



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2019 – 08:23 PM EST

PDB ID : 6C0L  
Title : Crystal structure of HIV-1 E138K mutant reverse transcriptase in complex with non-nucleoside inhibitor K-5a2  
Authors : Yang, Y.; Nguyen, L.A.; Smithline, Z.B.; Steitz, T.A.  
Deposited on : 2018-01-01  
Resolution : 1.95 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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.0 (224370), CSD as540be (2019)  
Xtriage (Phenix) : 1.13  
EDS : 2.4  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.4

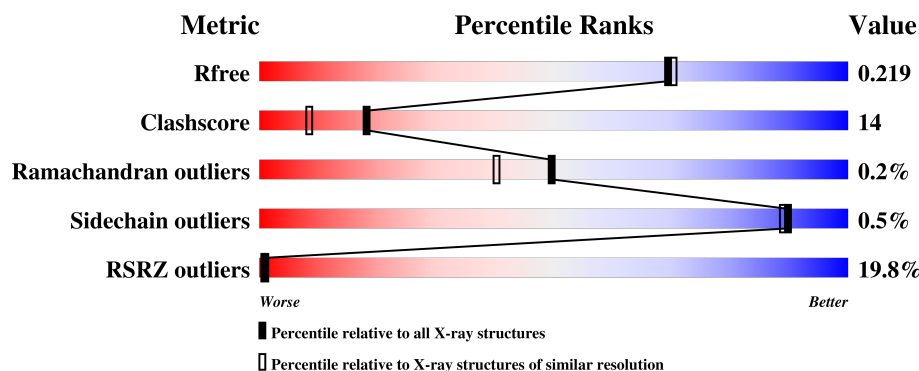
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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))
$R_{free}$	111664	2220 (1.96-1.96)
Clashscore	122126	2333 (1.96-1.96)
Ramachandran outliers	120053	2314 (1.96-1.96)
Sidechain outliers	120020	2314 (1.96-1.96)
RSRZ outliers	108989	2174 (1.96-1.96)

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. 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	557	<div> <div>18%</div> <div>75%</div> <div>24%</div> </div>
2	B	428	<div> <div>21%</div> <div>76%</div> <div>19%</div> <div>• •</div> </div>

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
6	SO4	A	607	-	-	X	-
6	SO4	B	501	-	-	-	X
7	EDO	A	611	-	-	X	-
7	EDO	A	617	-	-	-	X
7	EDO	A	620	-	-	-	X
7	EDO	A	621	-	-	-	X
7	EDO	A	622	-	-	-	X
7	EDO	B	513	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9001 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 Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	556	Total	C	N	O	S	0	7	0
			4579	2963	763	844	9			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP P03366
A	0	VAL	-	expression tag	UNP P03366
A	172	ALA	LYS	engineered mutation	UNP P03366
A	173	ALA	LYS	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366

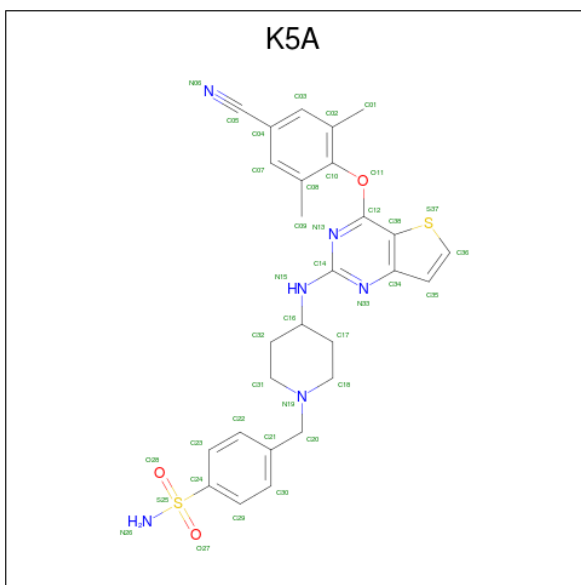
- Molecule 2 is a protein called Reverse transcriptase p51 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	414	Total	C	N	O	S	0	8	0
			3492	2277	578	630	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	138	LYS	GLU	engineered mutation	UNP P03366
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is 4-[(4-{[4-(4-cyano-2,6-dimethylphenoxy)thieno[3,2-d]pyrimidin-2-yl]amino}piperidin-1-yl)methyl]benzene-1-sulfonamide (three-letter code: K5A) (formula: C<sub>27</sub>H<sub>28</sub>N<sub>6</sub>O<sub>3</sub>S<sub>2</sub>) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			38	27	6	3	2		

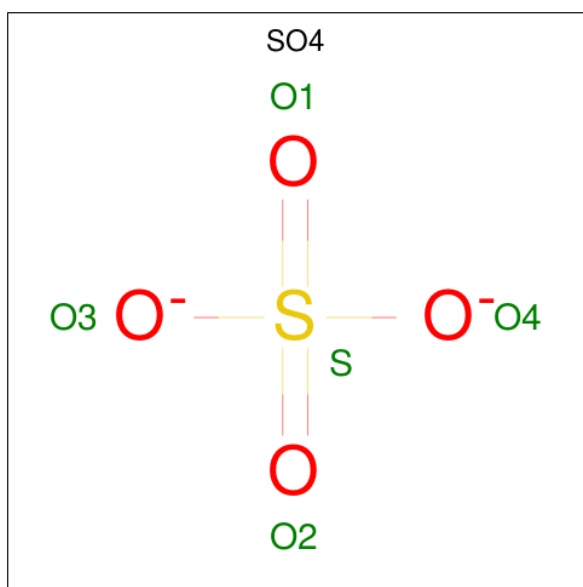
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

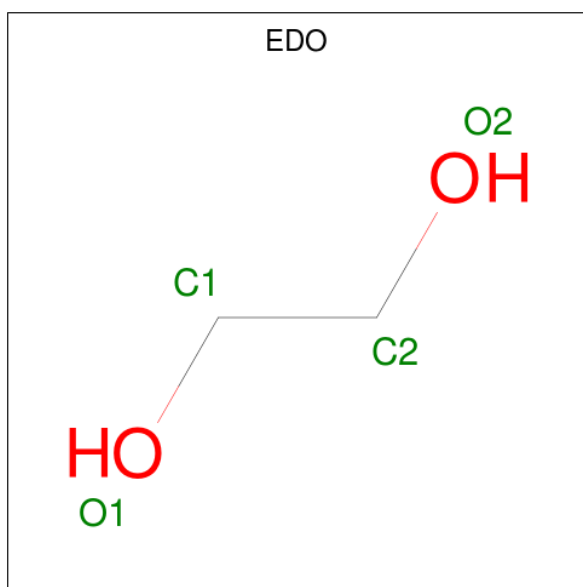
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Na 1 1	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula:  $\text{O}_4\text{S}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

*Continued on next page...*

*Continued from previous page...*

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

- Molecule 8 is water.

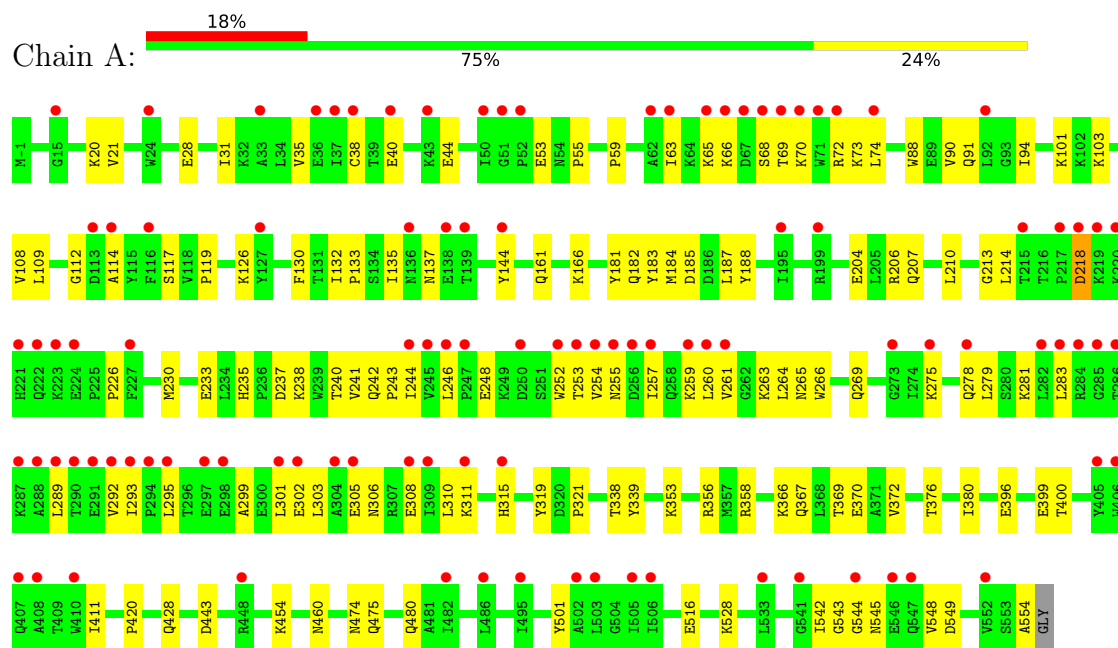
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	417	Total O 417 417	0	0
8	B	329	Total O 329 329	0	0



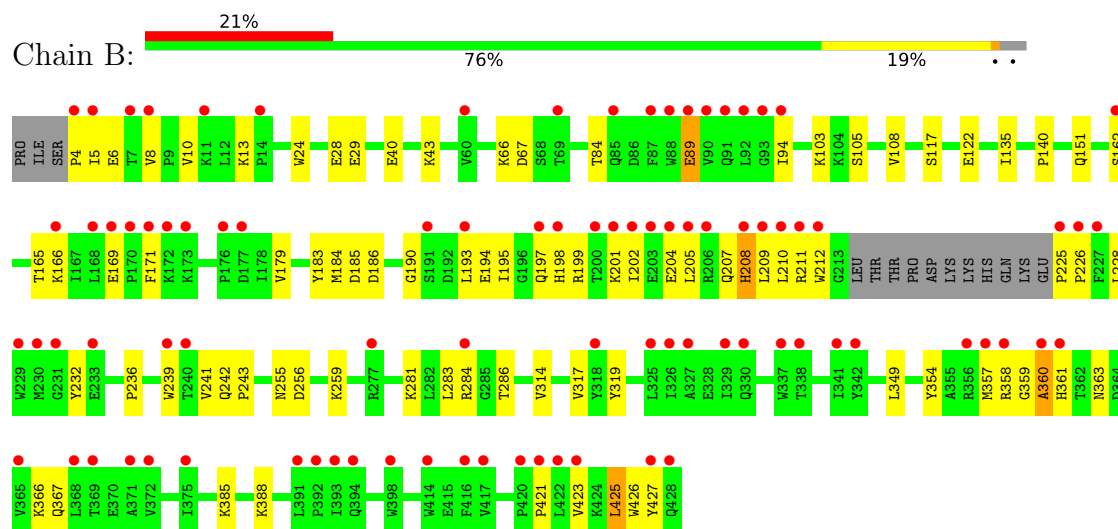
### 3 Residue-property plots [i](#)

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: Reverse transcriptase/ribonuclease H



#### • Molecule 2: Reverse transcriptase p51 subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	163.37Å 72.79Å 109.32Å 90.00° 100.25° 90.00°	Depositor
Resolution (Å)	43.16 – 1.95 43.15 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.3 (43.16-1.95) 99.4 (43.15-1.95)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.02 (at 1.95Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, $R_{free}$	0.185 , 0.219 0.186 , 0.219	Depositor DCC
$R_{free}$ test set	4578 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.8	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 67.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	9001	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, MG, EDO, K5A, SO4

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	0.36	0/4700	0.50	0/6390
2	B	0.39	0/3596	0.52	0/4887
All	All	0.37	0/8296	0.51	0/11277

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4579	0	4619	146	0
2	B	3492	0	3506	93	0
3	A	38	0	0	1	0
4	A	1	0	0	0	0
5	A	1	0	0	0	0
6	A	20	0	0	2	0
6	B	20	0	0	0	0
7	A	64	0	96	20	0
7	B	40	0	60	8	0
8	A	417	0	0	16	0
8	B	329	0	0	22	0
All	All	9001	0	8281	238	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 14.

All (238) 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:544:GLY:HA2	2:B:286[B]:THR:HG22	1.42	0.98
1:A:259:LYS:HE2	1:A:263:LYS:HE3	1.49	0.95
2:B:255:ASN:HB3	7:B:513:EDO:H12	1.53	0.91
2:B:360:ALA:HB2	2:B:366:LYS:HD3	1.56	0.85
2:B:184:MET:HE3	8:B:790:HOH:O	1.80	0.81
1:A:544:GLY:CA	2:B:286[B]:THR:HG22	2.13	0.78
1:A:181:TYR:HA	7:A:611:EDO:H22	1.67	0.76
1:A:241:VAL:HG12	1:A:242:GLN:O	1.85	0.76
2:B:162:SER:O	2:B:166:LYS:HD3	1.87	0.73
2:B:225:PRO:HB2	2:B:228:LEU:HB3	1.71	0.72
2:B:281:LYS:O	2:B:284:ARG:HG3	1.90	0.72
2:B:184:MET:HE2	8:B:696:HOH:O	1.91	0.71
2:B:209:LEU:HD21	8:B:872:HOH:O	1.90	0.71
1:A:182:GLN:H	7:A:611:EDO:H22	1.57	0.69
2:B:225:PRO:HG2	2:B:228:LEU:HD23	1.73	0.69
1:A:399:GLU:HG2	7:A:615:EDO:H12	1.75	0.69
2:B:108:VAL:HB	2:B:232:TYR:HB3	1.74	0.69
1:A:321:PRO:HD2	7:A:621:EDO:H11	1.76	0.68
2:B:317:VAL:CG1	2:B:349:LEU:HD23	2.24	0.68
1:A:65:LYS:HE2	1:A:72:ARG:NH2	2.09	0.67
1:A:184[B]:MET:HG2	1:A:185:ASP:N	2.07	0.67
2:B:360:ALA:HB1	2:B:363:ASN:HB3	1.76	0.67
1:A:40:GLU:O	1:A:44:GLU:HG3	1.95	0.66
1:A:181:TYR:CD1	7:A:611:EDO:H21	2.29	0.66
1:A:88:TRP:CD1	1:A:90:VAL:HG12	2.30	0.66
1:A:240:THR:OG1	1:A:315[A]:HIS:ND1	2.29	0.65
2:B:165:THR:O	2:B:169:GLU:HG2	1.96	0.65
1:A:28:GLU:HG3	1:A:135:ILE:HD12	1.79	0.65
2:B:256:ASP:OD1	7:B:513:EDO:H11	1.97	0.65
1:A:240:THR:HG22	1:A:241:VAL:N	2.13	0.64
7:A:613:EDO:H11	8:A:1033:HOH:O	1.98	0.64
1:A:257:ILE:CG2	1:A:283:LEU:HD11	2.28	0.64
1:A:206:ARG:NH2	1:A:218:ASP:OD1	2.30	0.64
2:B:205:LEU:O	2:B:205:LEU:HD23	1.96	0.64
1:A:137:ASN:HB2	7:A:620:EDO:H22	1.80	0.63
1:A:306:ASN:O	1:A:310:LEU:HD13	1.99	0.63
1:A:91:GLN:HB2	1:A:183:TYR:HE1	1.64	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ALA:HB1	1:A:214:LEU:HD13	1.82	0.61
2:B:198:HIS:O	2:B:202:ILE:HG12	2.00	0.61
2:B:255:ASN:CB	7:B:513:EDO:H12	2.29	0.60
1:A:380[A]:ILE:HD11	7:B:510:EDO:H21	1.84	0.60
1:A:91:GLN:HB2	1:A:183:TYR:CE1	2.38	0.59
1:A:69:THR:HG22	1:A:69:THR:O	2.02	0.59
1:A:101:LYS:HD3	1:A:321:PRO:CG	2.33	0.58
1:A:259:LYS:CE	1:A:263:LYS:HE3	2.30	0.58
1:A:65:LYS:HG2	1:A:66:LYS:H	1.68	0.58
1:A:63:ILE:O	1:A:63:ILE:HD12	2.04	0.58
2:B:314:VAL:HG23	8:B:630:HOH:O	2.04	0.57
2:B:425:LEU:H	2:B:425:LEU:HD23	1.69	0.57
1:A:112:GLY:HA2	1:A:185:ASP:OD1	2.04	0.57
1:A:253:THR:HG22	1:A:254:VAL:N	2.20	0.57
2:B:359:GLY:O	2:B:360:ALA:HB3	2.04	0.57
2:B:4:PRO:HG2	2:B:117:SER:O	2.04	0.57
2:B:195:ILE:HA	2:B:198:HIS:HB3	1.85	0.57
2:B:319:TYR:OH	2:B:385:LYS:HE2	2.03	0.57
8:A:1051:HOH:O	7:B:507:EDO:H12	2.03	0.56
1:A:183:TYR:O	1:A:184[B]:MET:HB3	2.04	0.56
1:A:358:ARG:NH2	8:A:711:HOH:O	2.38	0.56
1:A:278:GLN:O	1:A:281:LYS:HB2	2.06	0.56
1:A:70:LYS:HE3	1:A:72:ARG:HE	1.70	0.55
1:A:260:LEU:O	1:A:264:LEU:HG	2.07	0.55
2:B:284:ARG:HG2	8:B:813:HOH:O	2.05	0.55
1:A:137:ASN:OD1	7:A:620:EDO:H12	2.07	0.55
1:A:68:SER:OG	1:A:70:LYS:HE2	2.06	0.55
1:A:246:LEU:HD22	1:A:260:LEU:CD1	2.37	0.55
1:A:108:VAL:HG22	1:A:188:TYR:CD2	2.42	0.55
1:A:275:LYS:NZ	1:A:305:GLU:OE2	2.23	0.55
2:B:193:LEU:HD13	2:B:197:GLN:HB2	1.89	0.55
2:B:360:ALA:O	2:B:367:GLN:NE2	2.36	0.55
2:B:186:ASP:HB2	8:B:615:HOH:O	2.07	0.54
1:A:260:LEU:HD21	1:A:303:LEU:HD13	1.88	0.54
1:A:88:TRP:HD1	1:A:90:VAL:HG12	1.68	0.54
1:A:65:LYS:HB3	1:A:68:SER:OG	2.07	0.54
1:A:233:GLU:OE2	1:A:243:PRO:HD3	2.08	0.54
1:A:428[A]:GLN:NE2	8:A:703:HOH:O	2.32	0.54
1:A:252:TRP:CD1	1:A:295:LEU:HD11	2.43	0.54
1:A:70:LYS:HE3	1:A:72:ARG:NE	2.23	0.54
2:B:425:LEU:HD23	2:B:425:LEU:N	2.22	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:225:PRO:HB2	2:B:228:LEU:CB	2.37	0.53
1:A:246:LEU:HG	1:A:310:LEU:HD22	1.89	0.53
7:B:512:EDO:H12	8:B:733:HOH:O	2.09	0.53
1:A:210:LEU:O	1:A:213:GLY:N	2.33	0.53
1:A:20:LYS:NZ	1:A:55:PRO:HB2	2.22	0.53
2:B:8:VAL:O	2:B:10:VAL:HG23	2.09	0.53
2:B:360:ALA:HA	8:B:784:HOH:O	2.08	0.53
1:A:188:TYR:HB3	3:A:601:K5A:C09	2.39	0.52
2:B:226:PRO:HD2	8:B:846:HOH:O	2.10	0.52
2:B:236:PRO:HA	2:B:239:TRP:CG	2.45	0.52
2:B:241:VAL:HG13	8:B:839:HOH:O	2.09	0.52
2:B:225:PRO:HG2	2:B:228:LEU:CD2	2.39	0.52
2:B:423:VAL:HA	2:B:426[B]:TRP:CD1	2.45	0.52
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.92	0.52
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.44	0.52
1:A:257:ILE:O	1:A:261:VAL:HG23	2.10	0.52
1:A:28:GLU:HG3	1:A:135:ILE:CD1	2.40	0.52
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.50	0.51
2:B:360:ALA:CB	2:B:363:ASN:HB3	2.41	0.51
1:A:31:ILE:O	1:A:35:VAL:HG23	2.11	0.51
2:B:202:ILE:HB	8:B:616:HOH:O	2.11	0.51
2:B:66:LYS:O	2:B:67:ASP:HB2	2.09	0.51
1:A:528:LYS:CE	7:A:609:EDO:H12	2.41	0.50
2:B:151:GLN:HB3	2:B:185:ASP:OD2	2.11	0.50
1:A:101:LYS:NZ	6:A:607:SO4:O1	2.37	0.50
2:B:421:PRO:HD2	8:B:661:HOH:O	2.11	0.50
1:A:292:VAL:C	1:A:293:ILE:HD12	2.32	0.50
2:B:162:SER:HB2	8:B:715:HOH:O	2.09	0.50
2:B:226:PRO:HG3	8:B:829:HOH:O	2.11	0.50
7:A:612:EDO:H21	8:A:911:HOH:O	2.11	0.50
1:A:181:TYR:HA	7:A:611:EDO:C2	2.39	0.49
1:A:65:LYS:HE3	1:A:68:SER:OG	2.12	0.49
2:B:423:VAL:HB	2:B:426[B]:TRP:HD1	1.76	0.49
2:B:242:GLN:HE22	2:B:427:TYR:HB3	1.78	0.49
1:A:516:GLU:HA	1:A:516:GLU:OE1	2.13	0.49
2:B:255:ASN:OD1	7:B:513:EDO:H12	2.12	0.49
1:A:338[B]:THR:HG23	8:A:756:HOH:O	2.13	0.48
2:B:317:VAL:HG12	2:B:349:LEU:HD23	1.94	0.48
1:A:246:LEU:HG	1:A:310:LEU:CD2	2.42	0.48
2:B:193:LEU:HD12	2:B:194:GLU:O	2.14	0.48
1:A:246:LEU:HD22	1:A:260:LEU:HD12	1.95	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:ASN:OD1	1:A:353:LYS:NZ	2.41	0.48
1:A:266:TRP:O	1:A:269:GLN:HG2	2.13	0.48
1:A:63:ILE:CD1	1:A:72:ARG:HB2	2.43	0.48
2:B:354:TYR:CD2	2:B:357:MET:HE1	2.48	0.48
1:A:94:ILE:HG21	1:A:230:MET:HE2	1.95	0.48
2:B:197:GLN:O	2:B:201:LYS:HB2	2.13	0.48
2:B:241:VAL:HG23	2:B:243:PRO:HD3	1.95	0.48
1:A:338[B]:THR:CG2	8:A:702:HOH:O	2.62	0.48
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.49	0.47
1:A:91:GLN:N	1:A:91:GLN:OE1	2.46	0.47
2:B:40:GLU:HG2	8:B:655:HOH:O	2.14	0.47
1:A:240:THR:CG2	1:A:241:VAL:N	2.78	0.47
2:B:103:LYS:HD3	2:B:103:LYS:HA	1.48	0.47
2:B:29:GLU:HG2	8:B:602:HOH:O	2.14	0.47
1:A:321:PRO:HD2	7:A:621:EDO:C1	2.43	0.47
1:A:53:GLU:OE1	1:A:53:GLU:N	2.30	0.47
1:A:63:ILE:HD11	1:A:72:ARG:HB2	1.97	0.47
1:A:543:GLY:HA3	2:B:283:LEU:O	2.14	0.47
1:A:338[B]:THR:HG22	8:A:702:HOH:O	2.14	0.47
2:B:208:HIS:O	2:B:212:TRP:HD1	1.97	0.47
1:A:204:GLU:O	1:A:207:GLN:HB3	2.15	0.47
1:A:283:LEU:N	1:A:283:LEU:HD12	2.30	0.47
2:B:171:PHE:HE1	2:B:204:GLU:HG2	1.81	0.46
1:A:543:GLY:N	2:B:283:LEU:O	2.48	0.46
2:B:28:GLU:HB2	2:B:135:ILE:HD11	1.96	0.46
2:B:207:GLN:HA	2:B:207:GLN:OE1	2.15	0.46
2:B:94:ILE:HD12	2:B:94:ILE:O	2.16	0.46
2:B:105:SER:O	2:B:190:GLY:HA2	2.15	0.46
2:B:255:ASN:ND2	8:B:618:HOH:O	2.48	0.46
1:A:257:ILE:HG21	1:A:283:LEU:HD11	1.98	0.46
2:B:171:PHE:HB2	2:B:208:HIS:HD2	1.80	0.46
1:A:279:LEU:HD23	1:A:299:ALA:HB1	1.97	0.45
2:B:89:GLU:H	2:B:89:GLU:CD	2.20	0.45
1:A:244:ILE:HG22	1:A:310:LEU:HD23	1.97	0.45
2:B:103:LYS:NZ	2:B:179:VAL:HG23	2.32	0.45
1:A:248:GLU:HG3	8:A:959:HOH:O	2.15	0.45
1:A:65:LYS:HE3	1:A:70:LYS:HE2	1.97	0.45
1:A:279:LEU:HG	1:A:302:GLU:OE2	2.16	0.45
1:A:101:LYS:HG2	1:A:319:TYR:O	2.17	0.45
1:A:369:THR:HG23	1:A:411:ILE:HD11	1.98	0.45
2:B:171:PHE:HB2	2:B:208:HIS:CD2	2.52	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:388:LYS:HE2	8:B:884:HOH:O	2.16	0.45
1:A:400:THR:OG1	7:A:615:EDO:H21	2.16	0.45
1:A:253:THR:HG22	1:A:289:LEU:O	2.17	0.44
1:A:254:VAL:HG23	1:A:293:ILE:CD1	2.47	0.44
1:A:63:ILE:HD11	1:A:72:ARG:CB	2.47	0.44
1:A:187:LEU:HA	1:A:187:LEU:HD23	1.83	0.44
2:B:360:ALA:HB2	2:B:366:LYS:CD	2.39	0.44
1:A:133:PRO:HB2	8:A:754:HOH:O	2.17	0.44
1:A:542:ILE:O	1:A:545:ASN:HB3	2.18	0.44
1:A:474:ASN:HB2	7:A:612:EDO:H12	1.98	0.43
1:A:94:ILE:HD13	1:A:230:MET:CE	2.48	0.43
1:A:241:VAL:HG11	1:A:244:ILE:HD11	2.00	0.43
1:A:253:THR:HG22	1:A:254:VAL:H	1.82	0.43
2:B:183:TYR:CE2	2:B:184:MET:HG2	2.53	0.43
1:A:241:VAL:HG13	1:A:266:TRP:HE1	1.83	0.43
2:B:208:HIS:O	2:B:212:TRP:CD1	2.71	0.43
1:A:166:LYS:HD2	8:A:709:HOH:O	2.17	0.43
1:A:109:LEU:N	1:A:109:LEU:HD12	2.33	0.43
1:A:480:GLN:HB2	8:A:851:HOH:O	2.18	0.43
1:A:253:THR:CG2	1:A:254:VAL:N	2.82	0.43
1:A:226:PRO:HG3	1:A:235:HIS:CE1	2.54	0.43
1:A:254:VAL:HG23	1:A:293:ILE:HD11	2.01	0.43
1:A:182:GLN:N	7:A:611:EDO:H22	2.29	0.43
2:B:122:GLU:HG3	8:B:753:HOH:O	2.19	0.43
1:A:137:ASN:HB2	7:A:620:EDO:C2	2.48	0.42
7:A:611:EDO:H12	2:B:140:PRO:HD3	2.00	0.42
1:A:103:LYS:HD3	8:A:724:HOH:O	2.19	0.42
1:A:73:LYS:HG2	1:A:74:LEU:N	2.34	0.42
2:B:94:ILE:CG1	2:B:94:ILE:O	2.68	0.42
1:A:257:ILE:HG22	1:A:283:LEU:HD11	2.00	0.42
2:B:28:GLU:CB	2:B:135:ILE:HD11	2.50	0.42
2:B:43:LYS:HG3	8:B:728:HOH:O	2.19	0.42
1:A:293:ILE:HD12	1:A:293:ILE:N	2.35	0.42
1:A:69:THR:CG2	1:A:69:THR:O	2.66	0.42
1:A:182:GLN:HB2	1:A:187:LEU:CD2	2.49	0.42
1:A:255:ASN:OD1	1:A:289:LEU:HD23	2.20	0.42
1:A:301:LEU:O	1:A:305:GLU:HG3	2.19	0.42
1:A:356[B]:ARG:HD3	1:A:367:GLN:NE2	2.34	0.42
1:A:454:LYS:HE3	1:A:554:ALA:HB2	2.01	0.42
1:A:366:LYS:O	1:A:370:GLU:HG3	2.20	0.42
1:A:376:THR:O	1:A:380[B]:ILE:HG12	2.19	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:GLN:HG3	7:A:612:EDO:O2	2.19	0.42
1:A:214:LEU:HA	1:A:214:LEU:HD23	1.77	0.42
1:A:88:TRP:CZ3	7:A:610:EDO:H11	2.55	0.42
2:B:5:ILE:HG22	2:B:6:GLU:N	2.34	0.42
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.55	0.42
2:B:13:LYS:HE3	2:B:84:THR:O	2.20	0.42
2:B:199:ARG:O	2:B:202:ILE:HB	2.20	0.42
2:B:228:LEU:HD12	2:B:228:LEU:O	2.19	0.42
2:B:208:HIS:CE1	2:B:211:ARG:HH22	2.37	0.42
2:B:361[B]:HIS:HA	8:B:859:HOH:O	2.19	0.42
2:B:423:VAL:HB	2:B:426[B]:TRP:CD1	2.55	0.41
1:A:243:PRO:HD2	8:A:973:HOH:O	2.20	0.41
1:A:308:GLU:HA	1:A:311:LYS:HG3	2.03	0.41
1:A:460:ASN:HA	2:B:286[A]:THR:O	2.20	0.41
2:B:361[A]:HIS:HA	8:B:859:HOH:O	2.19	0.41
1:A:443:ASP:HB2	1:A:548:VAL:HG13	2.03	0.41
1:A:443:ASP:OD2	1:A:549:ASP:HA	2.20	0.41
2:B:24:TRP:CD2	7:B:505:EDO:H21	2.54	0.41
2:B:358:ARG:HG3	2:B:358:ARG:H	1.61	0.41
1:A:254:VAL:CG1	1:A:289:LEU:HA	2.50	0.41
2:B:103:LYS:HZ2	2:B:179:VAL:HG23	1.85	0.41
1:A:237:ASP:O	1:A:238:LYS:HD3	2.21	0.41
1:A:420:PRO:HG3	8:A:822:HOH:O	2.19	0.41
1:A:254:VAL:HB	1:A:289:LEU:HA	2.03	0.41
2:B:210:LEU:O	2:B:210:LEU:HD23	2.21	0.41
2:B:255:ASN:O	2:B:259:LYS:HG3	2.21	0.41
1:A:117:SER:O	1:A:119:PRO:HD3	2.20	0.41
1:A:372:VAL:HG11	1:A:411:ILE:HG23	2.03	0.41
1:A:68:SER:HB2	1:A:70:LYS:HD3	2.02	0.41
1:A:126:LYS:HE2	8:A:893:HOH:O	2.20	0.40
1:A:311:LYS:HB2	1:A:311:LYS:NZ	2.36	0.40
1:A:101:LYS:HE3	6:A:607:SO4:O2	2.20	0.40
1:A:255:ASN:HB2	1:A:289:LEU:HB3	2.04	0.40
1:A:396:GLU:HG3	7:A:615:EDO:O1	2.21	0.40
1:A:338[B]:THR:HG22	1:A:339:TYR:N	2.37	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	561/557 (101%)	542 (97%)	19 (3%)	0	100	100
2	B	418/428 (98%)	396 (95%)	20 (5%)	2 (0%)	31	18
All	All	979/985 (99%)	938 (96%)	39 (4%)	2 (0%)	49	40

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	360	ALA
2	B	89	GLU

### 5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	501/495 (101%)	499 (100%)	2 (0%)	92	91
2	B	383/390 (98%)	381 (100%)	2 (0%)	90	89
All	All	884/885 (100%)	880 (100%)	4 (0%)	90	89

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	161	GLN
1	A	218	ASP
2	B	208	HIS
2	B	425	LEU

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

Mol	Chain	Res	Type
2	B	182	GLN

### 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 37 ligands modelled in this entry, 2 are monoatomic - leaving 35 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	$\# Z  > 2$
3	K5A	A	601	-	41,42,42	1.55	6 (14%)	51,61,61	2.54	18 (35%)
6	SO4	A	604	-	4,4,4	0.16	0	6,6,6	0.06	0
6	SO4	A	605	-	4,4,4	0.16	0	6,6,6	0.11	0
6	SO4	A	606	-	4,4,4	0.17	0	6,6,6	0.09	0
6	SO4	A	607	-	4,4,4	0.14	0	6,6,6	0.11	0
7	EDO	A	608	-	3,3,3	0.41	0	2,2,2	0.60	0
7	EDO	A	609	-	3,3,3	0.44	0	2,2,2	0.37	0
7	EDO	A	610	-	3,3,3	0.46	0	2,2,2	0.41	0
7	EDO	A	611	-	3,3,3	0.45	0	2,2,2	0.32	0
7	EDO	A	612	-	3,3,3	0.46	0	2,2,2	0.43	0
7	EDO	A	613	-	3,3,3	0.44	0	2,2,2	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	EDO	A	614	-	3,3,3	0.45	0	2,2,2	0.38	0
7	EDO	A	615	-	3,3,3	0.45	0	2,2,2	0.39	0
7	EDO	A	616	-	3,3,3	0.45	0	2,2,2	0.41	0
7	EDO	A	617	-	3,3,3	0.47	0	2,2,2	0.35	0
7	EDO	A	618	-	3,3,3	0.43	0	2,2,2	0.42	0
7	EDO	A	619	-	3,3,3	0.38	0	2,2,2	0.48	0
7	EDO	A	620	-	3,3,3	0.47	0	2,2,2	0.27	0
7	EDO	A	621	-	3,3,3	0.47	0	2,2,2	0.34	0
7	EDO	A	622	-	3,3,3	0.45	0	2,2,2	0.31	0
7	EDO	A	623	-	3,3,3	0.44	0	2,2,2	0.37	0
6	SO4	B	501	-	4,4,4	0.16	0	6,6,6	0.08	0
6	SO4	B	502	-	4,4,4	0.15	0	6,6,6	0.05	0
6	SO4	B	503	-	4,4,4	0.16	0	6,6,6	0.06	0
6	SO4	B	504	-	4,4,4	0.16	0	6,6,6	0.09	0
7	EDO	B	505	-	3,3,3	0.46	0	2,2,2	0.19	0
7	EDO	B	506	-	3,3,3	0.49	0	2,2,2	0.15	0
7	EDO	B	507	-	3,3,3	0.47	0	2,2,2	0.35	0
7	EDO	B	508	-	3,3,3	0.48	0	2,2,2	0.29	0
7	EDO	B	509	-	3,3,3	0.46	0	2,2,2	0.52	0
7	EDO	B	510	-	3,3,3	0.46	0	2,2,2	0.45	0
7	EDO	B	511	-	3,3,3	0.48	0	2,2,2	0.33	0
7	EDO	B	512	-	3,3,3	0.52	0	2,2,2	0.44	0
7	EDO	B	513	-	3,3,3	0.43	0	2,2,2	0.38	0
7	EDO	B	514	-	3,3,3	0.45	0	2,2,2	0.37	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	K5A	A	601	-	-	2/20/30/30	0/5/5/5
7	EDO	A	608	-	-	1/1/1/1	-
7	EDO	A	609	-	-	0/1/1/1	-
7	EDO	A	610	-	-	1/1/1/1	-
7	EDO	A	611	-	-	1/1/1/1	-
7	EDO	A	612	-	-	0/1/1/1	-
7	EDO	A	613	-	-	0/1/1/1	-
7	EDO	A	614	-	-	0/1/1/1	-
7	EDO	A	615	-	-	0/1/1/1	-
7	EDO	A	616	-	-	0/1/1/1	-
7	EDO	A	617	-	-	0/1/1/1	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	A	618	-	-	0/1/1/1	-
7	EDO	A	619	-	-	0/1/1/1	-
7	EDO	A	620	-	-	0/1/1/1	-
7	EDO	A	621	-	-	0/1/1/1	-
7	EDO	A	622	-	-	0/1/1/1	-
7	EDO	A	623	-	-	0/1/1/1	-
7	EDO	B	505	-	-	1/1/1/1	-
7	EDO	B	506	-	-	0/1/1/1	-
7	EDO	B	507	-	-	0/1/1/1	-
7	EDO	B	508	-	-	0/1/1/1	-
7	EDO	B	509	-	-	0/1/1/1	-
7	EDO	B	510	-	-	1/1/1/1	-
7	EDO	B	511	-	-	1/1/1/1	-
7	EDO	B	512	-	-	0/1/1/1	-
7	EDO	B	513	-	-	0/1/1/1	-
7	EDO	B	514	-	-	1/1/1/1	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	K5A	C14-N15	4.32	1.40	1.34
3	A	601	K5A	C18-N19	3.93	1.57	1.47
3	A	601	K5A	C12-N13	3.54	1.38	1.31
3	A	601	K5A	C14-N13	3.01	1.44	1.34
3	A	601	K5A	S25-N26	2.77	1.66	1.60
3	A	601	K5A	C24-S25	-2.25	1.73	1.77

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	K5A	C03-C04-C05	6.59	127.77	119.51
3	A	601	K5A	C20-N19-C18	6.16	124.31	111.04
3	A	601	K5A	C07-C04-C05	-5.46	112.66	119.51
3	A	601	K5A	C21-C20-N19	-5.42	102.73	113.14
3	A	601	K5A	C29-C24-C23	-5.05	113.32	120.43
3	A	601	K5A	C22-C23-C24	4.87	124.54	119.45
3	A	601	K5A	C17-C18-N19	4.21	117.72	111.09
3	A	601	K5A	C30-C29-C24	3.83	123.46	119.45
3	A	601	K5A	C23-C24-S25	3.56	125.09	119.74
3	A	601	K5A	C01-C02-C10	3.15	125.95	120.84
3	A	601	K5A	C14-N15-C16	3.15	127.07	123.59
3	A	601	K5A	C31-N19-C18	2.92	115.30	108.86

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	K5A	O28-S25-C24	2.91	110.68	107.36
3	A	601	K5A	C20-N19-C31	-2.27	106.16	111.04
3	A	601	K5A	C01-C02-C03	-2.27	115.28	119.49
3	A	601	K5A	C31-C32-C16	2.13	114.24	110.44
3	A	601	K5A	C32-C31-N19	2.12	114.44	111.09
3	A	601	K5A	N15-C14-N13	2.04	120.01	117.09

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	K5A	C21-C20-N19-C18
7	B	510	EDO	O1-C1-C2-O2
7	B	511	EDO	O1-C1-C2-O2
7	A	611	EDO	O1-C1-C2-O2
7	A	610	EDO	O1-C1-C2-O2
7	A	608	EDO	O1-C1-C2-O2
7	B	514	EDO	O1-C1-C2-O2
7	B	505	EDO	O1-C1-C2-O2
3	A	601	K5A	C17-C16-N15-C14

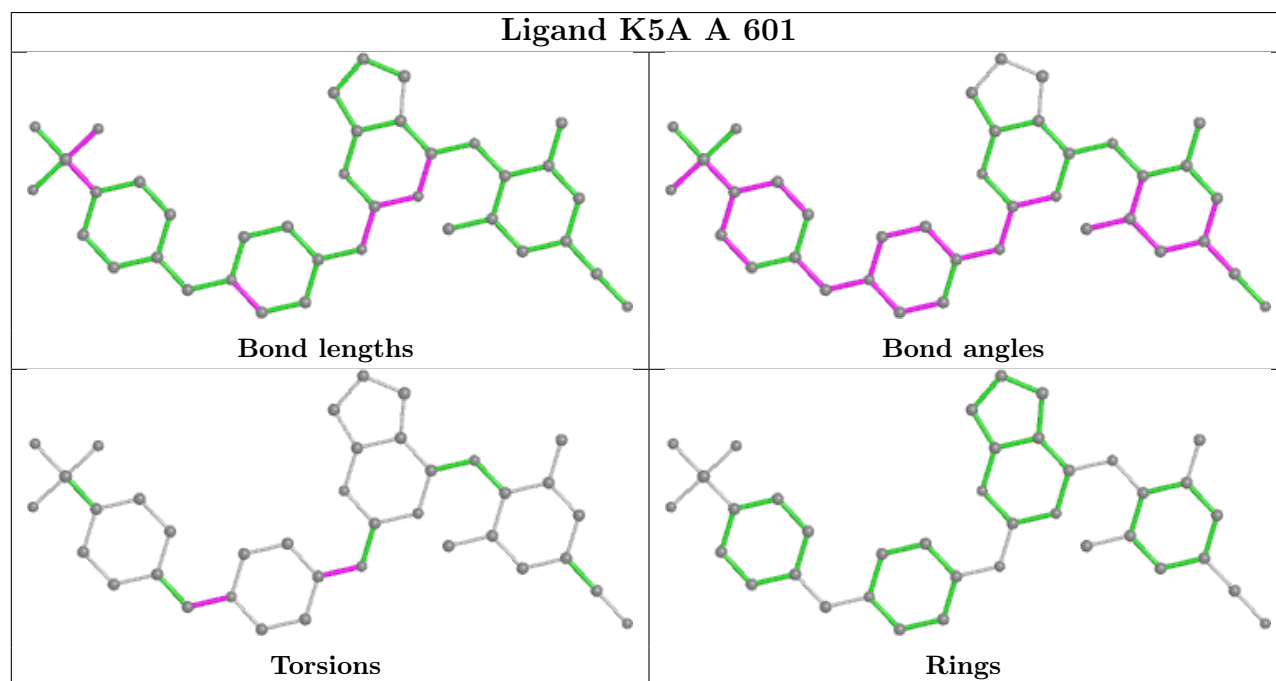
There are no ring outliers.

14 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	K5A	1	0
7	A	609	EDO	1	0
7	A	610	EDO	1	0
7	A	611	EDO	6	0
7	A	612	EDO	3	0
7	A	613	EDO	1	0
7	A	615	EDO	3	0
7	A	620	EDO	3	0
7	A	621	EDO	2	0
7	B	505	EDO	1	0
7	B	507	EDO	1	0
7	B	510	EDO	1	0
7	B	512	EDO	1	0
7	B	513	EDO	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	556/557 (99%)	1.01	103 (18%)  	40, 75, 157, 221	0
2	B	414/428 (96%)	1.11	89 (21%)  	40, 66, 136, 275	0
All	All	970/985 (98%)	1.06	192 (19%)  	40, 71, 150, 275	0

All (192) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	91	GLN	11.9
1	A	257	ILE	11.8
2	B	4	PRO	10.6
2	B	90	VAL	9.8
1	A	292	VAL	9.7
1	A	290	THR	9.3
2	B	92	LEU	9.2
1	A	286	THR	9.2
1	A	221	HIS	8.1
2	B	89	GLU	7.6
1	A	67	ASP	7.6
1	A	301	LEU	7.4
1	A	252	TRP	7.2
1	A	68	SER	6.8
1	A	295	LEU	6.4
1	A	293	ILE	6.3
2	B	5	ILE	6.2
2	B	230	MET	6.2
1	A	260	LEU	6.1
1	A	261	VAL	6.0
1	A	220	LYS	5.9
2	B	226	PRO	5.9
1	A	66	LYS	5.8
2	B	227	PHE	5.6

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	168	LEU	5.5
1	A	254	VAL	5.5
2	B	358	ARG	5.4
1	A	282	LEU	5.3
1	A	304	ALA	5.2
1	A	289	LEU	5.2
2	B	229	TRP	5.1
2	B	202	ILE	4.9
2	B	210	LEU	4.8
1	A	72	ARG	4.8
1	A	218	ASP	4.7
1	A	287	LYS	4.7
1	A	297	GLU	4.7
2	B	212	TRP	4.7
1	A	69	THR	4.7
1	A	283	LEU	4.6
1	A	294	PRO	4.6
2	B	209	LEU	4.6
1	A	114	ALA	4.5
1	A	244	ILE	4.5
2	B	391	LEU	4.4
2	B	357	MET	4.4
1	A	24	TRP	4.4
1	A	195	ILE	4.3
1	A	63	ILE	4.3
1	A	227	PHE	4.3
1	A	309	ILE	4.2
1	A	406	TRP	4.2
2	B	166	LYS	4.2
1	A	311	LYS	4.1
1	A	74	LEU	4.1
2	B	172	LYS	4.1
1	A	138	GLU	3.9
2	B	87	PHE	3.9
2	B	393	ILE	3.9
1	A	222	GLN	3.9
2	B	197	GLN	3.8
2	B	204	GLU	3.8
1	A	288	ALA	3.8
1	A	284	ARG	3.7
1	A	273	GLY	3.7
2	B	337	TRP	3.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	256	ASP	3.6
1	A	116	PHE	3.6
2	B	372	VAL	3.6
2	B	205	LEU	3.5
2	B	368	LEU	3.5
1	A	215	THR	3.5
2	B	169	GLU	3.5
1	A	144	TYR	3.5
1	A	298	GLU	3.4
2	B	88	TRP	3.4
1	A	65	LYS	3.4
1	A	199	ARG	3.4
1	A	246	LEU	3.4
2	B	231	GLY	3.3
2	B	326[A]	ILE	3.3
2	B	414	TRP	3.3
1	A	217	PRO	3.3
2	B	14	PRO	3.3
2	B	11	LYS	3.2
1	A	136	ASN	3.2
1	A	245	VAL	3.2
1	A	291	GLU	3.2
1	A	223	LYS	3.2
1	A	71	TRP	3.1
1	A	305	GLU	3.1
2	B	392	PRO	3.1
1	A	503	LEU	3.1
2	B	200	THR	3.1
2	B	7	THR	3.1
2	B	176	PRO	3.0
2	B	69	THR	3.0
2	B	338	THR	3.0
2	B	398	TRP	3.0
2	B	325	LEU	3.0
2	B	422	LEU	3.0
2	B	198	HIS	3.0
1	A	546	GLU	3.0
2	B	171	PHE	3.0
1	A	38	CYS	3.0
2	B	365	VAL	3.0
1	A	92	LEU	2.9
1	A	37	ILE	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	170	PRO	2.9
1	A	405	TYR	2.9
1	A	219	LYS	2.9
1	A	533	LEU	2.9
1	A	315[A]	HIS	2.8
2	B	329	ILE	2.8
1	A	506	ILE	2.8
2	B	201	LYS	2.8
2	B	206	ARG	2.8
2	B	93	GLY	2.8
2	B	421	PRO	2.8
1	A	408	ALA	2.7
2	B	240	THR	2.7
2	B	416	PHE	2.7
2	B	427	TYR	2.7
2	B	360	ALA	2.7
2	B	341	ILE	2.7
1	A	502	ALA	2.6
2	B	375	ILE	2.6
2	B	239	TRP	2.6
2	B	211	ARG	2.6
1	A	50	ILE	2.6
2	B	8	VAL	2.6
1	A	36	GLU	2.6
1	A	302	GLU	2.6
2	B	417	VAL	2.6
1	A	250	ASP	2.6
2	B	208	HIS	2.5
2	B	342	TYR	2.5
1	A	275	LYS	2.5
2	B	191	SER	2.5
1	A	253	THR	2.5
2	B	284	ARG	2.5
2	B	371	ALA	2.4
1	A	552	VAL	2.4
1	A	127	TYR	2.4
2	B	277	ARG	2.4
1	A	407	GLN	2.4
1	A	448	ARG	2.3
2	B	361[A]	HIS	2.3
1	A	482	ILE	2.3
2	B	60[A]	VAL	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	193	LEU	2.3
1	A	247	PRO	2.3
2	B	318	TYR	2.3
1	A	51	GLY	2.3
1	A	70	LYS	2.3
2	B	394[A]	GLN	2.3
1	A	255	ASN	2.3
1	A	544	GLY	2.2
2	B	330	GLN	2.2
1	A	62	ALA	2.2
2	B	369	THR	2.2
2	B	177	ASP	2.2
1	A	541	GLY	2.2
2	B	85	GLN	2.2
1	A	15	GLY	2.2
1	A	410[A]	TRP	2.2
1	A	43	LYS	2.2
1	A	52	PRO	2.2
2	B	225	PRO	2.2
1	A	547	GLN	2.2
1	A	113	ASP	2.2
2	B	423	VAL	2.2
2	B	203	GLU	2.2
1	A	259	LYS	2.2
1	A	33	ALA	2.2
2	B	356	ARG	2.1
1	A	285	GLY	2.1
2	B	173	LYS	2.1
1	A	224	GLU	2.1
2	B	94	ILE	2.1
2	B	428	GLN	2.1
2	B	327	ALA	2.1
1	A	495	ILE	2.1
1	A	505	ILE	2.1
1	A	308	GLU	2.1
1	A	40	GLU	2.1
2	B	420	PRO	2.1
2	B	162	SER	2.0
1	A	486	LEU	2.0
1	A	139	THR	2.0
1	A	278	GLN	2.0
2	B	233	GLU	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 carbohydrates 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<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.

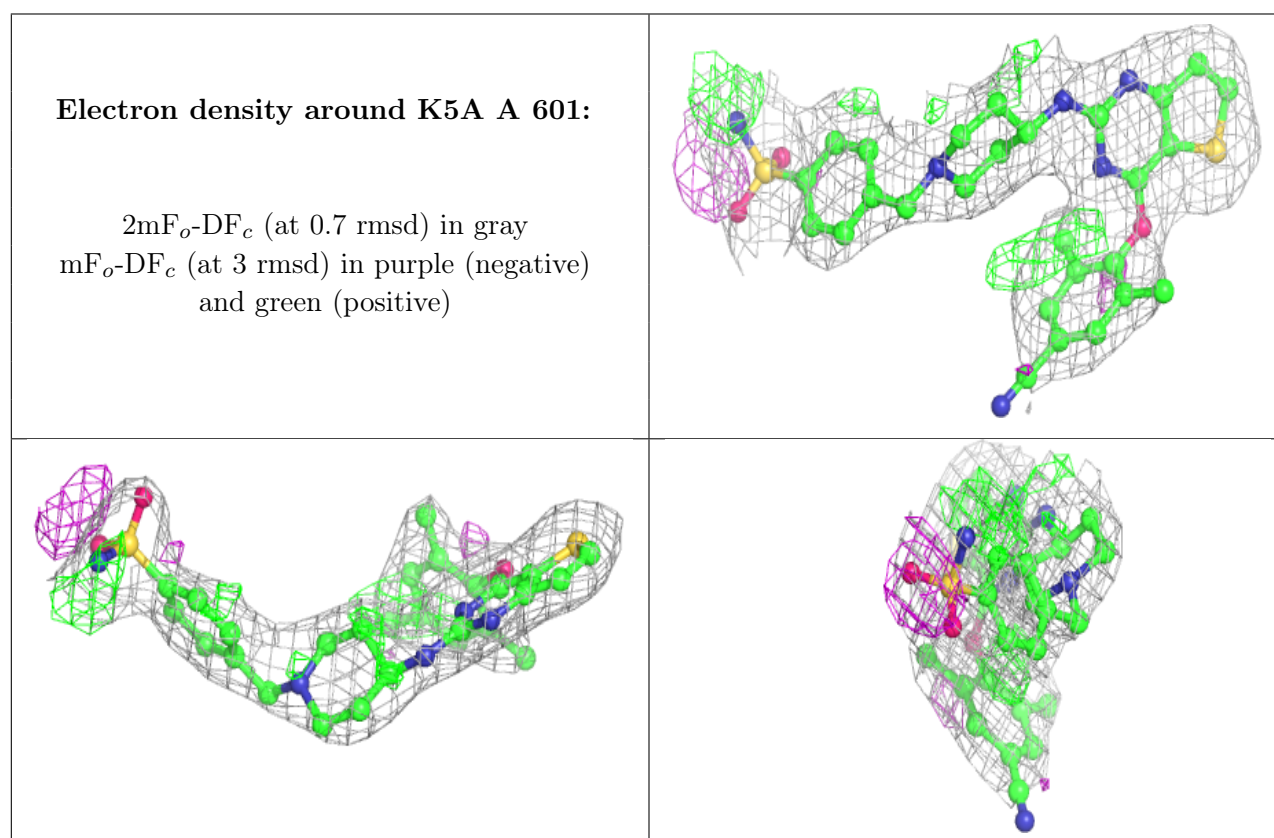
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	EDO	A	621	4/4	0.51	0.58	117,117,118,119	0
6	SO4	B	501	5/5	0.55	0.47	211,211,211,212	0
7	EDO	A	617	4/4	0.67	0.46	107,108,110,111	0
7	EDO	B	507	4/4	0.71	0.31	105,106,110,114	0
7	EDO	A	620	4/4	0.71	0.48	99,99,100,100	0
7	EDO	A	622	4/4	0.73	0.46	117,118,118,119	0
7	EDO	A	618	4/4	0.74	0.27	100,100,100,101	0
7	EDO	B	514	4/4	0.75	0.40	114,116,117,118	0
7	EDO	A	616	4/4	0.77	0.21	90,92,92,93	0
6	SO4	A	606	5/5	0.78	0.17	141,142,143,145	0
7	EDO	A	612	4/4	0.78	0.12	73,77,82,87	0
7	EDO	A	615	4/4	0.81	0.43	113,116,117,118	0
7	EDO	B	510	4/4	0.81	0.28	74,78,78,81	0
7	EDO	B	511	4/4	0.82	0.20	84,87,91,93	0
7	EDO	A	610	4/4	0.83	0.15	86,88,88,89	0
7	EDO	A	611	4/4	0.84	0.39	113,115,117,120	0
7	EDO	B	512	4/4	0.84	0.32	79,81,84,88	0
7	EDO	B	506	4/4	0.86	0.20	63,65,65,66	0
7	EDO	A	613	4/4	0.86	0.21	97,97,98,101	0
7	EDO	B	509	4/4	0.86	0.17	89,89,91,94	0
7	EDO	B	508	4/4	0.87	0.16	88,88,92,96	0
4	MG	A	602	1/1	0.87	0.15	66,66,66,66	0
7	EDO	A	614	4/4	0.87	0.18	96,98,101,103	0
5	NA	A	603	1/1	0.88	0.53	100,100,100,100	0
6	SO4	B	504	5/5	0.89	0.31	142,142,143,144	0
3	K5A	A	601	38/38	0.90	0.15	54,82,116,117	0
6	SO4	A	604	5/5	0.90	0.29	145,146,148,148	0

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	EDO	B	513	4/4	0.90	0.24	102,102,102,103	0
6	SO4	B	502	5/5	0.91	0.45	165,166,168,168	0
7	EDO	A	609	4/4	0.92	0.17	74,76,79,83	0
7	EDO	B	505	4/4	0.93	0.23	59,59,63,66	0
7	EDO	A	608	4/4	0.94	0.20	55,65,70,81	0
7	EDO	A	623	4/4	0.94	0.15	91,92,93,96	0
6	SO4	B	503	5/5	0.95	0.25	150,150,150,150	0
7	EDO	A	619	4/4	0.97	0.21	72,75,77,77	0
6	SO4	A	605	5/5	0.97	0.08	100,103,106,109	0
6	SO4	A	607	5/5	0.98	0.14	93,97,98,103	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.



## 6.5 Other polymers ⓘ

There are no such residues in this entry.