



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 09:07 PM BST

PDB ID : 6C0J  
Title : Crystal structure of HIV-1 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 : 1.92 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

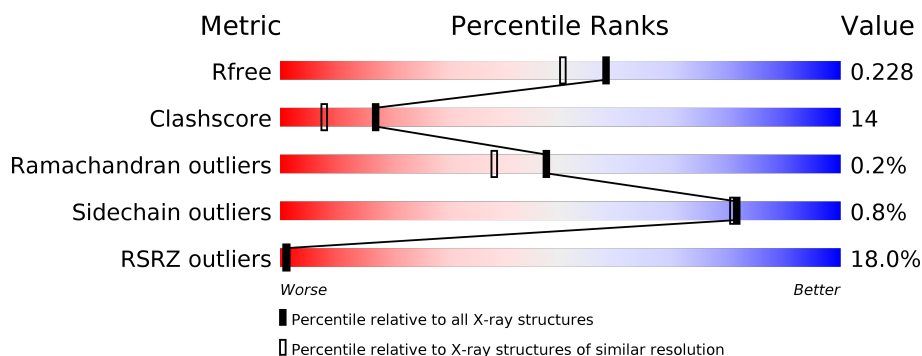
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.92 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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	557	<div> <div>19%</div> <div>78%</div> <div>21%</div> <div>.</div> </div>
2	B	428	<div> <div>17%</div> <div>75%</div> <div>21%</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	EDO	A	609	-	-	X	-
6	EDO	A	618	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8947 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	6	0
			4565	2952	761	843	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

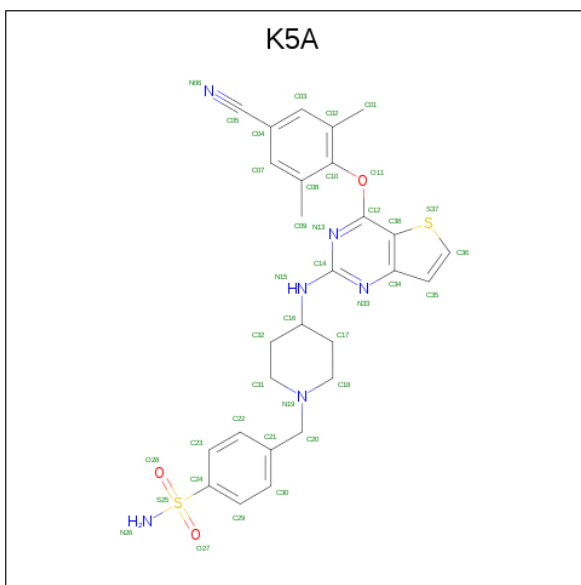
- Molecule 2 is a protein called Reverse transcriptase p51 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	414	Total	C	N	O	S	0	7	0
			3486	2273	574	632	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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).

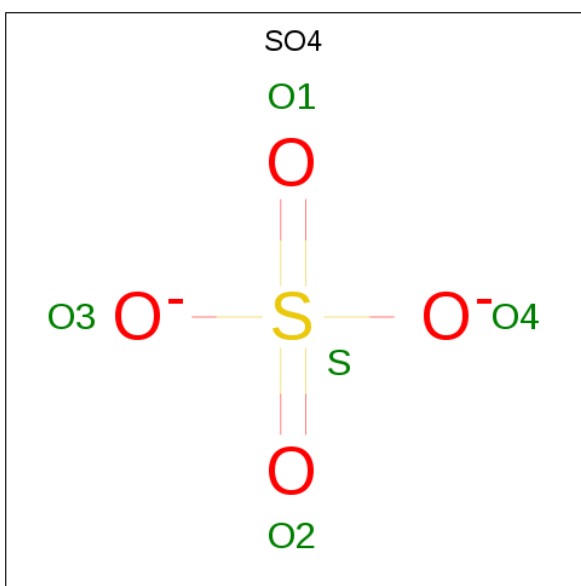


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			38	27	6	3	2		

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

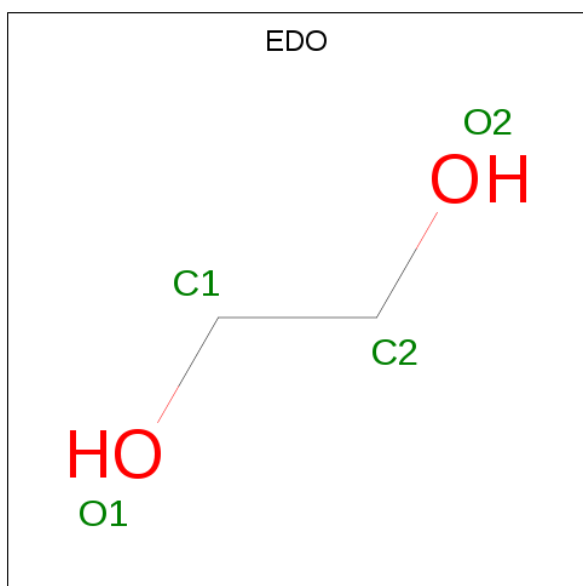
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 6 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
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	414	Total O 414 414	0	0

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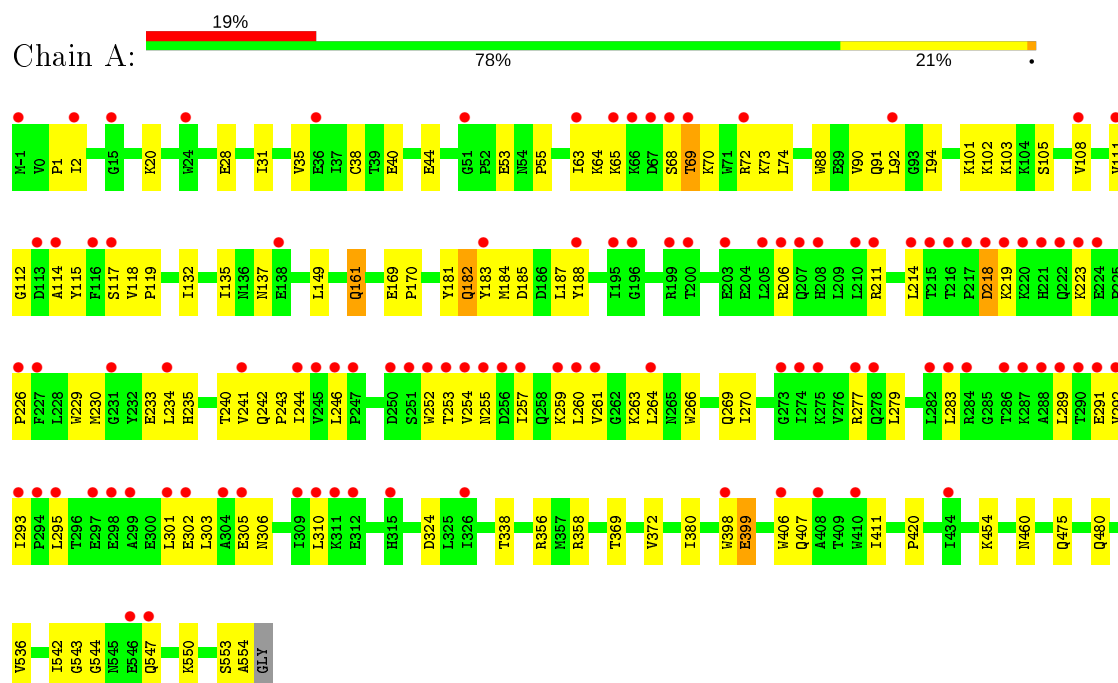
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	316	Total 316	O 316	0	0



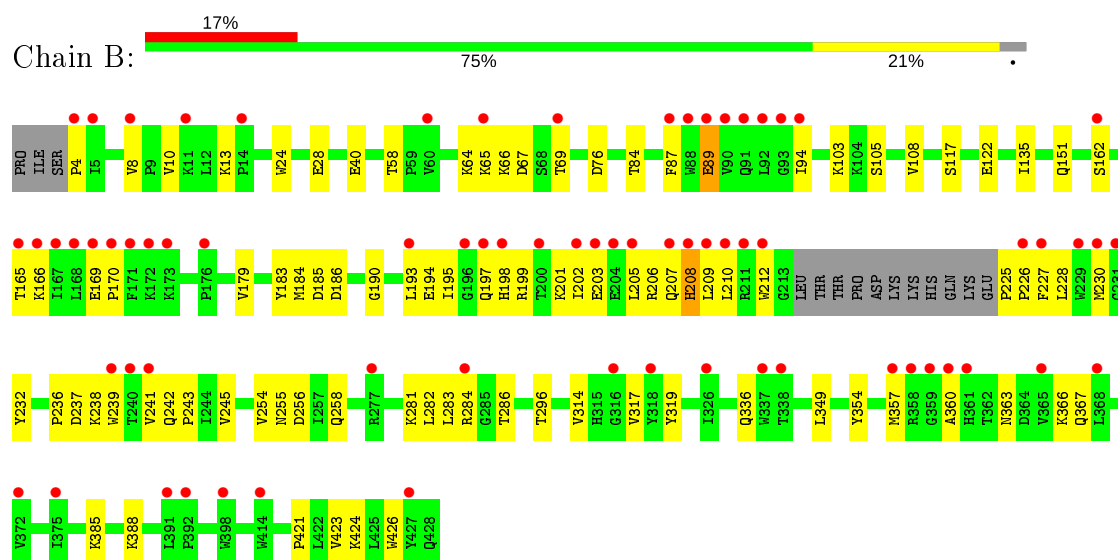
### 3 Residue-property plots

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: 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, $\alpha$ , $\beta$ , $\gamma$	163.26Å 72.78Å 109.55Å 90.00° 100.38° 90.00°	Depositor
Resolution (Å)	49.01 – 1.92 49.01 – 1.92	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.01-1.92) 99.3 (49.01-1.92)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.05 (at 1.92Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, $R_{free}$	0.183 , 0.226 0.186 , 0.228	Depositor DCC
$R_{free}$ test set	4795 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.1	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 69.1	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	8947	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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: MG, SO4, K5A, EDO

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	0/4684	0.49	0/6367
2	B	0.35	0/3590	0.50	0/4880
All	All	0.36	0/8274	0.50	0/11247

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	4565	0	4610	141	0
2	B	3486	0	3492	89	0
3	A	38	0	0	2	0
4	A	1	0	0	0	0
5	A	15	0	0	0	0
5	B	20	0	0	1	0
6	A	52	0	78	16	0
6	B	40	0	60	11	0
7	A	414	0	0	11	0
7	B	316	0	0	22	0
All	All	8947	0	8240	231	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 (231) 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)
2:B:360:ALA:HB2	2:B:366:LYS:HD3	1.38	1.03
1:A:259:LYS:HE2	1:A:263:LYS:HE3	1.41	1.01
2:B:255:ASN:HB3	6:B:513:EDO:H12	1.44	0.99
1:A:544:GLY:HA2	2:B:286[B]:THR:HG22	1.45	0.98
1:A:399:GLU:HG2	6:A:613:EDO:H12	1.44	0.97
1:A:240:THR:HG22	1:A:241:VAL:N	1.81	0.95
6:B:514:EDO:H12	7:B:804:HOH:O	1.76	0.85
1:A:137:ASN:HB2	6:A:618:EDO:H22	1.59	0.84
1:A:356[A]:ARG:HH12	6:A:616:EDO:H22	1.44	0.82
2:B:184:MET:HE3	7:B:759:HOH:O	1.80	0.82
1:A:181:TYR:HA	6:A:609:EDO:H22	1.62	0.81
1:A:182:GLN:HG3	1:A:187:LEU:CD2	2.12	0.80
1:A:241:VAL:HG12	1:A:242:GLN:O	1.83	0.79
1:A:240:THR:CG2	1:A:241:VAL:N	2.43	0.79
2:B:225:PRO:HG2	2:B:228:LEU:HD23	1.65	0.77
1:A:182:GLN:HG3	1:A:187:LEU:HD21	1.66	0.77
1:A:65:LYS:HG3	1:A:72:ARG:HH21	1.47	0.76
2:B:281:LYS:O	2:B:284:ARG:HG3	1.86	0.76
1:A:544:GLY:CA	2:B:286[B]:THR:HG22	2.17	0.73
1:A:184[B]:MET:HG2	1:A:185:ASP:N	2.02	0.73
2:B:360:ALA:HB1	2:B:363:ASN:HB3	1.71	0.72
1:A:356[A]:ARG:NH1	6:A:616:EDO:H22	2.03	0.72
2:B:162:SER:O	2:B:166:LYS:HD3	1.89	0.72
1:A:206:ARG:NH2	1:A:218:ASP:OD1	2.23	0.71
1:A:181:TYR:CD1	6:A:609:EDO:H21	2.26	0.69
1:A:257:ILE:CG2	1:A:283:LEU:HD11	2.23	0.69
2:B:256:ASP:OD1	6:B:513:EDO:H11	1.94	0.67
1:A:88:TRP:CD1	1:A:90:VAL:HG12	2.29	0.67
1:A:338[B]:THR:CG2	7:A:738:HOH:O	2.42	0.67
1:A:114:ALA:CB	1:A:214:LEU:HD22	2.24	0.66
7:A:871:HOH:O	6:B:514:EDO:H12	1.94	0.66
2:B:65:LYS:HE2	2:B:227:PHE:HB3	1.76	0.66
1:A:338[B]:THR:HG22	7:A:738:HOH:O	1.96	0.66
1:A:183:TYR:O	1:A:184[B]:MET:HB3	1.95	0.65
2:B:184:MET:HE2	7:B:793:HOH:O	1.94	0.65
2:B:87:PHE:HB2	7:B:854:HOH:O	1.97	0.64
2:B:255:ASN:CB	6:B:513:EDO:H12	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:TYR:HA	6:A:609:EDO:C2	2.28	0.64
1:A:65:LYS:HE3	1:A:68:SER:HB3	1.80	0.63
2:B:243:PRO:HD2	7:B:785:HOH:O	1.96	0.63
2:B:319:TYR:OH	2:B:385:LYS:HE2	1.97	0.63
1:A:182:GLN:H	6:A:609:EDO:H22	1.64	0.63
1:A:28:GLU:HG3	1:A:135:ILE:HD12	1.80	0.63
2:B:28:GLU:HB2	2:B:135:ILE:HD11	1.80	0.63
1:A:240:THR:CG2	1:A:241:VAL:H	2.12	0.62
1:A:101:LYS:HE3	7:A:786:HOH:O	2.00	0.62
2:B:209:LEU:HD21	7:B:874:HOH:O	2.00	0.62
1:A:356[B]:ARG:NH2	6:A:615:EDO:H22	2.16	0.61
2:B:317:VAL:CG1	2:B:349:LEU:HD23	2.30	0.61
2:B:282:LEU:CD2	2:B:296:THR:HG23	2.30	0.60
1:A:40:GLU:O	1:A:44:GLU:HG3	2.02	0.60
1:A:233:GLU:OE2	1:A:243:PRO:HD3	2.01	0.60
1:A:188:TYR:HB3	3:A:601:K5A:C09	2.31	0.60
2:B:205:LEU:O	2:B:205:LEU:HD23	2.01	0.60
1:A:108:VAL:HG22	1:A:188:TYR:CD2	2.37	0.59
1:A:114:ALA:HB1	1:A:214:LEU:HD22	1.83	0.59
2:B:65:LYS:HZ3	2:B:230:MET:HG2	1.66	0.59
1:A:219:LYS:HE2	1:A:223:LYS:NZ	2.18	0.59
1:A:306:ASN:O	1:A:310:LEU:HD13	2.04	0.58
2:B:193:LEU:HD13	2:B:197:GLN:HB2	1.85	0.58
2:B:4:PRO:HG2	2:B:117:SER:O	2.02	0.58
1:A:88:TRP:HD1	1:A:90:VAL:HG12	1.67	0.58
6:B:512:EDO:H12	7:B:712:HOH:O	2.02	0.58
1:A:182:GLN:H	6:A:609:EDO:C2	2.16	0.58
1:A:1:PRO:O	1:A:211:ARG:NH2	2.36	0.58
2:B:108:VAL:HB	2:B:232:TYR:HB3	1.86	0.57
6:A:610:EDO:H21	7:A:883:HOH:O	2.04	0.57
2:B:354:TYR:CD2	2:B:357:MET:HE1	2.40	0.57
1:A:70:LYS:HE3	1:A:72:ARG:HE	1.69	0.57
2:B:165:THR:O	2:B:169:GLU:HG2	2.05	0.57
2:B:282:LEU:HD21	2:B:296:THR:HG23	1.84	0.57
2:B:122:GLU:HG3	7:B:755:HOH:O	2.05	0.57
2:B:24:TRP:CD2	6:B:505:EDO:H21	2.40	0.56
1:A:182:GLN:HG3	1:A:187:LEU:HD23	1.86	0.56
2:B:170:PRO:HG2	2:B:208:HIS:NE2	2.21	0.56
1:A:69:THR:HG22	1:A:69:THR:O	2.06	0.55
2:B:28:GLU:CB	2:B:135:ILE:HD11	2.37	0.55
1:A:241:VAL:HG13	1:A:266:TRP:HE1	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:225:PRO:HB2	2:B:228:LEU:HB3	1.89	0.55
1:A:246:LEU:HD22	1:A:260:LEU:HD12	1.89	0.55
1:A:246:LEU:HD22	1:A:260:LEU:CD1	2.37	0.55
1:A:253:THR:HG22	1:A:254:VAL:N	2.22	0.55
1:A:64:LYS:NZ	1:A:69:THR:HG23	2.22	0.54
2:B:151:GLN:HB3	2:B:185:ASP:OD2	2.07	0.54
1:A:73:LYS:HB3	1:A:73:LYS:NZ	2.21	0.54
2:B:225:PRO:HB2	2:B:228:LEU:CB	2.37	0.54
1:A:480:GLN:HB2	7:A:980:HOH:O	2.06	0.54
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.48	0.54
1:A:112:GLY:HA2	1:A:185:ASP:OD1	2.07	0.54
1:A:252:TRP:CD1	1:A:295:LEU:HD11	2.42	0.54
2:B:241:VAL:HG23	2:B:243:PRO:HD3	1.89	0.54
2:B:336:GLN:NE2	7:B:614:HOH:O	2.41	0.54
1:A:257:ILE:O	1:A:261:VAL:HG23	2.08	0.53
2:B:195:ILE:HA	2:B:198:HIS:HB3	1.89	0.53
2:B:360:ALA:HB3	7:B:646:HOH:O	2.09	0.52
1:A:253:THR:HG22	1:A:289:LEU:O	2.10	0.52
1:A:454:LYS:CE	1:A:554:ALA:HB2	2.39	0.52
1:A:259:LYS:CE	1:A:263:LYS:HE3	2.27	0.52
1:A:31:ILE:O	1:A:35:VAL:HG23	2.09	0.52
1:A:102:LYS:O	1:A:103:LYS:HD3	2.10	0.52
2:B:40:GLU:HG2	7:B:656:HOH:O	2.10	0.52
2:B:208:HIS:O	2:B:212:TRP:HD1	1.93	0.51
1:A:63:ILE:CD1	1:A:72:ARG:HB2	2.41	0.51
2:B:198:HIS:O	2:B:202:ILE:HG12	2.11	0.51
1:A:91:GLN:HB2	1:A:183:TYR:CE1	2.45	0.51
1:A:454:LYS:HE3	1:A:554:ALA:HB2	1.92	0.51
2:B:226:PRO:HD2	7:B:856:HOH:O	2.10	0.51
1:A:260:LEU:HD21	1:A:303:LEU:HD13	1.91	0.51
2:B:203:GLU:OE1	2:B:206:ARG:NH1	2.44	0.50
2:B:360:ALA:O	2:B:367:GLN:NE2	2.44	0.50
1:A:28:GLU:HG3	1:A:135:ILE:CD1	2.41	0.50
1:A:94:ILE:HG21	1:A:230:MET:HE2	1.93	0.50
2:B:360:ALA:HB2	2:B:366:LYS:CD	2.27	0.50
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.47	0.49
1:A:266:TRP:O	1:A:269:GLN:HG2	2.12	0.49
1:A:254:VAL:HG23	1:A:293:ILE:HD11	1.94	0.49
1:A:254:VAL:HB	1:A:289:LEU:HA	1.95	0.49
1:A:254:VAL:HG11	1:A:289:LEU:HD12	1.95	0.49
1:A:91:GLN:HB2	1:A:183:TYR:HE1	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:LEU:HD12	7:A:710:HOH:O	2.13	0.49
1:A:543:GLY:HA3	2:B:283:LEU:O	2.13	0.49
1:A:454:LYS:NZ	1:A:554:ALA:HB2	2.28	0.49
1:A:358:ARG:NH2	7:A:723:HOH:O	2.45	0.48
1:A:65:LYS:CG	1:A:72:ARG:HH21	2.21	0.48
2:B:241:VAL:HG13	7:B:844:HOH:O	2.12	0.48
1:A:226:PRO:HG3	1:A:235:HIS:CE1	2.48	0.48
1:A:536:VAL:HB	1:A:542:ILE:HD13	1.96	0.48
1:A:246:LEU:HG	1:A:310:LEU:HD22	1.95	0.48
1:A:73:LYS:HG2	1:A:74:LEU:N	2.29	0.48
2:B:237:ASP:OD2	2:B:238:LYS:HE2	2.13	0.48
1:A:240:THR:HG23	1:A:270:ILE:HG21	1.95	0.48
1:A:283:LEU:N	1:A:283:LEU:HD12	2.28	0.48
1:A:550:LYS:HE3	7:A:743:HOH:O	2.14	0.47
1:A:257:ILE:HG21	1:A:283:LEU:HD11	1.95	0.47
2:B:103:LYS:HD3	2:B:103:LYS:HA	1.47	0.47
1:A:63:ILE:HD11	1:A:72:ARG:HB2	1.96	0.47
1:A:68:SER:C	1:A:70:LYS:H	2.16	0.47
2:B:28:GLU:HB2	2:B:135:ILE:CD1	2.44	0.47
1:A:292:VAL:C	1:A:293:ILE:HD12	2.35	0.47
2:B:105:SER:O	2:B:190:GLY:HA2	2.14	0.47
1:A:356[B]:ARG:HH22	6:A:615:EDO:H22	1.78	0.47
2:B:183:TYR:CE2	2:B:184:MET:HG2	2.50	0.47
2:B:13:LYS:HE3	2:B:84:THR:O	2.15	0.46
2:B:314:VAL:HG23	7:B:665:HOH:O	2.14	0.46
2:B:8:VAL:O	2:B:10:VAL:HG23	2.16	0.46
1:A:260:LEU:O	1:A:264:LEU:HG	2.16	0.46
1:A:20:LYS:NZ	1:A:55:PRO:HB2	2.29	0.46
1:A:254:VAL:CG1	1:A:289:LEU:HD12	2.46	0.46
2:B:354:TYR:CB	2:B:357:MET:HE2	2.45	0.46
2:B:66:LYS:O	2:B:67:ASP:HB2	2.15	0.46
2:B:423:VAL:HG21	7:B:607:HOH:O	2.16	0.46
1:A:241:VAL:HG13	1:A:266:TRP:NE1	2.31	0.46
2:B:354:TYR:HD2	2:B:357:MET:HE1	1.79	0.46
1:A:88:TRP:CZ3	6:A:608:EDO:H11	2.51	0.46
2:B:186:ASP:HB2	7:B:604:HOH:O	2.15	0.46
1:A:91:GLN:N	1:A:91:GLN:OE1	2.48	0.45
1:A:219:LYS:HE2	1:A:223:LYS:HZ1	1.81	0.45
2:B:242:GLN:HA	7:B:785:HOH:O	2.17	0.45
1:A:369:THR:HG23	1:A:411:ILE:HD11	1.99	0.45
1:A:65:LYS:HE2	1:A:70:LYS:HE2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:LYS:HG3	1:A:72:ARG:NH2	2.24	0.45
2:B:65:LYS:HZ1	2:B:230:MET:HB2	1.82	0.45
2:B:210:LEU:O	2:B:210:LEU:HD23	2.17	0.45
2:B:89:GLU:H	2:B:89:GLU:CD	2.19	0.45
2:B:94:ILE:CG1	2:B:94:ILE:O	2.65	0.45
1:A:301:LEU:O	1:A:305:GLU:HG3	2.17	0.44
1:A:90:VAL:HG21	1:A:161:GLN:HG2	2.00	0.44
1:A:277:ARG:HH12	6:A:615:EDO:C1	2.30	0.44
2:B:186:ASP:OD1	6:B:508:EDO:H12	2.17	0.44
1:A:244:ILE:HG22	1:A:310:LEU:HD23	2.00	0.44
1:A:279:LEU:HG	1:A:302:GLU:OE2	2.18	0.44
1:A:111:VAL:HG22	1:A:185:ASP:O	2.16	0.44
1:A:380[A]:ILE:HD11	6:B:510:EDO:H21	2.00	0.44
2:B:423:VAL:HA	2:B:426[B]:TRP:CD1	2.53	0.44
2:B:64:LYS:HE2	2:B:69:THR:O	2.17	0.44
2:B:207:GLN:HA	2:B:207:GLN:OE1	2.18	0.43
1:A:253:THR:HG22	1:A:254:VAL:H	1.83	0.43
1:A:254:VAL:CG1	1:A:289:LEU:HA	2.49	0.43
1:A:372:VAL:HG11	1:A:411:ILE:HD12	2.01	0.43
2:B:228:LEU:HD12	2:B:228:LEU:O	2.18	0.43
2:B:236:PRO:HA	2:B:239:TRP:CG	2.54	0.43
1:A:475:GLN:HG3	6:A:610:EDO:O2	2.18	0.43
1:A:64:LYS:HZ2	1:A:69:THR:HG23	1.82	0.43
1:A:543:GLY:N	2:B:283:LEU:O	2.49	0.43
7:A:871:HOH:O	6:B:514:EDO:C1	2.61	0.43
1:A:460:ASN:HA	2:B:286[A]:THR:O	2.19	0.43
2:B:103:LYS:NZ	2:B:179:VAL:HG23	2.34	0.43
1:A:182:GLN:CG	1:A:187:LEU:HD23	2.47	0.43
2:B:94:ILE:HG13	2:B:94:ILE:O	2.19	0.43
1:A:229:TRP:CE3	1:A:234:LEU:HD11	2.54	0.42
1:A:70:LYS:HE3	1:A:72:ARG:NE	2.33	0.42
2:B:58:THR:HG23	2:B:76:ASP:O	2.19	0.42
1:A:553:SER:O	1:A:554:ALA:C	2.57	0.42
1:A:63:ILE:O	1:A:63:ILE:HD12	2.19	0.42
1:A:65:LYS:CE	1:A:70:LYS:HE2	2.50	0.42
1:A:2:ILE:HA	1:A:211:ARG:HH21	1.85	0.42
1:A:254:VAL:HG23	1:A:293:ILE:CD1	2.49	0.42
1:A:255:ASN:OD1	1:A:289:LEU:HD23	2.19	0.42
2:B:424:LYS:NZ	5:B:502:SO4:O3	2.51	0.42
1:A:241:VAL:CG1	1:A:266:TRP:CD1	3.03	0.42
1:A:420:PRO:HG3	7:A:862:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:94:ILE:HD12	2:B:94:ILE:O	2.20	0.42
1:A:112:GLY:O	1:A:115:TYR:HB3	2.19	0.41
2:B:254:VAL:O	2:B:258:GLN:HG3	2.20	0.41
1:A:291:GLU:O	1:A:293:ILE:HD12	2.19	0.41
1:A:53:GLU:OE1	1:A:53:GLU:N	2.44	0.41
1:A:70:LYS:HE3	1:A:72:ARG:HG3	2.03	0.41
2:B:388:LYS:HE2	7:B:869:HOH:O	2.19	0.41
6:B:507:EDO:H12	7:B:891:HOH:O	2.20	0.41
1:A:398:TRP:CH2	1:A:411:ILE:HG12	2.56	0.41
2:B:193:LEU:HD12	2:B:194:GLU:O	2.21	0.41
1:A:118:VAL:HG11	1:A:149:LEU:HD11	2.03	0.41
1:A:187:LEU:HA	1:A:187:LEU:HD23	1.90	0.41
1:A:406:TRP:CE2	1:A:407:GLN:HG3	2.56	0.41
1:A:547:GLN:N	1:A:547:GLN:OE1	2.53	0.41
1:A:90:VAL:N	1:A:91:GLN:OE1	2.54	0.41
2:B:162:SER:HB2	7:B:706:HOH:O	2.19	0.41
2:B:245:VAL:HG22	7:B:611:HOH:O	2.21	0.41
1:A:182:GLN:N	6:A:609:EDO:H22	2.33	0.41
2:B:195:ILE:HD11	2:B:199:ARG:CZ	2.50	0.41
2:B:225:PRO:HB2	2:B:228:LEU:HB2	2.03	0.41
2:B:421:PRO:HD2	7:B:689:HOH:O	2.21	0.41
1:A:188:TYR:CB	3:A:601:K5A:C09	2.99	0.41
1:A:63:ILE:C	1:A:63:ILE:HD12	2.40	0.41
1:A:63:ILE:HD11	1:A:72:ARG:CB	2.51	0.41
1:A:169:GLU:HB3	1:A:170:PRO:CD	2.51	0.40
1:A:117:SER:O	1:A:119:PRO:HD3	2.21	0.40
2:B:197:GLN:O	2:B:201:LYS:HB2	2.22	0.40
1:A:253:THR:CG2	1:A:254:VAL:N	2.84	0.40
1:A:214:LEU:HA	1:A:214:LEU:HD23	1.88	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	560/557 (100%)	541 (97%)	18 (3%)	1 (0%)	47	38
2	B	417/428 (97%)	397 (95%)	19 (5%)	1 (0%)	47	38
All	All	977/985 (99%)	938 (96%)	37 (4%)	2 (0%)	47	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	THR
2	B	89	GLU

### 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	500/495 (101%)	494 (99%)	6 (1%)	71	69
2	B	382/390 (98%)	381 (100%)	1 (0%)	92	93
All	All	882/885 (100%)	875 (99%)	7 (1%)	81	81

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	SER
1	A	161	GLN
1	A	182	GLN
1	A	218	ASP
1	A	324	ASP
1	A	399	GLU
2	B	208	HIS

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 1 is monoatomic - leaving 31 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	$\# Z  > 2$
6	EDO	A	609	-	3,3,3	0.45	0	2,2,2	0.25	0
6	EDO	A	612	-	3,3,3	0.45	0	2,2,2	0.35	0
6	EDO	A	613	-	3,3,3	0.44	0	2,2,2	0.36	0
6	EDO	B	510	-	3,3,3	0.47	0	2,2,2	0.39	0
6	EDO	A	615	-	3,3,3	0.44	0	2,2,2	0.37	0
6	EDO	A	618	-	3,3,3	0.46	0	2,2,2	0.34	0
6	EDO	B	512	-	3,3,3	0.49	0	2,2,2	0.35	0
6	EDO	A	611	-	3,3,3	0.44	0	2,2,2	0.43	0
6	EDO	A	617	-	3,3,3	0.47	0	2,2,2	0.36	0
6	EDO	A	614	-	3,3,3	0.43	0	2,2,2	0.40	0
6	EDO	B	506	-	3,3,3	0.46	0	2,2,2	0.22	0
5	SO4	A	604	-	4,4,4	0.14	0	6,6,6	0.10	0
5	SO4	A	603	-	4,4,4	0.15	0	6,6,6	0.05	0
6	EDO	A	616	-	3,3,3	0.45	0	2,2,2	0.34	0
6	EDO	A	606	-	3,3,3	0.42	0	2,2,2	0.45	0
6	EDO	B	514	-	3,3,3	0.46	0	2,2,2	0.34	0
5	SO4	B	504	-	4,4,4	0.14	0	6,6,6	0.08	0
6	EDO	B	507	-	3,3,3	0.46	0	2,2,2	0.32	0
5	SO4	B	503	-	4,4,4	0.13	0	6,6,6	0.05	0
6	EDO	A	610	-	3,3,3	0.43	0	2,2,2	0.43	0
6	EDO	B	508	-	3,3,3	0.46	0	2,2,2	0.30	0
5	SO4	A	605	-	4,4,4	0.13	0	6,6,6	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	SO4	B	502	-	4,4,4	0.14	0	6,6,6	0.04	0
6	EDO	A	607	-	3,3,3	0.43	0	2,2,2	0.46	0
6	EDO	B	505	-	3,3,3	0.43	0	2,2,2	0.34	0
6	EDO	B	513	-	3,3,3	0.41	0	2,2,2	0.39	0
5	SO4	B	501	-	4,4,4	0.14	0	6,6,6	0.05	0
6	EDO	A	608	-	3,3,3	0.47	0	2,2,2	0.30	0
3	K5A	A	601	-	40,42,42	1.65	6 (15%)	50,61,61	2.51	16 (32%)
6	EDO	B	509	-	3,3,3	0.41	0	2,2,2	0.60	0
6	EDO	B	511	-	3,3,3	0.44	0	2,2,2	0.35	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
6	EDO	A	609	-	-	0/1/1/1	-
6	EDO	A	612	-	-	0/1/1/1	-
6	EDO	A	613	-	-	0/1/1/1	-
6	EDO	B	510	-	-	1/1/1/1	-
6	EDO	A	615	-	-	1/1/1/1	-
6	EDO	A	618	-	-	0/1/1/1	-
6	EDO	B	512	-	-	1/1/1/1	-
6	EDO	A	611	-	-	0/1/1/1	-
6	EDO	A	617	-	-	1/1/1/1	-
6	EDO	A	614	-	-	1/1/1/1	-
6	EDO	B	506	-	-	1/1/1/1	-
6	EDO	A	616	-	-	1/1/1/1	-
6	EDO	A	606	-	-	1/1/1/1	-
6	EDO	B	514	-	-	0/1/1/1	-
6	EDO	B	507	-	-	1/1/1/1	-
6	EDO	A	610	-	-	1/1/1/1	-
6	EDO	B	508	-	-	0/1/1/1	-
6	EDO	A	607	-	-	0/1/1/1	-
6	EDO	B	505	-	-	1/1/1/1	-
6	EDO	B	513	-	-	0/1/1/1	-
6	EDO	A	608	-	-	1/1/1/1	-
3	K5A	A	601	-	-	3/20/30/30	0/5/5/5
6	EDO	B	509	-	-	0/1/1/1	-
6	EDO	B	511	-	-	0/1/1/1	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	K5A	C14-N15	4.93	1.41	1.34
3	A	601	K5A	C18-N19	4.10	1.58	1.46
3	A	601	K5A	C12-N13	3.79	1.38	1.31
3	A	601	K5A	C14-N13	3.14	1.44	1.34
3	A	601	K5A	S25-N26	2.84	1.66	1.60
3	A	601	K5A	C24-S25	-2.27	1.73	1.77

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	K5A	C03-C04-C05	6.16	127.72	119.54
3	A	601	K5A	C20-N19-C18	6.01	124.43	111.06
3	A	601	K5A	C21-C20-N19	-5.30	102.83	113.12
3	A	601	K5A	C29-C24-C23	-5.12	113.30	120.44
3	A	601	K5A	C07-C04-C05	-5.10	112.76	119.54
3	A	601	K5A	C22-C23-C24	4.88	124.50	119.45
3	A	601	K5A	C17-C18-N19	4.13	117.52	111.11
3	A	601	K5A	C30-C29-C24	3.91	123.49	119.45
3	A	601	K5A	C23-C24-S25	3.65	125.03	119.73
3	A	601	K5A	C01-C02-C10	3.21	126.00	120.82
3	A	601	K5A	C31-N19-C18	2.99	115.56	108.83
3	A	601	K5A	O28-S25-C24	2.92	110.61	107.35
3	A	601	K5A	C32-C31-N19	2.33	114.73	111.11
3	A	601	K5A	C01-C02-C03	-2.29	115.26	119.49
3	A	601	K5A	O11-C12-C38	2.24	119.34	115.69
3	A	601	K5A	C31-C32-C16	2.11	114.21	110.50

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	K5A	C21-C20-N19-C18
6	B	510	EDO	O1-C1-C2-O2
6	A	615	EDO	O1-C1-C2-O2
6	B	506	EDO	O1-C1-C2-O2
6	A	606	EDO	O1-C1-C2-O2
6	A	608	EDO	O1-C1-C2-O2
3	A	601	K5A	C23-C24-S25-O28
3	A	601	K5A	C29-C24-S25-O28
6	B	512	EDO	O1-C1-C2-O2
6	A	614	EDO	O1-C1-C2-O2
6	B	507	EDO	O1-C1-C2-O2

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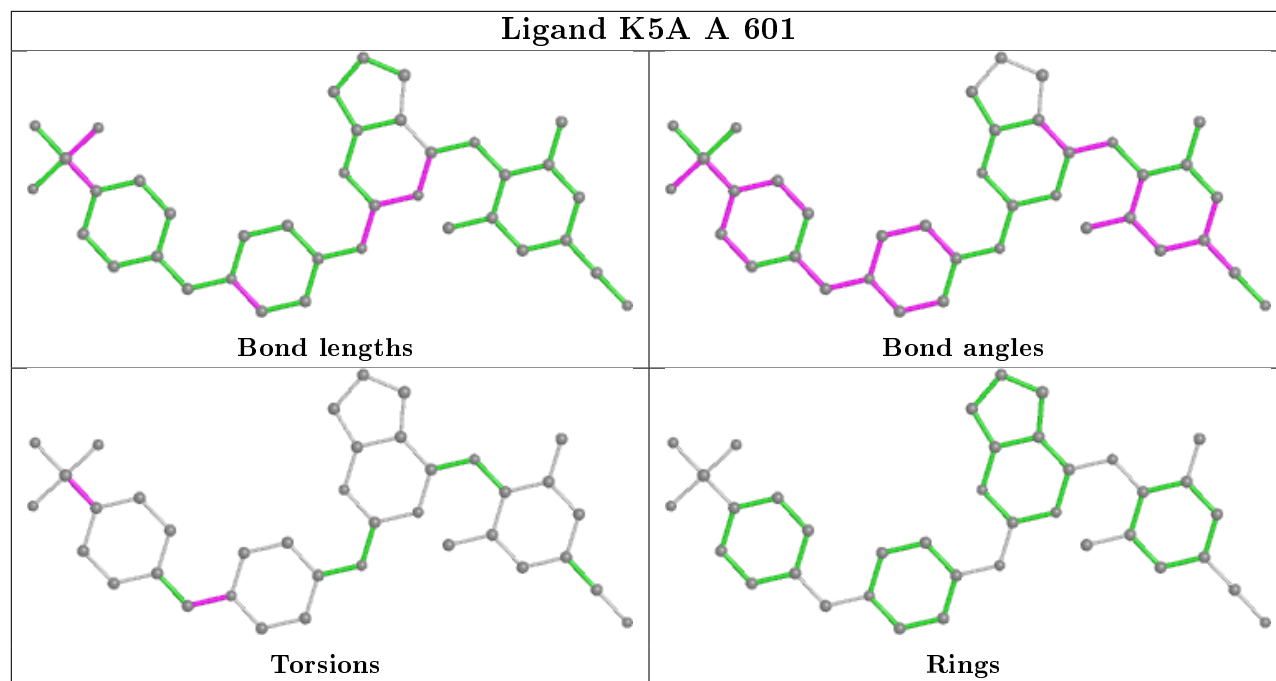
Mol	Chain	Res	Type	Atoms
6	B	505	EDO	O1-C1-C2-O2
6	A	617	EDO	O1-C1-C2-O2
6	A	616	EDO	O1-C1-C2-O2
6	A	610	EDO	O1-C1-C2-O2

There are no ring outliers.

16 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	609	EDO	6	0
6	A	613	EDO	1	0
6	B	510	EDO	1	0
6	A	615	EDO	3	0
6	A	618	EDO	1	0
6	B	512	EDO	1	0
6	A	616	EDO	2	0
6	B	514	EDO	3	0
6	B	507	EDO	1	0
6	A	610	EDO	2	0
6	B	508	EDO	1	0
5	B	502	SO4	1	0
6	B	505	EDO	1	0
6	B	513	EDO	3	0
6	A	608	EDO	1	0
3	A	601	K5A	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 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%)	1.10	104 (18%)  	39, 72, 149, 220	0
2	B	414/428 (96%)	1.08	71 (17%)  	39, 65, 136, 267	0
All	All	970/985 (98%)	1.09	175 (18%)  	39, 69, 142, 267	0

All (175) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	4	PRO	14.2
2	B	92	LEU	12.7
2	B	91	GLN	12.5
1	A	286	THR	12.2
2	B	90	VAL	12.0
1	A	67	ASP	10.3
1	A	257	ILE	10.3
1	A	290	THR	10.1
1	A	292	VAL	10.0
1	A	221	HIS	8.8
1	A	68	SER	8.4
2	B	358	ARG	8.1
2	B	359	GLY	7.8
1	A	301	LEU	7.4
2	B	89	GLU	7.1
1	A	261	VAL	7.1
1	A	220	LYS	7.1
1	A	289	LEU	6.9
1	A	295	LEU	6.8
1	A	252	TRP	6.5
2	B	210	LEU	6.5
1	A	283	LEU	6.4
2	B	209	LEU	6.3
2	B	229	TRP	6.2

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Mol	Chain	Res	Type	RSRZ
1	A	114	ALA	6.2
1	A	254	VAL	6.2
1	A	223	LYS	6.0
1	A	297	GLU	5.7
2	B	88	TRP	5.6
1	A	294	PRO	5.6
1	A	260	LEU	5.6
2	B	230	MET	5.4
1	A	24	TRP	5.4
1	A	222	GLN	5.3
1	A	69	THR	5.3
2	B	227	PHE	5.3
1	A	244	ILE	5.3
1	A	215	THR	5.2
1	A	293	ILE	5.1
1	A	298	GLU	5.0
1	A	218	ASP	5.0
1	A	214	LEU	5.0
2	B	212	TRP	5.0
1	A	227	PHE	4.9
2	B	226	PRO	4.8
2	B	202	ILE	4.8
1	A	304	ALA	4.7
2	B	231	GLY	4.7
1	A	282	LEU	4.6
2	B	197	GLN	4.6
1	A	245	VAL	4.6
1	A	195	ILE	4.4
2	B	168	LEU	4.4
1	A	15	GLY	4.3
1	A	287	LYS	4.2
1	A	311	LYS	4.2
2	B	5	ILE	4.2
2	B	357	MET	4.1
1	A	219	LYS	4.0
1	A	208	HIS	4.0
1	A	199	ARG	4.0
2	B	166	LYS	3.9
1	A	216	THR	3.9
1	A	546	GLU	3.9
1	A	217	PRO	3.8
1	A	66	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	246	LEU	3.7
1	A	256	ASP	3.7
1	A	309	ILE	3.7
1	A	92	LEU	3.7
1	A	284	ARG	3.7
2	B	200	THR	3.6
2	B	93	GLY	3.6
2	B	204	GLU	3.6
1	A	211	ARG	3.5
2	B	172	LYS	3.5
1	A	291	GLU	3.5
2	B	169	GLU	3.4
2	B	211	ARG	3.4
1	A	247	PRO	3.4
1	A	273	GLY	3.4
2	B	87	PHE	3.4
2	B	203	GLU	3.3
2	B	318	TYR	3.3
2	B	170	PRO	3.3
2	B	360	ALA	3.2
1	A	251	SER	3.2
2	B	193	LEU	3.2
1	A	288	ALA	3.2
1	A	207	GLN	3.1
1	A	250	ASP	3.1
1	A	188	TYR	3.1
1	A	116	PHE	3.0
1	A	72	ARG	3.0
1	A	302	GLU	3.0
1	A	255	ASN	2.9
2	B	198	HIS	2.9
2	B	196	GLY	2.9
2	B	240	THR	2.8
2	B	205	LEU	2.8
1	A	206	ARG	2.8
1	A	117	SER	2.8
1	A	111	VAL	2.8
1	A	234	LEU	2.8
2	B	391	LEU	2.7
2	B	326	ILE	2.7
1	A	315[A]	HIS	2.7
1	A	259	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	210	LEU	2.6
2	B	337	TRP	2.6
2	B	60[A]	VAL	2.6
2	B	372	VAL	2.6
2	B	207	GLN	2.6
2	B	14	PRO	2.6
1	A	224	GLU	2.6
2	B	365	VAL	2.5
1	A	547	GLN	2.5
1	A	275	LYS	2.5
2	B	427[A]	TYR	2.5
1	A	312	GLU	2.5
1	A	408	ALA	2.5
1	A	241	VAL	2.5
1	A	226	PRO	2.4
2	B	239	TRP	2.4
2	B	65	LYS	2.4
1	A	203	GLU	2.4
2	B	94	ILE	2.4
2	B	375	ILE	2.4
2	B	241	VAL	2.4
1	A	305	GLU	2.4
1	A	200	THR	2.4
1	A	274	ILE	2.4
1	A	183	TYR	2.4
1	A	299	ALA	2.4
2	B	162	SER	2.4
1	A	277	ARG	2.4
1	A	65	LYS	2.4
1	A	410	TRP	2.4
2	B	167	ILE	2.4
1	A	113	ASP	2.3
1	A	264	LEU	2.3
1	A	-1	MET	2.3
1	A	406	TRP	2.3
1	A	51	GLY	2.3
2	B	173	LYS	2.3
1	A	2	ILE	2.3
2	B	208	HIS	2.3
2	B	338	THR	2.3
1	A	108	VAL	2.3
2	B	398	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	310	LEU	2.3
2	B	277	ARG	2.2
1	A	398	TRP	2.2
2	B	414	TRP	2.2
1	A	205	LEU	2.2
1	A	231	GLY	2.2
1	A	278	GLN	2.2
2	B	11	LYS	2.2
2	B	284	ARG	2.2
1	A	196	GLY	2.1
2	B	171	PHE	2.1
2	B	8	VAL	2.1
2	B	176	PRO	2.1
2	B	361	HIS	2.1
1	A	63	ILE	2.1
1	A	434	ILE	2.1
2	B	165	THR	2.1
2	B	368	LEU	2.1
2	B	69	THR	2.1
1	A	326	ILE	2.1
2	B	316	GLY	2.1
1	A	253	THR	2.1
1	A	138	GLU	2.1
1	A	36	GLU	2.0
2	B	392	PRO	2.0

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

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

## 6.3 Carbohydrates ⓘ

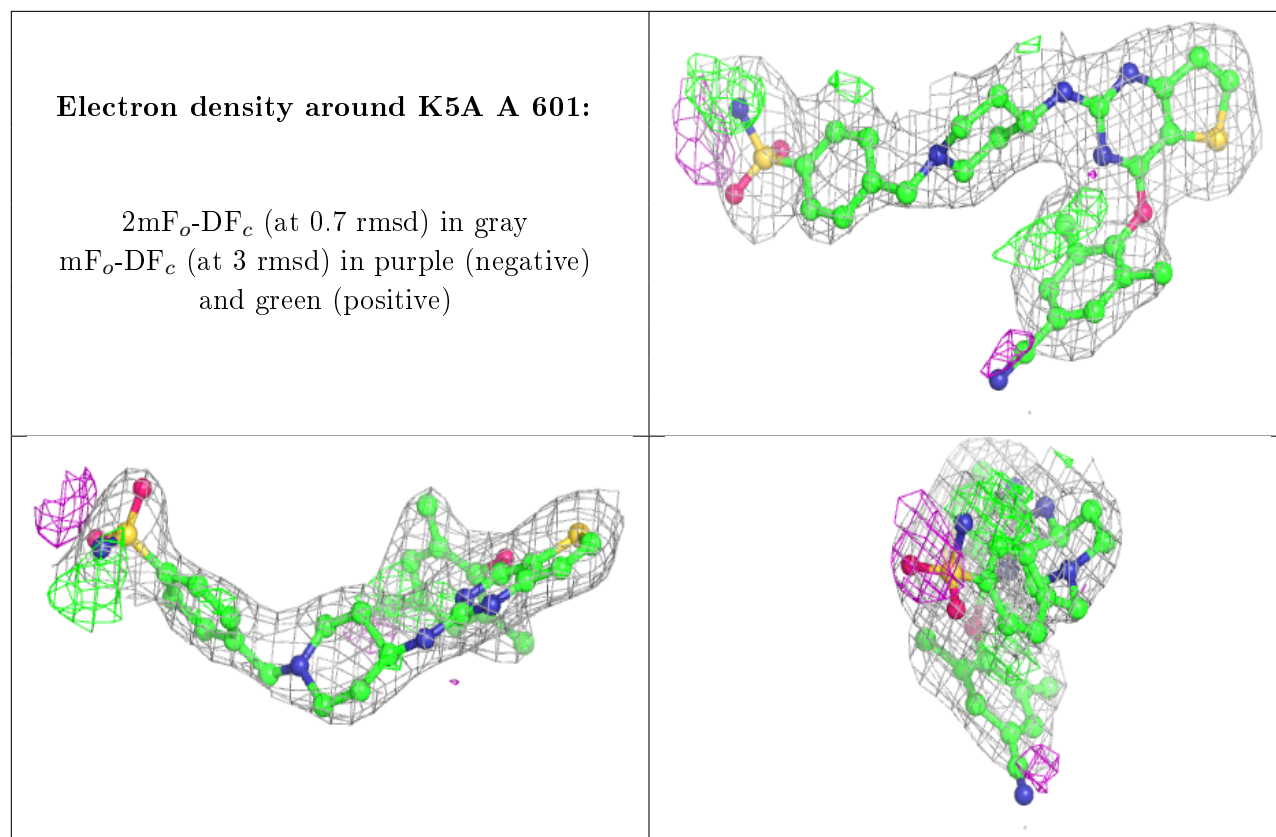
There are no monosaccharides in this entry.

## 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, 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( $\text{\AA}^2$ )	Q<0.9
6	EDO	B	507	4/4	0.60	0.26	85,90,96,102	0
6	EDO	B	514	4/4	0.64	0.22	31,34,39,43	0
6	EDO	A	617	4/4	0.64	0.28	92,97,99,103	0
6	EDO	A	613	4/4	0.74	0.35	102,106,108,110	0
5	SO4	B	501	5/5	0.75	0.30	206,206,206,208	0
6	EDO	A	610	4/4	0.77	0.14	71,76,80,86	0
6	EDO	A	618	4/4	0.78	0.46	31,34,39,43	0
6	EDO	B	510	4/4	0.79	0.27	71,73,79,83	0
6	EDO	A	615	4/4	0.81	0.39	99,102,102,108	0
5	SO4	A	605	5/5	0.81	0.22	136,137,139,143	0
6	EDO	A	616	4/4	0.81	0.10	104,106,107,108	0
4	MG	A	602	1/1	0.82	0.13	64,64,64,64	0
6	EDO	A	608	4/4	0.84	0.13	86,87,89,91	0
6	EDO	B	512	4/4	0.85	0.19	80,80,80,83	0
6	EDO	A	609	4/4	0.86	0.21	91,94,97,100	0
6	EDO	A	614	4/4	0.86	0.27	87,89,90,92	0
6	EDO	B	513	4/4	0.87	0.29	85,86,86,90	0
6	EDO	B	508	4/4	0.87	0.18	83,87,93,100	0
6	EDO	A	611	4/4	0.87	0.17	86,86,89,89	0
6	EDO	B	511	4/4	0.87	0.15	75,83,91,94	0
3	K5A	A	601	38/38	0.88	0.17	55,89,133,135	0
6	EDO	B	509	4/4	0.88	0.19	86,87,89,91	0
6	EDO	A	612	4/4	0.88	0.15	96,97,97,97	0
5	SO4	A	604	5/5	0.90	0.14	101,102,106,114	0
5	SO4	B	504	5/5	0.90	0.24	131,131,132,136	0
5	SO4	A	603	5/5	0.90	0.23	131,132,133,135	0
6	EDO	A	607	4/4	0.92	0.19	72,73,81,83	0
5	SO4	B	502	5/5	0.93	0.31	159,160,160,162	0
6	EDO	B	506	4/4	0.94	0.21	60,64,67,72	0
5	SO4	B	503	5/5	0.95	0.23	148,148,150,150	0
6	EDO	A	606	4/4	0.95	0.21	54,65,68,82	0
6	EDO	B	505	4/4	0.95	0.22	56,58,63,65	0

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.