



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 27, 2016 – 05:11 PM EDT

PDB ID : 5TF5  
Title : CRYSTAL STRUCTURE OF HUMAN KAT-2 IN COMPLEX WITH A REVERSIBLE INHIBITOR  
Authors : Nematollahi, A.; Sun, G.; Church, W.B.  
Deposited on : 2016-09-24  
Resolution : 1.81 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

<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027939

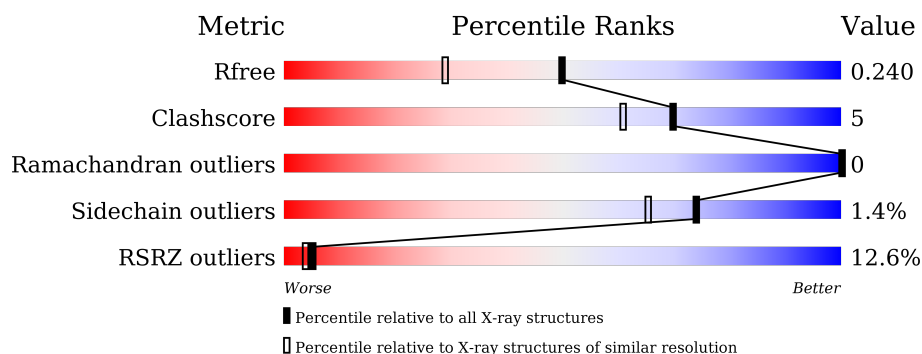
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.81 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))
$R_{free}$	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	425	<div> <div>14%</div> <div> <div></div> <div>91%</div> <div>8%</div> </div> </div>
1	B	425	<div> <div>12%</div> <div> <div></div> <div>92%</div> <div>7%</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
1	LLP	B	263	-	-	X	-
2	7AR	B	501	-	-	X	X

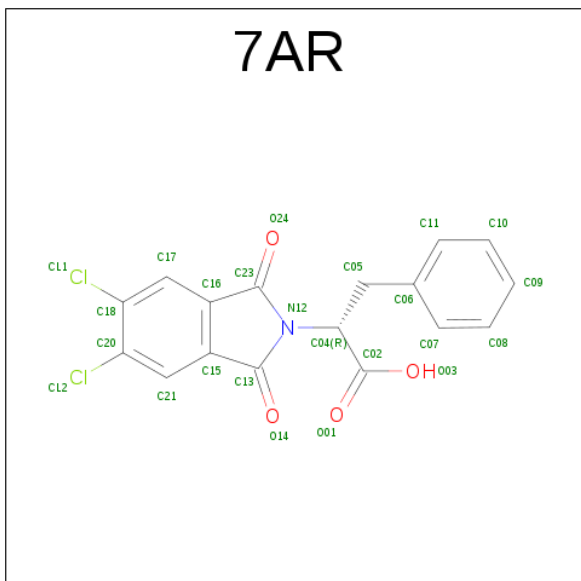
i

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 Kynurenine/alpha-aminoadipate aminotransferase, mitochondrial.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	425	Total 6687	C 2147	H 3340	N 560	O 621	P 1	S 18	0	0	0
1	B	425	Total 6687	C 2147	H 3340	N 560	O 621	P 1	S 18	0	0	0

- Molecule 2 is (2R)-2-(5,6-dichloro-1,3-dioxo-1,3-dihydro-2H-isoindol-2-yl)-3-phenylpropanoic acid (three-letter code: 7AR) (formula:  $C_{17}H_{11}Cl_2NO_4$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Cl	N	O	0	0
			24	17	2	1	4		

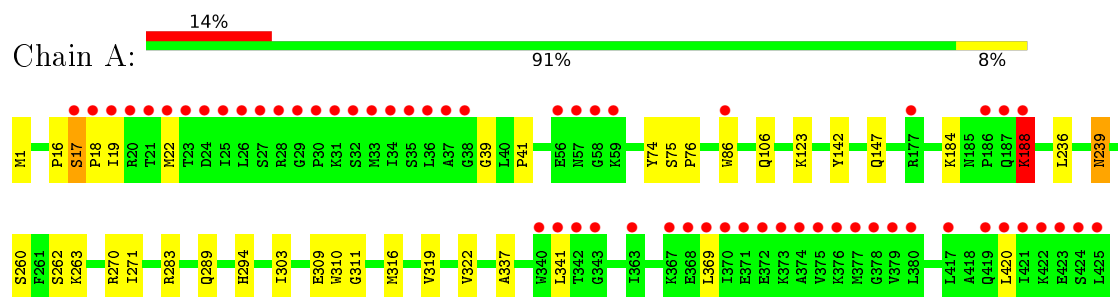
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	326	Total 326	O 326	0	0
3	B	356	Total 356	O 356	0	0

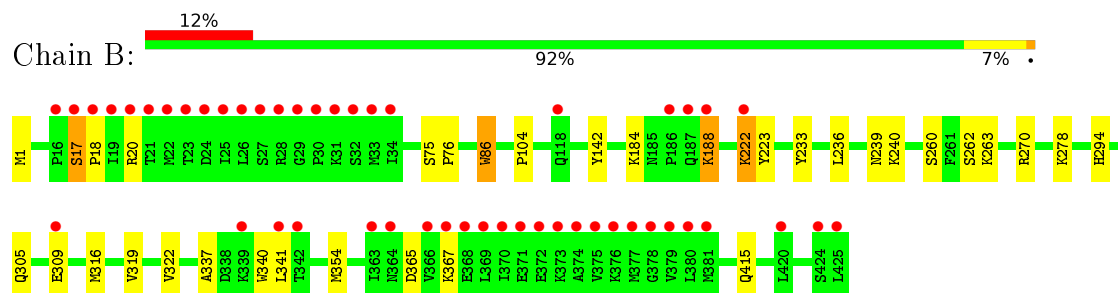
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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: Kynurenine/alpha-aminoadipate aminotransferase, mitochondrial



- Molecule 1: Kynurenine/alpha-aminoadipate aminotransferase, mitochondrial



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.88Å 99.28Å 107.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.13 – 1.81 47.41 – 1.81	Depositor EDS
% Data completeness (in resolution range)	98.3 (46.13-1.81) 89.6 (47.41-1.81)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.43 (at 1.81Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, $R_{free}$	0.219 , 0.245 0.215 , 0.240	Depositor DCC
$R_{free}$ test set	1799 reflections (2.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	16.2	Xtriage
Anisotropy	0.673	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 47.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	14080	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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: LLP, 7AR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.32	0/3404	0.49	0/4620
1	B	0.34	0/3404	0.52	1/4620 (0.0%)
All	All	0.33	0/6808	0.51	1/9240 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	222	LYS	CD-CE-NZ	5.54	124.45	111.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	17	SER	Peptide
1	A	188	LYS	Peptide
1	B	17	SER	Peptide
1	B	188	LYS	Peptide



## 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	3347	3340	3358	27	1
1	B	3347	3340	3358	36	1
2	B	24	0	0	20	0
3	A	326	0	0	2	4
3	B	356	0	0	1	4
All	All	7400	6680	6716	61	5

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (61) 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:B:263:LLP:H4'1	2:B:501:7AR:C04	1.79	1.12
1:B:263:LLP:NZ	2:B:501:7AR:C06	2.53	0.72
1:B:263:LLP:NZ	2:B:501:7AR:C11	2.58	0.67
1:B:263:LLP:C4'	2:B:501:7AR:C07	2.75	0.65
1:B:263:LLP:C4'	2:B:501:7AR:C06	2.77	0.63
1:B:263:LLP:H4'1	2:B:501:7AR:C07	2.29	0.63
1:B:260:SER:HG	1:B:262:SER:HG	1.48	0.61
1:B:263:LLP:HD3	2:B:501:7AR:C10	2.31	0.61
1:A:294:HIS:CE1	1:B:270:ARG:HD3	2.38	0.58
1:A:239:ASN:OD1	1:A:239:ASN:N	2.35	0.58
1:A:39:GLY:O	2:B:501:7AR:C06	2.52	0.57
1:A:16:PRO:O	3:A:501:HOH:O	2.17	0.56
1:A:270:ARG:HD3	1:B:294:HIS:CE1	2.42	0.55
1:B:263:LLP:H4'1	2:B:501:7AR:C06	2.38	0.54
1:A:17:SER:HB3	1:A:18:PRO:CD	2.37	0.54
1:B:17:SER:HB3	1:B:18:PRO:HD3	1.90	0.53
1:B:263:LLP:C4'	2:B:501:7AR:C04	2.70	0.53
1:A:19:ILE:HG12	2:B:501:7AR:O24	2.10	0.52
1:B:236:LEU:HD21	1:B:322:VAL:HG12	1.93	0.51
1:B:142:TYR:CE2	2:B:501:7AR:O14	2.64	0.51
1:B:354:MET:SD	2:B:501:7AR:C10	3.00	0.49
1:B:17:SER:HB3	1:B:18:PRO:CD	2.42	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:SER:HG	1:A:262:SER:HG	1.61	0.49
1:A:142:TYR:HB2	1:A:263:LLP:H2'3	1.95	0.49
1:B:86:TRP:CD1	1:B:86:TRP:C	2.86	0.48
1:A:337:ALA:HA	1:A:341:LEU:HD23	1.95	0.48
1:A:147:GLN:OE1	3:A:502:HOH:O	2.20	0.47
1:A:316:MET:O	1:A:319:VAL:HG22	2.14	0.47
1:A:39:GLY:O	2:B:501:7AR:C11	2.62	0.47
1:A:86:TRP:HH2	1:A:311:GLY:C	2.18	0.47
1:B:142:TYR:HB2	1:B:263:LLP:H2'3	1.96	0.47
1:B:233:TYR:OH	2:B:501:7AR:C08	2.63	0.47
1:A:41:PRO:HD3	2:B:501:7AR:C11	2.45	0.46
1:B:316:MET:O	1:B:319:VAL:HG22	2.16	0.46
1:B:365:ASP:OD1	1:B:367:LYS:HG2	2.16	0.45
1:A:86:TRP:CD1	1:A:86:TRP:C	2.89	0.45
1:B:104:PRO:HB3	1:B:278:LYS:HD3	1.98	0.45
1:A:17:SER:HB3	1:A:18:PRO:HD3	1.98	0.45
1:B:260:SER:OG	1:B:263:LLP:OP1	2.28	0.45
1:B:305:GLN:O	1:B:309:GLU:HG2	2.18	0.44
1:B:222:LYS:HD3	1:B:223:TYR:CE2	2.52	0.44
1:A:236:LEU:HD21	1:A:322:VAL:HG12	2.00	0.44
1:B:270:ARG:NH2	3:B:614:HOH:O	2.49	0.44
1:A:271:ILE:HG13	1:A:303:ILE:HD12	1.98	0.44
1:A:309:GLU:HG3	1:A:310:TRP:N	2.34	0.43
1:A:75:SER:HB2	1:A:76:PRO:CD	2.48	0.43
1:B:340:TRP:CE2	1:B:415:GLN:HG3	2.54	0.43
1:B:17:SER:C	1:B:20:ARG:HE	2.22	0.42
1:B:263:LLP:H4'1	2:B:501:7AR:C05	2.45	0.42
1:A:22:MET:HE3	2:B:501:7AR:CL1	2.56	0.42
1:A:283:ARG:N	1:A:283:ARG:HD2	2.35	0.42
1:B:75:SER:HB2	1:B:76:PRO:CD	2.49	0.42
1:B:340:TRP:CZ2	1:B:415:GLN:CG	3.02	0.42
1:B:354:MET:SD	2:B:501:7AR:C09	3.08	0.41
1:A:17:SER:HB2	1:A:289:GLN:HB3	2.03	0.41
1:A:188:LYS:CG	1:A:188:LYS:O	2.69	0.41
1:B:17:SER:CB	1:B:18:PRO:CD	2.99	0.41
1:A:74:TYR:CE2	2:B:501:7AR:C05	3.03	0.40
1:B:337:ALA:HA	1:B:341:LEU:HD23	2.02	0.40
1:B:340:TRP:CZ2	1:B:415:GLN:HG3	2.56	0.40
1:A:369:LEU:HD11	1:A:420:LEU:HB3	2.02	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:786:HOH:O	3:B:922:HOH:O[1_655]	2.00	0.20
3:A:738:HOH:O	3:B:920:HOH:O[3_745]	2.04	0.16
1:A:106:GLN:OE1	1:B:240:LYS:HZ2[2_655]	1.48	0.12
3:A:531:HOH:O	3:B:879:HOH:O[3_745]	2.09	0.11
3:A:810:HOH:O	3:B:951:HOH:O[2_655]	2.15	0.05

## 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	422/425 (99%)	404 (96%)	18 (4%)	0	100	100
1	B	422/425 (99%)	400 (95%)	22 (5%)	0	100	100
All	All	844/850 (99%)	804 (95%)	40 (5%)	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	369/369 (100%)	364 (99%)	5 (1%)	74	65
1	B	369/369 (100%)	364 (99%)	5 (1%)	74	65
All	All	738/738 (100%)	728 (99%)	10 (1%)	74	65

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

Mol	Chain	Res	Type
1	A	1	MET
1	A	123	LYS
1	A	184	LYS
1	A	188	LYS
1	A	239	ASN
1	B	1	MET
1	B	86	TRP
1	B	184	LYS
1	B	188	LYS
1	B	239	ASN

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	LLP	A	263	1	22,24,25	4.97	7 (31%)	28,32,34	2.12	7 (25%)
1	LLP	B	263	1	22,24,25	5.09	8 (36%)	28,32,34	2.04	7 (25%)

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
1	LLP	A	263	1	-	1/15/17/19	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	B	263	1	-	1/15/17/19	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	263	LLP	C6-N1	2.06	1.38	1.34
1	B	263	LLP	C6-C5	2.45	1.42	1.37
1	A	263	LLP	C6-C5	2.53	1.43	1.37
1	A	263	LLP	C2-N1	2.82	1.39	1.33
1	B	263	LLP	C2-N1	2.90	1.39	1.33
1	B	263	LLP	C4-C4'	4.60	1.54	1.46
1	A	263	LLP	C4-C4'	5.52	1.56	1.46
1	B	263	LLP	C4-C5	7.84	1.52	1.42
1	A	263	LLP	C4-C5	8.28	1.52	1.42
1	A	263	LLP	C4-C3	9.40	1.53	1.40
1	A	263	LLP	C4'-NZ	9.49	1.55	1.27
1	B	263	LLP	C4'-NZ	9.52	1.55	1.27
1	B	263	LLP	C4-C3	9.84	1.53	1.40
1	A	263	LLP	C3-C2	15.47	1.51	1.40
1	B	263	LLP	C3-C2	16.36	1.52	1.40

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	263	LLP	C3-C4-C5	-5.85	114.02	118.26
1	B	263	LLP	C3-C4-C5	-5.57	114.22	118.26
1	A	263	LLP	C2'-C2-C3	-3.12	117.74	120.90
1	B	263	LLP	C2'-C2-C3	-2.72	118.15	120.90
1	A	263	LLP	O-C-CA	-2.50	119.02	125.72
1	B	263	LLP	O-C-CA	-2.15	119.94	125.72
1	A	263	LLP	C2'-C2-N1	2.02	122.41	117.96
1	B	263	LLP	C2'-C2-N1	2.05	122.49	117.96
1	B	263	LLP	CE-NZ-C4'	2.66	127.08	119.14
1	A	263	LLP	CE-NZ-C4'	2.83	127.59	119.14
1	B	263	LLP	OP3-P-OP1	3.25	121.23	110.63
1	A	263	LLP	OP3-P-OP2	3.92	121.82	107.44
1	A	263	LLP	CD-CE-NZ	5.32	119.70	110.94
1	B	263	LLP	CD-CE-NZ	5.53	120.05	110.94

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	263	LLP	C4-C4'-NZ-CE
1	A	263	LLP	C4-C4'-NZ-CE

There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	263	LLP	1	0
1	B	263	LLP	12	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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$
2	7AR	B	501	-	22,26,26	3.35	8 (36%)	32,38,38	1.59	5 (15%)

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
2	7AR	B	501	-	-	0/8/28/28	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	7AR	C15-C13	-5.12	1.40	1.48

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	7AR	C13-N12	-4.61	1.31	1.40
2	B	501	7AR	C16-C23	-4.37	1.41	1.48
2	B	501	7AR	C23-N12	-4.01	1.32	1.40
2	B	501	7AR	C20-CL2	2.02	1.78	1.73
2	B	501	7AR	C18-CL1	2.21	1.79	1.73
2	B	501	7AR	O24-C23	8.63	1.40	1.22
2	B	501	7AR	O14-C13	8.65	1.40	1.22

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	7AR	C06-C05-C04	-4.35	105.33	113.98
2	B	501	7AR	C16-C15-C13	-2.55	106.06	108.28
2	B	501	7AR	C21-C15-C13	2.31	133.03	129.29
2	B	501	7AR	C17-C16-C23	3.02	134.19	129.29
2	B	501	7AR	C15-C13-N12	3.24	108.70	105.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	7AR	20	0

## 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	424/425 (99%)	0.96	58 (13%) 4 3	13, 24, 88, 153	0
1	B	424/425 (99%)	0.78	49 (11%) 6 5	12, 22, 88, 154	0
All	All	848/850 (99%)	0.87	107 (12%) 5 4	12, 23, 90, 154	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	26	LEU	19.6
1	B	18	PRO	18.6
1	B	26	LEU	17.5
1	A	23	THR	15.8
1	B	27	SER	15.2
1	A	28	ARG	14.7
1	B	23	THR	13.9
1	A	18	PRO	13.0
1	B	20	ARG	12.3
1	A	21	THR	12.0
1	B	17	SER	11.7
1	B	25	ILE	11.3
1	A	27	SER	11.0
1	B	21	THR	10.9
1	A	342	THR	10.7
1	B	30	PRO	10.6
1	A	25	ILE	10.2
1	B	370	ILE	10.1
1	B	22	MET	10.0
1	B	29	GLY	9.8
1	A	22	MET	9.8
1	A	370	ILE	9.6
1	B	19	ILE	9.5
1	A	376	LYS	9.4

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	28	ARG	9.4
1	B	31	LYS	9.3
1	B	374	ALA	9.2
1	A	29	GLY	8.8
1	A	32	SER	8.8
1	A	19	ILE	8.4
1	B	376	LYS	8.3
1	A	368	GLU	8.2
1	A	374	ALA	8.2
1	A	34	ILE	8.2
1	A	30	PRO	8.1
1	B	24	ASP	8.0
1	A	24	ASP	8.0
1	B	379	VAL	7.8
1	A	20	ARG	7.7
1	A	380	LEU	7.7
1	B	372	GLU	7.4
1	A	31	LYS	7.2
1	B	32	SER	7.2
1	A	188	LYS	7.0
1	A	377	MET	6.9
1	A	378	GLY	6.9
1	A	373	LYS	6.6
1	B	188	LYS	6.5
1	A	33	MET	6.5
1	A	372	GLU	6.3
1	B	342	THR	6.2
1	A	375	VAL	6.2
1	A	425	LEU	6.1
1	B	375	VAL	6.0
1	B	368	GLU	6.0
1	A	379	VAL	5.9
1	B	369	LEU	5.7
1	B	425	LEU	5.7
1	A	424	SER	5.7
1	B	377	MET	5.5
1	B	373	LYS	5.4
1	B	367	LYS	5.2
1	B	33	MET	5.0
1	A	59	LYS	4.6
1	A	367	LYS	4.6
1	A	371	GLU	4.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	363	ILE	4.5
1	A	17	SER	4.4
1	B	186	PRO	4.4
1	A	35	SER	4.3
1	B	371	GLU	4.3
1	B	378	GLY	4.2
1	A	422	LYS	4.2
1	B	420	LEU	4.2
1	A	369	LEU	4.0
1	B	34	ILE	3.9
1	B	380	LEU	3.8
1	A	341	LEU	3.6
1	A	57	ASN	3.5
1	A	58	GLY	3.3
1	A	187	GLN	3.3
1	B	363	ILE	3.2
1	A	36	LEU	3.1
1	B	16	PRO	2.8
1	A	37	ALA	2.7
1	B	364	ASN	2.6
1	B	341	LEU	2.6
1	B	222	LYS	2.6
1	A	340	TRP	2.5
1	A	419	GLN	2.4
1	A	38	GLY	2.4
1	A	86	TRP	2.4
1	A	421	ILE	2.3
1	B	424	SER	2.3
1	B	381	MET	2.3
1	B	118	GLN	2.2
1	A	177	ARG	2.2
1	A	56	GLU	2.2
1	B	309	GLU	2.2
1	A	343	GLY	2.2
1	A	417	LEU	2.1
1	B	339	LYS	2.1
1	A	420	LEU	2.1
1	B	187	GLN	2.1
1	B	366	VAL	2.1
1	A	186	PRO	2.1
1	A	423	GLU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	LLP	B	263	24/25	0.83	0.26	-	4,19,79,86	0
1	LLP	A	263	24/25	0.82	0.25	-	8,20,81,90	0

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	7AR	B	501	24/24	0.43	0.51	1.12	36,60,97,117	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.