



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 8, 2021 – 04:03 PM EST

PDB ID : 7LQU  
Title : Crystal Structure of HIV-1 RT in Complex with NBD-14075  
Authors : Losada, N.; Ruiz, F.X.; Gruber, K.; Das, K.; Arnold, E.  
Deposited on : 2021-02-15  
Resolution : 2.60 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 : 2.23.2  
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) : 2.23.2

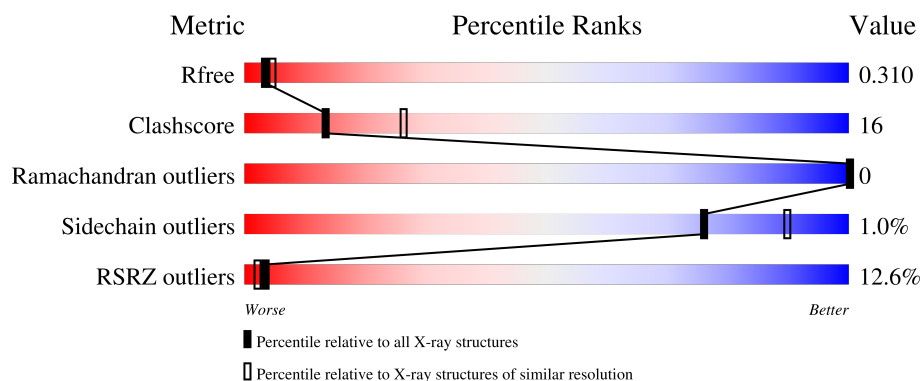
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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  $\geq 3$ , 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>16%</div> <div>71%</div> <div>28%</div> </div>
2	B	429	<div> <div>7%</div> <div>68%</div> <div>28%</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
4	SO4	B	501	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8072 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 p66.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	556	Total	C	N	O	S	0	1	0
			4521	2926	751	836	8			

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

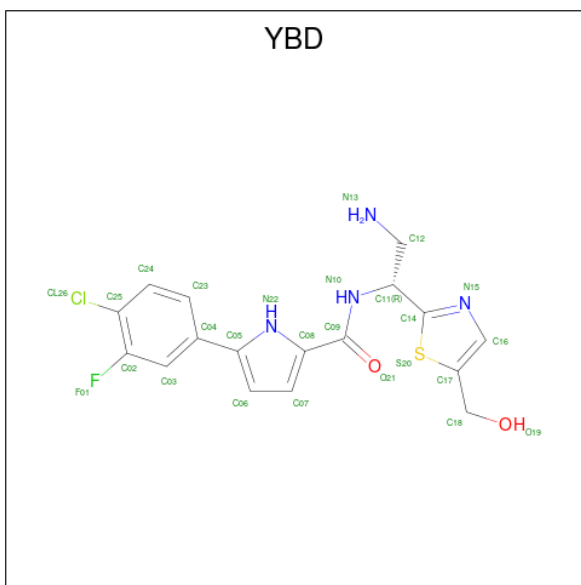
- Molecule 2 is a protein called Reverse transcriptase p51.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	412	Total	C	N	O	S	0	0	0
			3409	2220	564	618	7			

There are 2 discrepancies between the modelled and reference sequences:

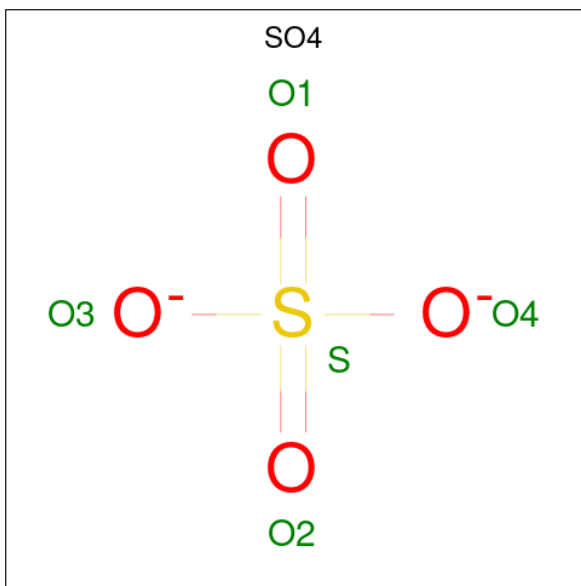
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP P03366
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is {N}-[(1 {R})-2-azanyl-1-[5-(hydroxymethyl)-1,3-thiazol-2-yl]ethyl]-5-(4-chloranyl-3-fluoranyl-phenyl)-1 {H}-pyrrole-2-carboxamide (three-letter code: YBD) (formula: C<sub>17</sub>H<sub>16</sub>ClFN<sub>4</sub>O<sub>2</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	Cl	F	N	O	S	0	0
			26	17	1	1	4	2	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula:  $\text{O}_4\text{S}$ ).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	63	Total 63	O 63	0	0
5	B	38	Total 38	O 38	0	0

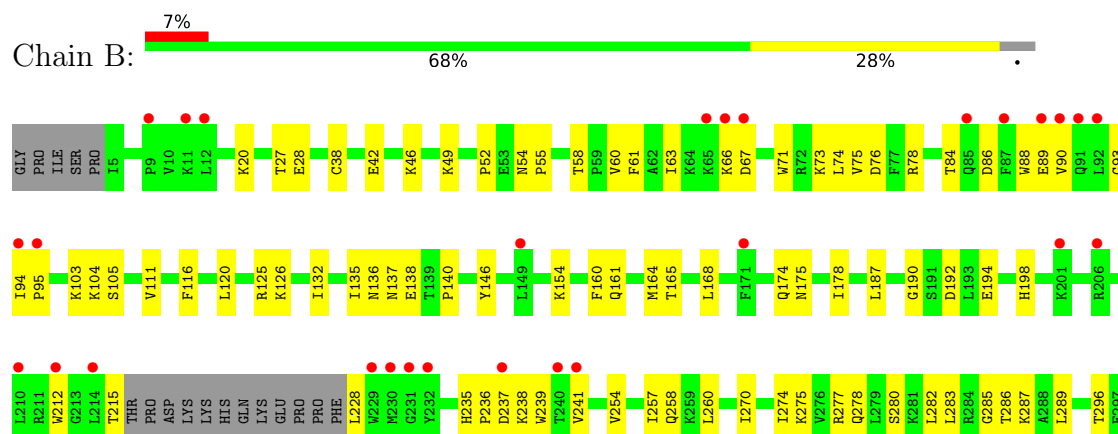
### 3 Residue-property plots [i](#)

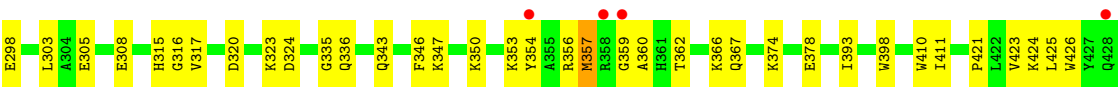
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Reverse transcriptase p66



#### • Molecule 2: Reverse transcriptase p51





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	161.68Å 73.05Å 107.29Å 90.00° 99.58° 90.00°	Depositor
Resolution (Å)	47.90 – 2.60 47.90 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.3 (47.90-2.60) 95.3 (47.90-2.60)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.53 (at 2.61Å)	Xtriage
Refinement program	PHENIX dev_3051	Depositor
R, $R_{free}$	0.248 , 0.310 0.248 , 0.310	Depositor DCC
$R_{free}$ test set	1795 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.0	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 48.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8072	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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: SO4, YBD

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	0.46	0/4643	0.60	0/6311
2	B	0.47	0/3506	0.64	0/4762
All	All	0.47	0/8149	0.62	0/11073

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	4521	0	4576	152	0
2	B	3409	0	3441	118	0
3	A	26	0	0	2	0
4	A	10	0	0	2	0
4	B	5	0	0	2	0
5	A	63	0	0	21	0
5	B	38	0	0	38	0
All	All	8072	0	8017	258	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 16.

All (258) 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:61:PHE:CZ	2:B:74:LEU:HD23	1.69	1.26
1:A:544:GLY:O	1:A:548:VAL:HG12	1.31	1.25
2:B:374:LYS:HE3	5:B:635:HOH:O	1.40	1.17
1:A:325:LEU:HG	1:A:387:PRO:HB3	1.38	1.01
2:B:95:PRO:HD2	5:B:628:HOH:O	1.60	1.01
2:B:315:HIS:HA	5:B:606:HOH:O	1.60	1.00
2:B:61:PHE:CZ	2:B:74:LEU:CD2	2.45	0.99
2:B:354:TYR:HB2	5:B:632:HOH:O	1.62	0.98
1:A:110:ASP:HB2	5:A:706:HOH:O	1.62	0.97
1:A:542:ILE:O	1:A:542:ILE:HG22	1.63	0.97
2:B:61:PHE:CE2	2:B:74:LEU:HD23	2.03	0.93
1:A:424:LYS:HB2	5:A:717:HOH:O	1.69	0.93
2:B:241:VAL:HB	5:B:629:HOH:O	1.68	0.92
1:A:137:ASN:HB2	5:A:711:HOH:O	1.71	0.91
1:A:441:TYR:CD2	1:A:544:GLY:HA3	2.05	0.91
2:B:315:HIS:HE1	5:B:633:HOH:O	1.54	0.90
1:A:116:PHE:HZ	5:A:707:HOH:O	1.58	0.87
2:B:94:ILE:HG13	2:B:161:GLN:NE2	1.89	0.87
2:B:94:ILE:HG23	5:B:628:HOH:O	1.74	0.87
1:A:441:TYR:CG	1:A:544:GLY:HA3	2.11	0.86
2:B:94:ILE:HD11	2:B:161:GLN:HG3	1.56	0.84
1:A:536:VAL:HB	1:A:542:ILE:HD13	1.59	0.84
2:B:357:MET:HE2	5:B:623:HOH:O	1.76	0.84
1:A:94:ILE:HG12	1:A:183:TYR:OH	1.77	0.84
1:A:441:TYR:HB3	1:A:544:GLY:HA3	1.60	0.83
1:A:441:TYR:CB	1:A:544:GLY:HA3	2.09	0.83
2:B:126:LYS:HB3	5:B:616:HOH:O	1.77	0.83
2:B:93:GLY:HA2	5:B:611:HOH:O	1.79	0.82
2:B:238:LYS:HE2	5:B:609:HOH:O	1.79	0.81
2:B:257:ILE:HG22	2:B:283:LEU:HD11	1.63	0.80
1:A:105:SER:HG	1:A:198:HIS:CE1	2.03	0.76
1:A:210:LEU:HD12	5:A:754:HOH:O	1.85	0.75
1:A:537:PRO:O	1:A:542:ILE:HD12	1.86	0.75
1:A:37:ILE:HD13	1:A:73:LYS:HB3	1.69	0.74
2:B:93:GLY:CA	5:B:611:HOH:O	2.36	0.73
1:A:109:LEU:HD22	1:A:217:PRO:HG2	1.72	0.72
1:A:229:TRP:HB2	3:A:601:YBD:C07	2.19	0.72
2:B:315:HIS:CE1	5:B:633:HOH:O	2.35	0.72
1:A:105:SER:OG	1:A:198:HIS:ND1	2.21	0.72
1:A:253:THR:HG22	1:A:292:VAL:HG22	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:GLN:HB3	5:A:729:HOH:O	1.91	0.70
1:A:92:LEU:HB3	5:B:625:HOH:O	1.90	0.70
1:A:203:GLU:HA	1:A:206:ARG:HD3	1.74	0.70
1:A:183:TYR:CE2	1:A:184:MET:HG2	2.26	0.70
2:B:235:HIS:HB3	2:B:238:LYS:HG2	1.73	0.70
2:B:66:LYS:NZ	2:B:67:ASP:OD2	2.24	0.68
1:A:86:ASP:HB2	5:B:604:HOH:O	1.95	0.67
2:B:282:LEU:HD21	2:B:296:THR:HG23	1.75	0.67
1:A:210:LEU:CD1	5:A:754:HOH:O	2.42	0.66
2:B:60:VAL:HG23	2:B:75:VAL:HG22	1.78	0.65
2:B:104:LYS:HA	2:B:237:ASP:HB2	1.78	0.65
2:B:354:TYR:HE1	5:B:635:HOH:O	1.79	0.65
1:A:544:GLY:O	1:A:548:VAL:CG1	2.26	0.65
1:A:210:LEU:HB2	5:A:754:HOH:O	1.97	0.64
1:A:548:VAL:CG2	5:A:734:HOH:O	2.45	0.64
1:A:90:VAL:HG11	2:B:140:PRO:HB3	1.78	0.64
1:A:441:TYR:HB3	1:A:544:GLY:CA	2.28	0.64
1:A:542:ILE:O	1:A:542:ILE:CG2	2.37	0.64
1:A:191:SER:OG	1:A:198:HIS:ND1	2.21	0.63
2:B:228:LEU:CD2	5:B:630:HOH:O	2.47	0.62
1:A:441:TYR:CB	1:A:544:GLY:CA	2.78	0.62
1:A:223:LYS:HB3	1:A:227:PHE:HE1	1.64	0.61
1:A:40:GLU:HA	1:A:43:LYS:HD2	1.82	0.61
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.00	0.61
1:A:325:LEU:CG	1:A:387:PRO:HB3	2.22	0.60
1:A:449:GLU:OE2	1:A:449:GLU:N	2.33	0.60
1:A:490:GLY:O	1:A:528:LYS:NZ	2.32	0.60
2:B:356:ARG:HG2	2:B:357:MET:H	1.65	0.60
2:B:270:ILE:HG12	2:B:346:PHE:HB3	1.83	0.59
1:A:542:ILE:HG23	2:B:283:LEU:HD23	1.85	0.59
1:A:551:LEU:HG	5:A:710:HOH:O	2.02	0.59
2:B:46:LYS:HE2	2:B:116:PHE:HB3	1.85	0.59
2:B:238:LYS:CD	5:B:609:HOH:O	2.50	0.58
1:A:56:TYR:O	1:A:143:ARG:NH2	2.30	0.58
2:B:95:PRO:CD	5:B:628:HOH:O	2.33	0.58
2:B:94:ILE:CG1	2:B:161:GLN:NE2	2.65	0.58
1:A:266:TRP:O	1:A:269:GLN:HG2	2.03	0.58
2:B:154:LYS:CD	5:B:613:HOH:O	2.51	0.58
2:B:136:ASN:HB2	5:B:610:HOH:O	2.05	0.57
2:B:360:ALA:HB2	5:B:608:HOH:O	2.03	0.57
1:A:277:ARG:HH12	1:A:356:ARG:NH2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:94:ILE:CD1	2:B:161:GLN:HG3	2.33	0.57
2:B:350:LYS:HE3	2:B:378:GLU:OE1	2.05	0.56
1:A:388:LYS:HE3	5:A:740:HOH:O	2.05	0.56
2:B:354:TYR:CB	5:B:632:HOH:O	2.37	0.56
1:A:543:GLY:HA3	2:B:285:GLY:O	2.05	0.56
2:B:360:ALA:HB1	2:B:367:GLN:NE2	2.21	0.56
1:A:183:TYR:CD2	1:A:184:MET:HG2	2.41	0.56
1:A:552:VAL:CG1	5:A:734:HOH:O	2.52	0.55
2:B:354:TYR:CA	5:B:632:HOH:O	2.53	0.55
2:B:89:GLU:HG3	2:B:90:VAL:H	1.72	0.55
2:B:86:ASP:OD1	2:B:154:LYS:NZ	2.36	0.55
1:A:116:PHE:CZ	5:A:707:HOH:O	2.43	0.55
1:A:356:ARG:HD3	1:A:367:GLN:NE2	2.22	0.55
1:A:404:GLU:OE2	1:A:431:LYS:NZ	2.32	0.55
2:B:421:PRO:HB2	2:B:423:VAL:HG12	1.87	0.55
1:A:516:GLU:O	1:A:520:GLN:HG3	2.07	0.55
1:A:257:ILE:HB	1:A:283:LEU:HD21	1.89	0.54
2:B:393:ILE:HD13	2:B:398:TRP:HB2	1.89	0.54
1:A:325:LEU:HG	1:A:387:PRO:CB	2.26	0.54
1:A:543:GLY:O	1:A:544:GLY:C	2.46	0.54
1:A:50:ILE:CG1	1:A:143:ARG:HB3	2.38	0.53
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.89	0.53
1:A:24:TRP:HE3	1:A:25:PRO:HD2	1.73	0.53
1:A:57:ASN:OD1	1:A:143:ARG:NH1	2.42	0.53
2:B:73:LYS:NZ	2:B:146:TYR:OH	2.42	0.53
1:A:7:THR:HG21	1:A:121:ASP:HA	1.91	0.53
1:A:17:ASP:O	1:A:83:ARG:HD3	2.09	0.52
1:A:543:GLY:HA3	2:B:283:LEU:O	2.09	0.52
1:A:324:ASP:O	1:A:343:GLN:HG2	2.10	0.52
1:A:441:TYR:CG	1:A:544:GLY:CA	2.89	0.52
2:B:324:ASP:O	2:B:343:GLN:HG2	2.09	0.52
2:B:320:ASP:OD2	2:B:323:LYS:HG3	2.10	0.52
1:A:223:LYS:HB3	1:A:227:PHE:CE1	2.44	0.52
1:A:548:VAL:HA	1:A:551:LEU:HB2	1.92	0.52
2:B:20:LYS:HE2	2:B:55:PRO:HB2	1.91	0.52
1:A:167:ILE:HD13	1:A:214:LEU:HD11	1.90	0.52
1:A:458:VAL:CG2	2:B:286:THR:HG21	2.40	0.52
2:B:94:ILE:CG2	5:B:628:HOH:O	2.47	0.52
1:A:547:GLN:NE2	5:A:708:HOH:O	2.41	0.51
2:B:136:ASN:HB3	2:B:138:GLU:HG3	1.92	0.51
1:A:252:TRP:CH2	1:A:260:LEU:HD22	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:SER:HB3	1:A:274:ILE:HB	1.92	0.51
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.93	0.51
1:A:238:LYS:HD2	1:A:315:HIS:CG	2.45	0.51
1:A:177:ASP:OD2	1:A:201:LYS:NZ	2.37	0.51
1:A:39:THR:HG22	1:A:43:LYS:HE3	1.93	0.51
2:B:61:PHE:HZ	2:B:74:LEU:CD2	2.17	0.51
2:B:360:ALA:O	2:B:362:THR:N	2.38	0.51
1:A:376:THR:O	1:A:380:ILE:HG12	2.10	0.51
1:A:254:VAL:HG23	1:A:291:GLU:O	2.11	0.51
1:A:199:ARG:O	1:A:203:GLU:HG2	2.11	0.51
1:A:207:GLN:HA	1:A:210:LEU:HD12	1.93	0.51
1:A:325:LEU:HD11	1:A:341:ILE:CG2	2.41	0.51
1:A:541:GLY:HA2	1:A:546:GLU:HB2	1.92	0.51
1:A:57:ASN:OD1	1:A:131:THR:OG1	2.23	0.50
1:A:458:VAL:HG23	2:B:286:THR:HG21	1.93	0.50
1:A:23:GLN:HG2	1:A:133:PRO:HD3	1.93	0.50
1:A:540:LYS:HB2	1:A:542:ILE:HG13	1.92	0.50
1:A:7:THR:CG2	1:A:121:ASP:HA	2.41	0.50
1:A:219:LYS:HG2	1:A:220:LYS:H	1.77	0.50
1:A:267:ALA:HB1	1:A:310:LEU:HD21	1.94	0.50
1:A:540:LYS:O	1:A:541:GLY:C	2.50	0.50
2:B:275:LYS:HD2	4:B:501:SO4:O4	2.12	0.50
1:A:115:TYR:OH	1:A:150:PRO:O	2.30	0.49
2:B:194:GLU:O	2:B:198:HIS:N	2.44	0.49
1:A:159:ILE:O	1:A:163:SER:OG	2.24	0.49
1:A:171:PHE:CD2	1:A:205:LEU:HD13	2.48	0.49
1:A:385:LYS:NZ	5:A:705:HOH:O	2.35	0.49
2:B:423:VAL:HA	2:B:426:TRP:CD1	2.47	0.49
2:B:335:GLY:HA3	2:B:356:ARG:HD3	1.94	0.48
1:A:203:GLU:HA	1:A:206:ARG:HH11	1.77	0.48
1:A:114:ALA:HA	5:A:726:HOH:O	2.14	0.48
2:B:237:ASP:C	5:B:609:HOH:O	2.51	0.48
2:B:354:TYR:CD1	2:B:374:LYS:HD2	2.48	0.48
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.53	0.48
1:A:379:SER:CB	1:A:387:PRO:HD3	2.44	0.47
2:B:174:GLN:HG3	2:B:175:ASN:OD1	2.14	0.47
2:B:359:GLY:HA3	2:B:366:LYS:NZ	2.29	0.47
1:A:441:TYR:CD2	1:A:544:GLY:CA	2.88	0.47
2:B:239:TRP:CZ3	2:B:350:LYS:HE2	2.49	0.47
1:A:50:ILE:HG12	1:A:143:ARG:HB3	1.96	0.47
2:B:86:ASP:HB3	2:B:88:TRP:CZ2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.55	0.47
1:A:356:ARG:HG2	1:A:357:MET:O	2.15	0.47
1:A:380:ILE:HD12	2:B:27:THR:HG22	1.97	0.47
1:A:443:ASP:HB2	1:A:548:VAL:HG13	1.97	0.47
1:A:551:LEU:N	5:A:710:HOH:O	2.47	0.47
2:B:154:LYS:HD3	5:B:613:HOH:O	2.13	0.46
1:A:547:GLN:CB	5:A:729:HOH:O	2.53	0.46
2:B:94:ILE:HD11	2:B:161:GLN:CG	2.38	0.46
1:A:443:ASP:OD1	1:A:444:GLY:N	2.44	0.46
2:B:94:ILE:HG13	2:B:161:GLN:CD	2.34	0.46
2:B:238:LYS:HD3	5:B:609:HOH:O	2.14	0.46
2:B:354:TYR:HA	5:B:632:HOH:O	2.14	0.46
1:A:35:VAL:HG22	1:A:132:ILE:HG21	1.98	0.46
1:A:447:ASN:O	1:A:451:LYS:N	2.48	0.46
2:B:317:VAL:HG22	2:B:347:LYS:HD2	1.98	0.46
1:A:105:SER:HG	1:A:198:HIS:CG	2.26	0.45
1:A:447:ASN:OD1	1:A:450:THR:HG23	2.16	0.45
1:A:419:THR:HA	1:A:420:PRO:HD3	1.72	0.45
1:A:537:PRO:O	1:A:542:ILE:CD1	2.60	0.45
1:A:424:LYS:HD3	1:A:426:TRP:CH2	2.51	0.45
1:A:544:GLY:HA2	2:B:286:THR:HG22	1.98	0.45
2:B:76:ASP:OD2	2:B:78:ARG:NH2	2.47	0.45
1:A:229:TRP:CB	3:A:601:YBD:C07	2.92	0.45
2:B:103:LYS:O	2:B:236:PRO:HG2	2.16	0.45
2:B:278:GLN:HG3	2:B:298:GLU:HB3	1.97	0.45
1:A:252:TRP:CE3	1:A:256:ASP:HB3	2.52	0.45
1:A:405:TYR:CE2	1:A:407:GLN:HB2	2.52	0.45
1:A:92:LEU:CG	5:B:625:HOH:O	2.64	0.45
1:A:93:GLY:HA3	2:B:137:ASN:CG	2.37	0.45
1:A:113:ASP:O	1:A:115:TYR:N	2.50	0.45
1:A:543:GLY:CA	2:B:285:GLY:O	2.65	0.45
1:A:115:TYR:CE2	1:A:156:SER:HB3	2.52	0.44
1:A:427:TYR:HB2	4:A:602:SO4:O3	2.18	0.44
2:B:228:LEU:HD21	5:B:630:HOH:O	2.16	0.44
1:A:228:LEU:HD22	1:A:233:GLU:CG	2.48	0.44
1:A:228:LEU:HD22	1:A:233:GLU:HG2	1.99	0.44
1:A:277:ARG:HH12	1:A:356:ARG:HH21	1.65	0.44
2:B:237:ASP:CB	5:B:609:HOH:O	2.65	0.44
2:B:336:GLN:HB3	2:B:353:LYS:NZ	2.33	0.44
1:A:269:GLN:HA	1:A:351:THR:O	2.18	0.44
2:B:28:GLU:HB2	2:B:135:ILE:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:THR:HB	2:B:154:LYS:HE2	1.99	0.44
2:B:277:ARG:N	4:B:501:SO4:O2	2.51	0.44
1:A:101:LYS:HE2	1:A:101:LYS:H	1.82	0.43
2:B:274:ILE:O	2:B:275:LYS:HD3	2.17	0.43
1:A:548:VAL:HG22	5:A:734:HOH:O	2.16	0.43
2:B:160:PHE:HD2	2:B:164:MET:HB2	1.83	0.43
2:B:236:PRO:HA	2:B:239:TRP:NE1	2.33	0.43
1:A:257:ILE:O	1:A:261:VAL:HG23	2.18	0.43
1:A:130:PHE:CE1	1:A:144:TYR:HB3	2.53	0.43
2:B:212:TRP:O	2:B:215:THR:HG22	2.19	0.43
2:B:257:ILE:CG2	2:B:283:LEU:HD11	2.41	0.43
1:A:88:TRP:HB3	2:B:52:PRO:HA	2.01	0.43
2:B:238:LYS:CE	5:B:609:HOH:O	2.47	0.43
2:B:254:VAL:O	2:B:258:GLN:HG3	2.18	0.43
1:A:149:LEU:HA	1:A:150:PRO:HD3	1.88	0.43
2:B:42:GLU:OE2	2:B:49:LYS:HG2	2.19	0.43
2:B:282:LEU:CD2	2:B:296:THR:HG23	2.44	0.43
2:B:236:PRO:HA	2:B:239:TRP:CE2	2.55	0.42
2:B:238:LYS:N	5:B:609:HOH:O	2.51	0.42
2:B:289:LEU:HD23	2:B:289:LEU:HA	1.81	0.42
1:A:122:GLU:OE1	1:A:125:ARG:HD2	2.20	0.42
1:A:311:LYS:HG3	1:A:312:GLU:N	2.35	0.42
1:A:369:THR:O	1:A:373[B]:GLN:HG2	2.20	0.42
1:A:122:GLU:HA	1:A:125:ARG:HG3	2.02	0.42
1:A:88:TRP:HB2	2:B:54:ASN:O	2.20	0.42
2:B:410:TRP:O	2:B:411:ILE:HG13	2.20	0.42
1:A:209:LEU:HB3	1:A:214:LEU:HB2	2.02	0.42
2:B:305:GLU:O	2:B:308:GLU:HB2	2.19	0.42
2:B:63:ILE:O	2:B:71:TRP:HA	2.20	0.42
1:A:547:GLN:C	5:A:710:HOH:O	2.58	0.42
2:B:175:ASN:HB3	2:B:178:ILE:HG12	2.02	0.41
1:A:92:LEU:CB	5:B:625:HOH:O	2.61	0.41
1:A:210:LEU:CB	5:A:754:HOH:O	2.64	0.41
2:B:136:ASN:ND2	5:B:610:HOH:O	2.51	0.41
1:A:42:GLU:OE2	1:A:49:LYS:HG3	2.20	0.41
1:A:233:GLU:O	1:A:239:TRP:HA	2.20	0.41
2:B:258:GLN:HG2	2:B:283:LEU:CD2	2.50	0.41
2:B:260:LEU:HD21	2:B:303:LEU:HD13	2.02	0.41
2:B:316:GLY:N	5:B:606:HOH:O	2.45	0.41
1:A:50:ILE:HG13	1:A:143:ARG:HB3	2.02	0.41
2:B:136:ASN:CB	5:B:610:HOH:O	2.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:MET:O	1:A:359:GLY:N	2.51	0.41
1:A:452:LEU:HD23	1:A:470:THR:HA	2.03	0.41
1:A:457:TYR:HE1	1:A:463:ARG:HG2	1.84	0.41
2:B:104:LYS:HB2	2:B:192:ASP:HA	2.02	0.41
2:B:165:THR:O	2:B:168:LEU:N	2.50	0.41
2:B:424:LYS:HG2	2:B:425:LEU:HD23	2.02	0.41
1:A:233:GLU:HG3	1:A:242:GLN:HA	2.02	0.41
2:B:61:PHE:CZ	2:B:74:LEU:HD21	2.49	0.41
2:B:105:SER:O	2:B:190:GLY:HA2	2.21	0.41
2:B:120:LEU:HD23	2:B:125:ARG:HG2	2.02	0.41
1:A:116:PHE:CZ	1:A:151:GLN:HG2	2.57	0.40
1:A:282:LEU:HD21	1:A:296:THR:HG23	2.02	0.40
1:A:512:LYS:NZ	4:A:603:SO4:O3	2.44	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	555/557 (100%)	506 (91%)	49 (9%)	0	100	100
2	B	408/429 (95%)	374 (92%)	34 (8%)	0	100	100
All	All	963/986 (98%)	880 (91%)	83 (9%)	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	496/495 (100%)	490 (99%)	6 (1%)	71	87
2	B	374/390 (96%)	370 (99%)	4 (1%)	73	88
All	All	870/885 (98%)	860 (99%)	10 (1%)	76	88

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	350	LYS
1	A	363	ASN
1	A	373[A]	GLN
1	A	373[B]	GLN
1	A	399	GLU
2	B	58	THR
2	B	280	SER
2	B	287	LYS
2	B	357	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	340	GLN
2	B	161	GLN
2	B	258	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

4 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	$\# Z  > 2$
4	SO4	A	603	-	4,4,4	0.33	0	6,6,6	0.05	0
3	YBD	A	601	-	25,28,28	2.59	8 (32%)	22,39,39	1.44	3 (13%)
4	SO4	A	602	-	4,4,4	0.32	0	6,6,6	0.05	0
4	SO4	B	501	-	4,4,4	0.32	0	6,6,6	0.05	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	YBD	A	601	-	-	2/10/20/20	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	YBD	C16-N15	7.49	1.47	1.36
3	A	601	YBD	C17-S20	-6.27	1.60	1.73
3	A	601	YBD	C09-N10	5.24	1.45	1.34
3	A	601	YBD	C14-S20	-3.34	1.63	1.73
3	A	601	YBD	C04-C05	2.71	1.53	1.48
3	A	601	YBD	C18-C17	2.25	1.53	1.50
3	A	601	YBD	C25-CL26	2.23	1.78	1.73
3	A	601	YBD	O21-C09	-2.12	1.19	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	YBD	C04-C05-N22	3.11	126.00	120.78
3	A	601	YBD	C06-C05-C04	-2.64	126.31	128.77
3	A	601	YBD	C08-C09-N10	2.52	119.88	115.20

There are no chirality outliers.

All (2) torsion outliers are listed below:

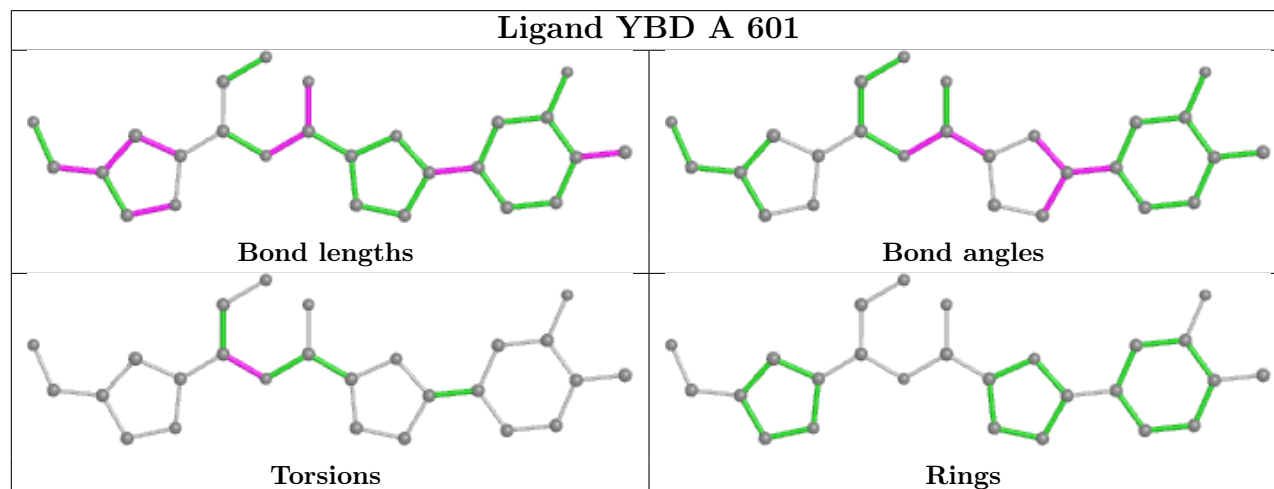
Mol	Chain	Res	Type	Atoms
3	A	601	YBD	C12-C11-N10-C09
3	A	601	YBD	C14-C11-N10-C09

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	603	SO4	1	0
3	A	601	YBD	2	0
4	A	602	SO4	1	0
4	B	501	SO4	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%)	0.91	90 (16%) ⓘ ⓘ	43, 95, 130, 145	0
2	B	412/429 (96%)	0.50	32 (7%) ⓘ ⓘ	41, 78, 116, 140	0
All	All	968/986 (98%)	0.74	122 (12%) ⓘ ⓘ	41, 85, 128, 145	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	553	SER	9.5
2	B	230	MET	8.7
1	A	288	ALA	8.4
1	A	552	VAL	8.2
2	B	89	GLU	7.6
1	A	289	LEU	7.6
1	A	551	LEU	6.7
1	A	279	LEU	6.6
2	B	90	VAL	6.6
1	A	294	PRO	6.4
1	A	227	PHE	6.2
1	A	92	LEU	6.2
2	B	232	TYR	6.1
1	A	293	ILE	6.0
1	A	282	LEU	5.8
1	A	554	ALA	5.7
1	A	295	LEU	5.6
1	A	303	LEU	5.5
1	A	246	LEU	5.4
1	A	91	GLN	5.4
1	A	218	ASP	5.4
1	A	296	THR	5.2
1	A	544	GLY	5.1
1	A	254	VAL	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	292	VAL	4.9
1	A	548	VAL	4.7
1	A	251	SER	4.7
1	A	550	LYS	4.6
1	A	299	ALA	4.6
1	A	300	GLU	4.6
1	A	304	ALA	4.6
2	B	358	ARG	4.6
1	A	221	HIS	4.6
1	A	310	LEU	4.6
1	A	90	VAL	4.5
1	A	214	LEU	4.4
1	A	283	LEU	4.3
2	B	67	ASP	4.3
1	A	252	TRP	4.2
1	A	546	GLU	4.1
2	B	214	LEU	4.1
2	B	359	GLY	3.9
2	B	237	ASP	3.9
1	A	195	ILE	3.9
1	A	248	GLU	3.8
1	A	250	ASP	3.8
2	B	12	LEU	3.8
2	B	241	VAL	3.8
1	A	286	THR	3.8
2	B	212	TRP	3.8
1	A	298	GLU	3.7
1	A	187	LEU	3.7
1	A	216	THR	3.6
1	A	549	ASP	3.6
1	A	222	GLN	3.6
1	A	290	THR	3.6
2	B	229	TRP	3.5
1	A	287	LYS	3.4
1	A	302	GLU	3.4
2	B	91	GLN	3.3
1	A	309	ILE	3.3
1	A	253	THR	3.2
1	A	184	MET	3.2
1	A	278	GLN	3.2
2	B	85	GLN	3.2
2	B	149	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	297	GLU	3.1
1	A	17	ASP	3.1
2	B	231	GLY	3.1
1	A	257	ILE	3.1
2	B	92	LEU	3.0
1	A	285	GLY	3.0
1	A	306	ASN	3.0
1	A	224	GLU	3.0
1	A	2	ILE	2.9
1	A	291	GLU	2.9
1	A	255	ASN	2.9
2	B	66	LYS	2.8
1	A	14	PRO	2.8
1	A	196	GLY	2.8
2	B	94	ILE	2.8
2	B	206	ARG	2.8
1	A	249	LYS	2.8
1	A	247	PRO	2.7
1	A	271	TYR	2.7
1	A	245	VAL	2.7
1	A	202	ILE	2.7
2	B	201	LYS	2.7
1	A	12	LEU	2.7
2	B	210	LEU	2.6
1	A	61	PHE	2.6
1	A	72	ARG	2.5
1	A	115	TYR	2.5
2	B	65	LYS	2.5
1	A	209	LEU	2.5
1	A	180	ILE	2.5
1	A	261	VAL	2.5
1	A	545	ASN	2.5
1	A	325	LEU	2.4
1	A	311	LYS	2.4
1	A	140	PRO	2.4
2	B	171	PHE	2.4
1	A	547	GLN	2.4
1	A	264	LEU	2.4
2	B	354	TYR	2.4
1	A	102	LYS	2.3
2	B	95	PRO	2.3
2	B	428	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	217	PRO	2.2
2	B	240	THR	2.2
1	A	67	ASP	2.2
1	A	308	GLU	2.2
1	A	313	PRO	2.2
1	A	315	HIS	2.1
2	B	87	PHE	2.1
2	B	9	PRO	2.1
1	A	205	LEU	2.1
1	A	189	VAL	2.1
1	A	281	LYS	2.1
1	A	100	LEU	2.0
2	B	11	LYS	2.0
1	A	277	ARG	2.0

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

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

## 6.3 Carbohydrates [i](#)

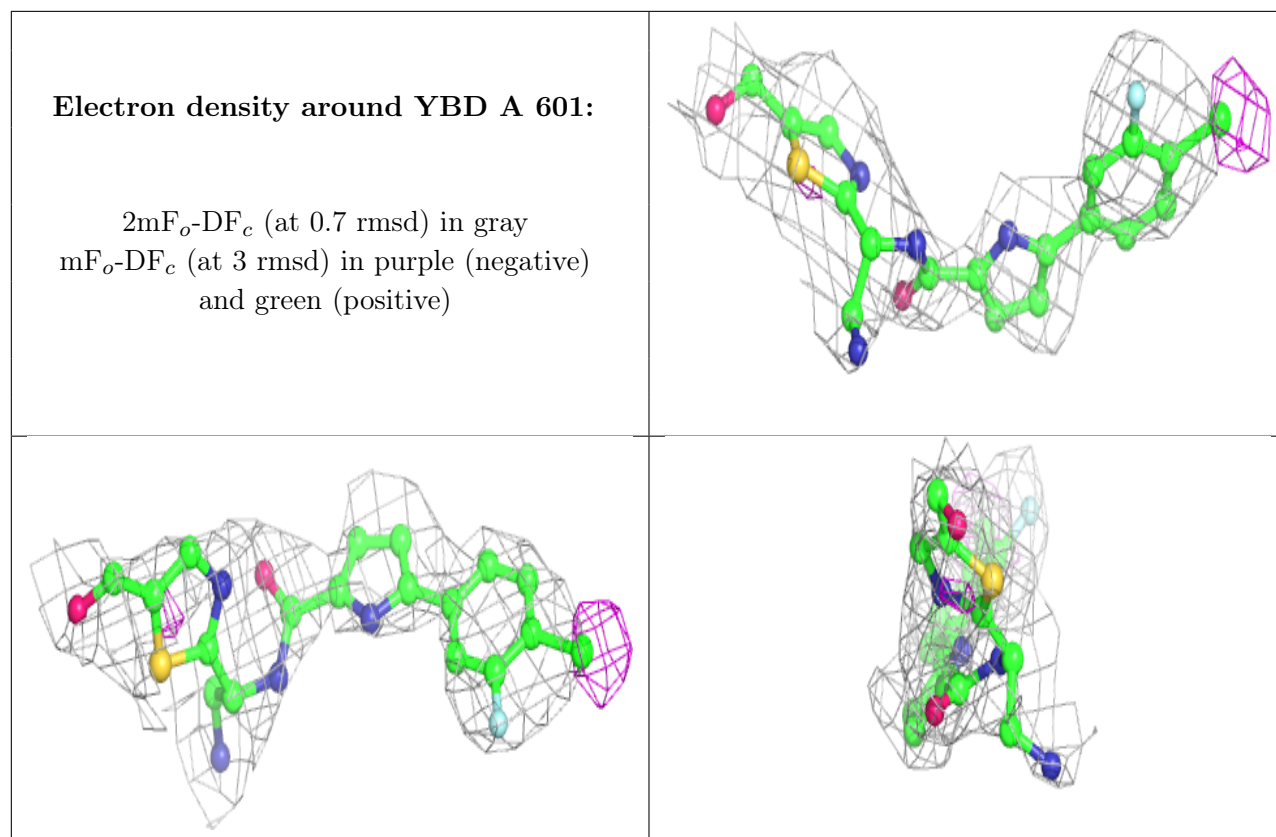
There are no monosaccharides in this entry.

## 6.4 Ligands [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( $\text{\AA}^2$ )	Q<0.9
3	YBD	A	601	26/26	0.75	0.31	97,107,111,114	0
4	SO4	B	501	5/5	0.83	0.38	94,95,97,99	0
4	SO4	A	603	5/5	0.89	0.16	96,98,99,99	0
4	SO4	A	602	5/5	0.95	0.32	91,92,92,93	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.