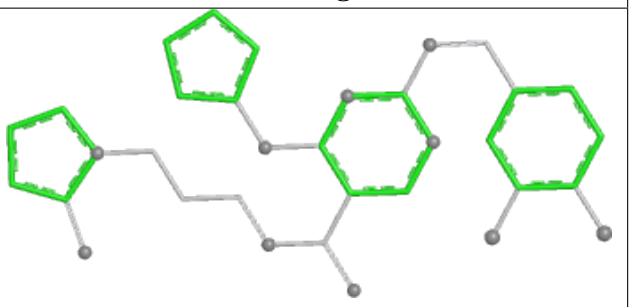
Bond lengths



Bond angles

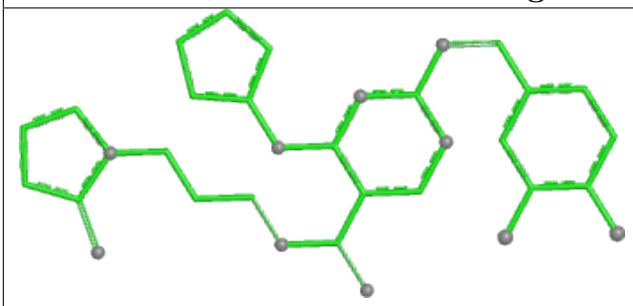


Torsions

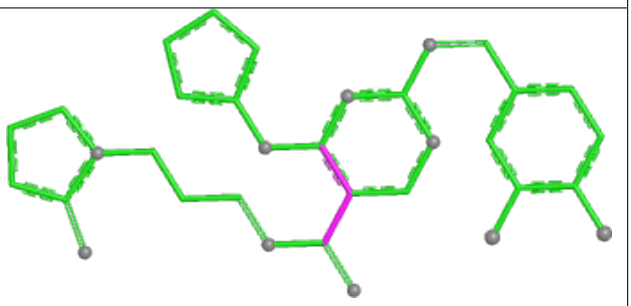


Rings

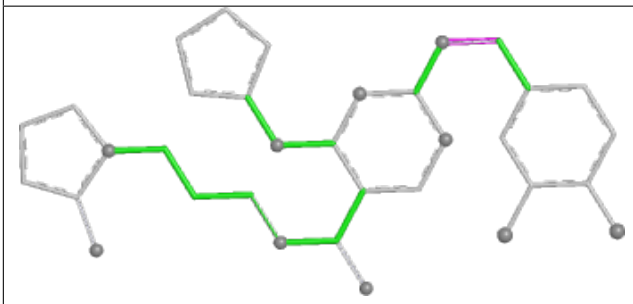
Ligand V6E B 401



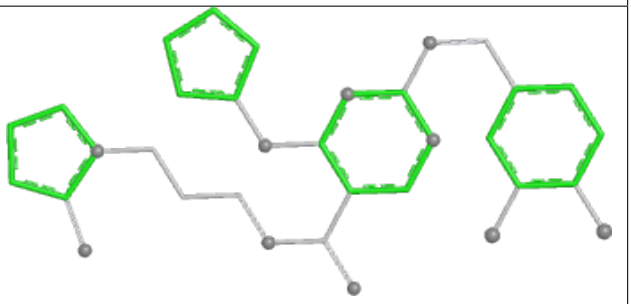
Bond lengths



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	298/353 (84%)	-0.16	2 (0%)	87	91	21, 31, 49, 74	0
1	B	297/353 (84%)	-0.14	3 (1%)	82	86	21, 31, 50, 61	0
1	C	297/353 (84%)	-0.06	4 (1%)	77	81	22, 33, 54, 73	0
1	D	297/353 (84%)	-0.09	6 (2%)	65	71	22, 34, 56, 76	0
All	All	1189/1412 (84%)	-0.11	15 (1%)	77	81	21, 32, 53, 76	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	6	VAL	8.0
1	D	223	LYS	5.5
1	A	6	VAL	4.8
1	B	6	VAL	4.6
1	D	7	LEU	3.8
1	B	177	GLY	3.7
1	C	84	ASP	3.7
1	D	238	ASN	3.5
1	C	85	GLY	3.1
1	A	7	LEU	3.0
1	D	6	VAL	2.9
1	B	236	LYS	2.9
1	D	52	PRO	2.7
1	C	234	LYS	2.5
1	D	176	ALA	2.3

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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

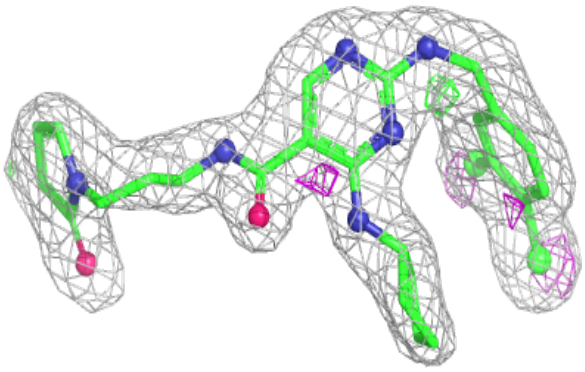
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

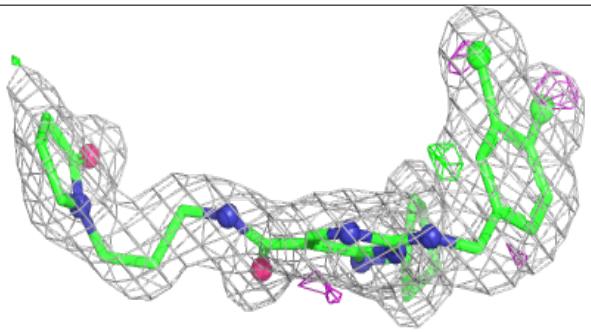
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	B	409	4/4	0.86	0.11	31,33,35,36	0
3	EDO	A	407	4/4	0.89	0.12	41,41,41,42	0
2	V6E	C	401	34/34	0.89	0.13	26,35,47,48	0
3	EDO	C	406	4/4	0.89	0.09	28,31,31,34	0
3	EDO	D	402	4/4	0.89	0.13	29,32,32,34	0
3	EDO	A	406	4/4	0.90	0.11	31,32,33,35	0
2	V6E	D	401	34/34	0.90	0.10	27,33,42,56	0
3	EDO	B	406	4/4	0.90	0.12	34,37,37,42	0
2	V6E	B	401	34/34	0.91	0.10	27,36,41,45	0
2	V6E	A	401	34/34	0.92	0.10	27,31,37,50	0
3	EDO	B	403	4/4	0.92	0.09	34,35,37,41	0
3	EDO	B	405	4/4	0.93	0.10	26,28,28,38	0
3	EDO	A	403	4/4	0.93	0.12	36,37,39,41	0
3	EDO	B	407	4/4	0.93	0.10	32,34,36,36	0
3	EDO	D	404	4/4	0.93	0.10	28,29,29,30	0
3	EDO	B	402	4/4	0.94	0.07	32,33,34,34	0
3	EDO	A	402	4/4	0.95	0.10	34,35,36,38	0
3	EDO	B	404	4/4	0.95	0.15	43,45,46,51	0
3	EDO	D	403	4/4	0.95	0.12	37,40,42,45	0
3	EDO	C	403	4/4	0.95	0.10	40,43,44,46	0
3	EDO	C	402	4/4	0.96	0.07	38,39,40,40	0
3	EDO	C	405	4/4	0.96	0.11	32,35,37,38	0
3	EDO	A	405	4/4	0.97	0.10	28,30,32,35	0
3	EDO	B	408	4/4	0.97	0.10	41,42,42,43	0
3	EDO	C	404	4/4	0.97	0.09	31,33,35,36	0
3	EDO	A	404	4/4	0.97	0.12	25,26,26,27	0

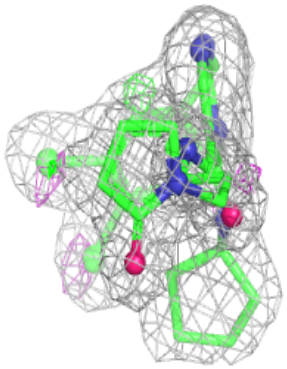
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around V6E C 401:

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

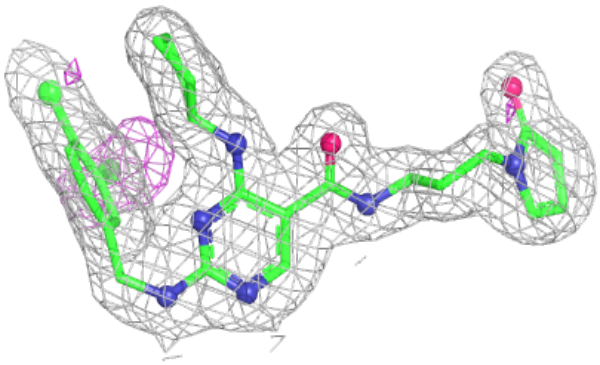


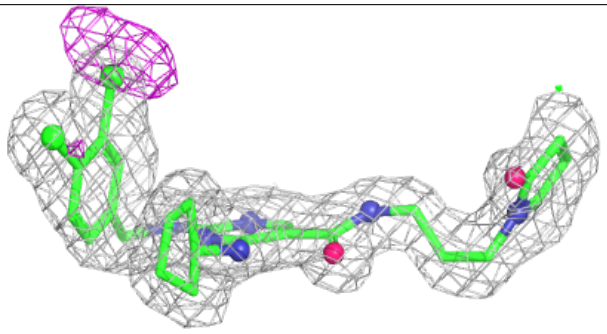


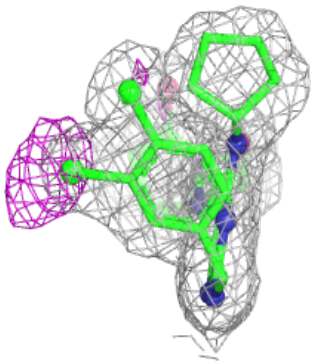


Electron density around V6E D 401:

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

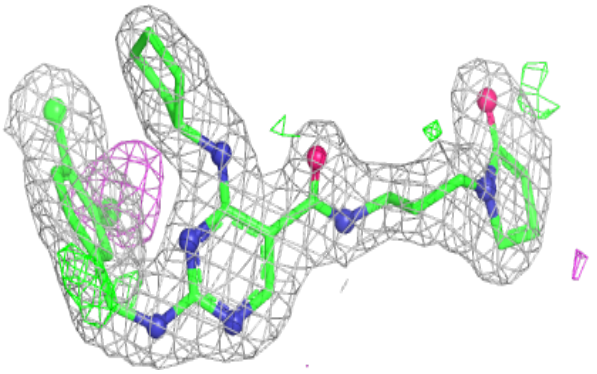


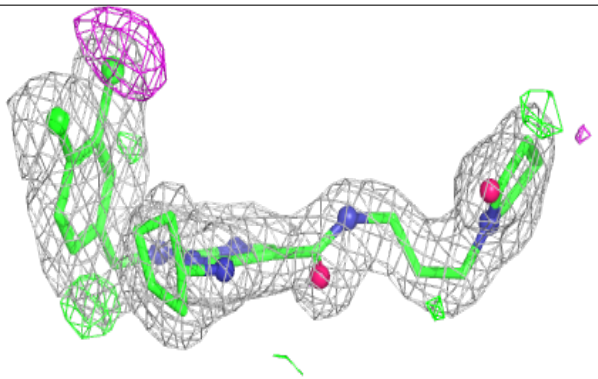




Electron density around V6E B 401:

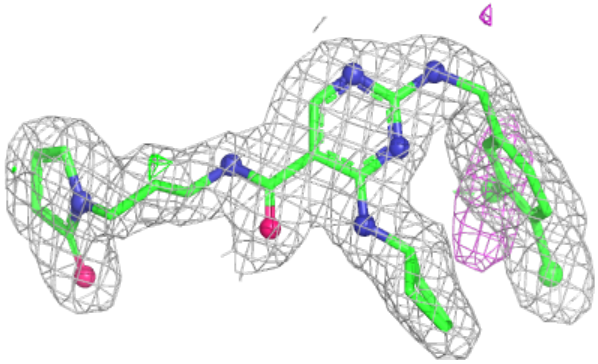
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

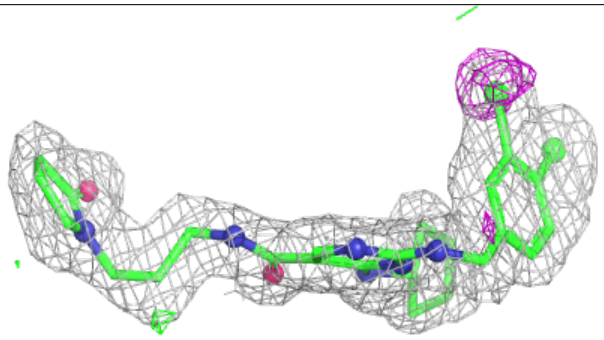


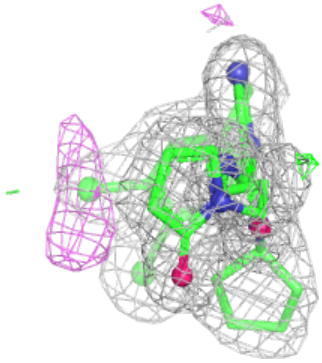


Electron density around V6E A 401:

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







6.5 Other polymers (i)

There are no such residues in this entry.