



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 13, 2023 – 05:05 pm GMT

PDB ID : 2XGO  
Title : XcOGT in complex with UDP-S-GlcNAc  
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Deposited on : 2010-06-07  
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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

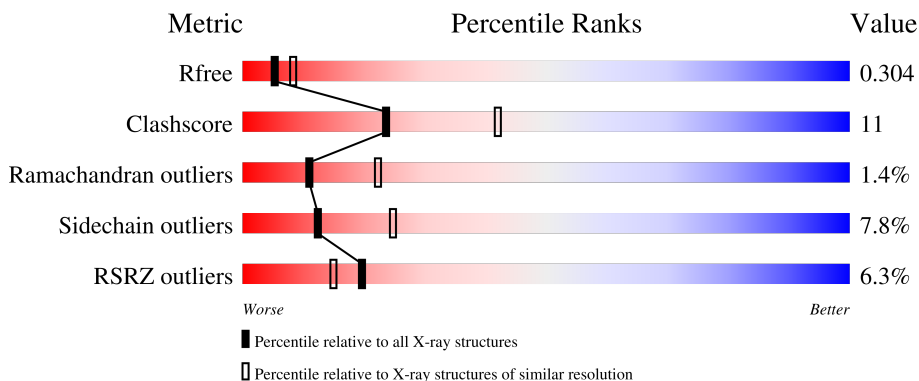
# 1 Overall quality at a glance

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	568	
1	B	568	

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
2	ZKD	A	1569	X	-	-	-

## 2 Entry composition [i](#)

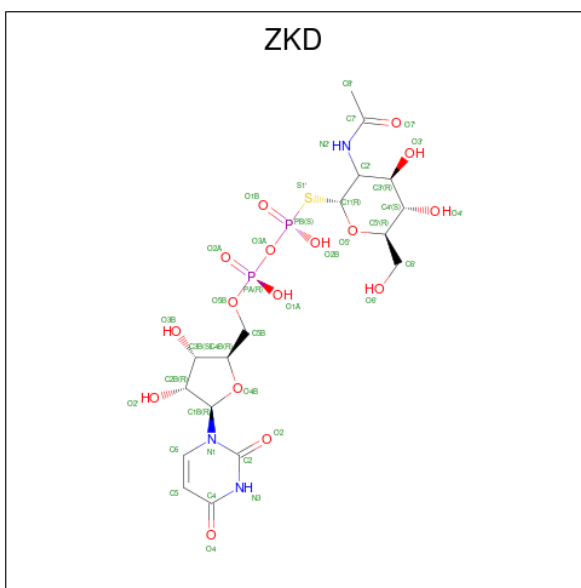
There are 3 unique types of molecules in this entry. The entry contains 8353 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 XCOGT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	548	Total	C	N	O	S	0	0	0
			4171	2635	771	749	16			
1	B	541	Total	C	N	O	S	0	0	0
			4104	2589	760	739	16			

- Molecule 2 is URIDINE-DIPHOSPHATE-1-DEOXY-1-THIO-N-ACETYLGLUCOSAMINE (three-letter code: ZKD) (formula:  $C_{17}H_{27}N_3O_{16}P_2S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
2	A	1	Total	C	N	O	P	S	0	0
			39	17	3	16	2	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
3	A	23	Total	O	0	0
			23	23		

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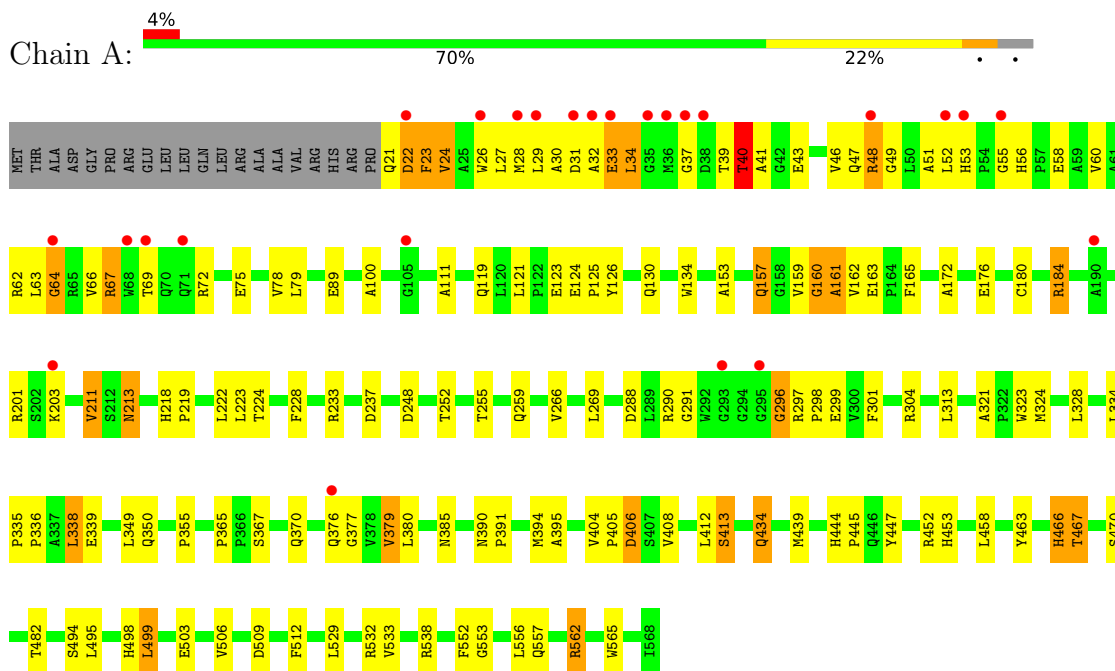
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	B	16	Total	O	0	0
			16	16		

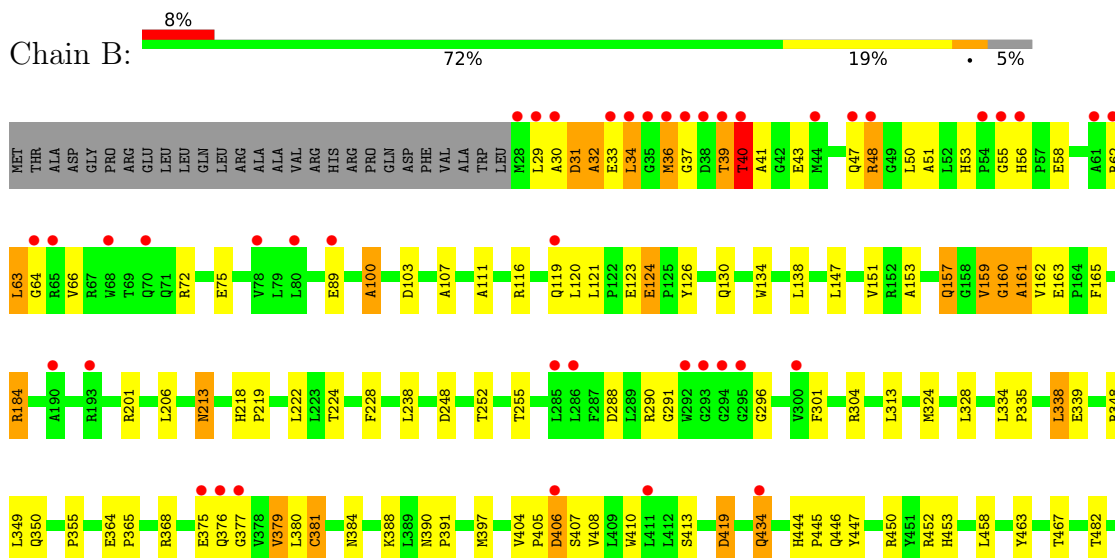
### 3 Residue-property plots

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: XCOGT



#### • Molecule 1: XCOGT





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.66Å 100.02Å 155.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.84 – 2.60 19.84 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.84-2.60) 91.5 (19.84-2.60)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.17 (at 2.59Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.259 , 0.309 0.258 , 0.304	Depositor DCC
$R_{free}$ test set	759 reflections (2.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	69.6	Xtrriage
Anisotropy	0.138	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 59.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8353	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZKD

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	0.70	1/4280 (0.0%)	0.79	7/5840 (0.1%)
1	B	0.63	1/4209 (0.0%)	0.77	9/5742 (0.2%)
All	All	0.67	2/8489 (0.0%)	0.78	16/11582 (0.1%)

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	5
1	B	0	6
All	All	0	11

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	180	CYS	CB-SG	-5.92	1.72	1.81
1	B	381	CYS	CB-SG	-5.39	1.73	1.81

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	562	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	B	562	ARG	NE-CZ-NH1	-8.50	116.05	120.30
1	B	562	ARG	NE-CZ-NH2	8.20	124.40	120.30
1	A	562	ARG	NE-CZ-NH2	-6.95	116.82	120.30
1	B	248	ASP	CB-CG-OD2	6.33	124.00	118.30
1	A	248	ASP	CB-CG-OD1	6.10	123.79	118.30
1	A	222	LEU	CA-CB-CG	6.04	129.19	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	407	SER	N-CA-C	-6.02	94.74	111.00
1	B	64	GLY	N-CA-C	-5.84	98.49	113.10
1	B	33	GLU	N-CA-C	5.78	126.59	111.00
1	B	222	LEU	CA-CB-CG	5.63	128.26	115.30
1	B	36	MET	C-N-CA	5.49	133.84	122.30
1	A	159	VAL	CB-CA-C	-5.28	101.37	111.40
1	A	237	ASP	CB-CG-OD1	5.23	123.00	118.30
1	B	36	MET	CA-C-N	5.19	126.58	116.20
1	A	562	ARG	CD-NE-CZ	5.01	130.62	123.60

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	160	GLY	Peptide
1	A	32	ALA	Peptide
1	A	40	THR	Peptide
1	A	406	ASP	Peptide
1	A	63	LEU	Peptide
1	B	160	GLY	Peptide
1	B	32	ALA	Peptide
1	B	39	THR	Peptide
1	B	40	THR	Peptide
1	B	406	ASP	Peptide
1	B	63	LEU	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	4171	0	4093	102	0
1	B	4104	0	4032	78	0
2	A	39	0	24	14	0
3	A	23	0	0	5	0
3	B	16	0	0	3	0
All	All	8353	0	8149	185	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 11.

All (185) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ARG:NH2	3:A:2003:HOH:O	1.98	0.95
1:A:213:ASN:HD22	1:A:213:ASN:H	1.12	0.92
1:A:48:ARG:HH11	1:A:48:ARG:HG3	1.36	0.90
1:B:213:ASN:HD22	1:B:213:ASN:H	1.21	0.84
1:B:377:GLY:O	3:B:2015:HOH:O	1.96	0.83
1:A:467:THR:HG21	2:A:1569:ZKD:H3B	1.61	0.83
1:B:153:ALA:O	1:B:157:GLN:HG2	1.80	0.81
1:B:48:ARG:HG3	1:B:48:ARG:HH11	1.45	0.79
2:A:1569:ZKD:H1'	2:A:1569:ZKD:C8'	2.14	0.77
1:B:72:ARG:HB3	1:B:75:GLU:OE1	1.84	0.77
1:A:434:GLN:HE21	1:A:434:GLN:HA	1.50	0.77
1:A:31:ASP:OD1	1:A:62:ARG:HD3	1.86	0.74
1:A:160:GLY:C	1:A:162:VAL:H	1.91	0.73
2:A:1569:ZKD:H6'	3:A:2021:HOH:O	1.89	0.72
1:A:72:ARG:HB3	1:A:75:GLU:OE1	1.89	0.71
1:A:213:ASN:HD22	1:A:213:ASN:N	1.84	0.70
1:B:159:VAL:HG22	1:B:159:VAL:O	1.93	0.69
1:A:126:TYR:HA	1:A:161:ALA:HB1	1.75	0.69
1:B:288:ASP:HB2	1:B:301:PHE:CZ	2.27	0.68
1:B:368:ARG:NH1	3:B:2015:HOH:O	2.27	0.67
1:B:365:PRO:HD3	1:B:452:ARG:HD2	1.76	0.67
1:B:384:ASN:HB3	1:B:388:LYS:HD2	1.77	0.66
1:A:201:ARG:O	1:A:565:TRP:HD1	1.79	0.66
1:B:434:GLN:HE21	1:B:434:GLN:HA	1.59	0.65
1:B:224:THR:HB	1:B:228:PHE:CE2	2.34	0.63
1:A:153:ALA:O	1:A:157:GLN:HG2	1.99	0.63
1:B:379:VAL:HG11	1:B:453:HIS:O	1.98	0.62
1:A:23:PHE:O	1:A:26:TRP:HB2	2.00	0.62
1:B:290:ARG:HB2	1:B:291:GLY:HA2	1.83	0.61
1:A:160:GLY:C	1:A:162:VAL:N	2.52	0.60
1:A:290:ARG:HE	1:A:296:GLY:C	2.04	0.60
1:B:130:GLN:HA	1:B:130:GLN:OE1	2.01	0.60
2:A:1569:ZKD:H1'	2:A:1569:ZKD:H8'B	1.83	0.60
1:A:130:GLN:HA	1:A:130:GLN:OE1	2.03	0.59
1:B:552:PHE:CE2	1:B:556:LEU:HD11	2.36	0.59
1:B:39:THR:O	1:B:39:THR:OG1	2.15	0.59
1:A:296:GLY:O	1:A:297:ARG:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:ASP:HB2	1:A:301:PHE:CZ	2.38	0.58
1:B:290:ARG:HE	1:B:296:GLY:C	2.07	0.58
1:B:553:GLY:O	1:B:557:GLN:HG3	2.03	0.58
1:B:328:LEU:HD11	1:B:349:LEU:HG	1.85	0.57
1:A:48:ARG:HH11	1:A:48:ARG:CG	2.13	0.57
1:B:163:GLU:HG2	1:B:184:ARG:HH21	1.68	0.57
1:B:163:GLU:HG2	1:B:184:ARG:NH2	2.20	0.57
1:B:444:HIS:HB3	1:B:445:PRO:HD3	1.85	0.57
1:A:466:HIS:HB3	3:A:2014:HOH:O	2.06	0.56
1:A:467:THR:HB	2:A:1569:ZKD:O2A	2.06	0.56
1:A:224:THR:HB	1:A:228:PHE:CE2	2.41	0.56
1:B:446:GLN:O	1:B:450:ARG:NH2	2.39	0.56
1:B:538:ARG:HB3	1:B:538:ARG:NH2	2.21	0.55
1:B:30:ALA:O	1:B:34:LEU:HB2	2.07	0.55
1:B:153:ALA:O	1:B:157:GLN:CG	2.53	0.55
1:A:529:LEU:O	1:A:533:VAL:HG23	2.06	0.54
1:B:213:ASN:HD22	1:B:213:ASN:N	1.95	0.54
1:A:553:GLY:O	1:A:557:GLN:HG3	2.07	0.54
1:A:40:THR:HA	1:A:43:GLU:H	1.73	0.54
1:B:529:LEU:O	1:B:533:VAL:HG23	2.07	0.54
1:A:252:THR:HG21	1:B:255:THR:OG1	2.07	0.54
1:A:379:VAL:HG11	1:A:453:HIS:O	2.08	0.54
1:A:467:THR:CG2	2:A:1569:ZKD:H3B	2.36	0.54
1:B:124:GLU:OE1	1:B:126:TYR:HB3	2.08	0.53
1:A:288:ASP:CG	1:A:290:ARG:HH21	2.12	0.53
1:A:298:PRO:HD2	1:A:299:GLU:OE1	2.09	0.53
1:A:365:PRO:HD3	1:A:452:ARG:HD2	1.90	0.53
2:A:1569:ZKD:H1'	2:A:1569:ZKD:H8'A	1.87	0.53
1:A:48:ARG:O	1:A:51:ALA:HB3	2.08	0.53
1:B:48:ARG:O	1:B:51:ALA:HB3	2.09	0.52
1:A:111:ALA:HB2	1:A:134:TRP:HD1	1.75	0.52
1:A:385:ASN:ND2	2:A:1569:ZKD:H8'B	2.25	0.52
1:B:503:GLU:OE2	1:B:532:ARG:NH1	2.37	0.52
1:A:290:ARG:HB2	1:A:291:GLY:HA2	1.90	0.51
1:B:31:ASP:OD1	1:B:62:ARG:HD3	2.09	0.51
1:A:444:HIS:HB3	1:A:445:PRO:HD3	1.92	0.51
1:B:288:ASP:CG	1:B:290:ARG:HH21	2.14	0.51
1:A:30:ALA:O	1:A:34:LEU:HB2	2.10	0.51
1:A:64:GLY:H	1:A:79:LEU:HD13	1.74	0.51
1:B:377:GLY:HA2	1:B:406:ASP:HB3	1.90	0.51
1:A:163:GLU:HG2	1:A:184:ARG:NH2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:ASN:HD21	2:A:1569:ZKD:C1'	2.24	0.51
1:B:34:LEU:HD11	1:B:66:VAL:HG22	1.93	0.51
1:A:434:GLN:HA	1:A:434:GLN:NE2	2.22	0.51
1:A:56:HIS:HD2	1:A:58:GLU:H	1.58	0.51
1:A:213:ASN:H	1:A:213:ASN:ND2	1.94	0.51
1:B:48:ARG:HG3	1:B:48:ARG:NH1	2.22	0.50
1:A:288:ASP:OD1	1:A:290:ARG:HB2	2.12	0.50
1:B:147:LEU:O	1:B:151:VAL:HG23	2.11	0.50
1:B:335:PRO:HD2	1:B:338:LEU:HB2	1.93	0.50
1:A:552:PHE:CE2	1:A:556:LEU:HD11	2.45	0.50
1:A:121:LEU:HB3	1:A:124:GLU:HB2	1.93	0.50
1:A:33:GLU:OE2	1:A:41:ALA:HB1	2.12	0.50
1:A:412:LEU:HD11	2:A:1569:ZKD:H5	1.93	0.50
1:A:33:GLU:CD	1:A:41:ALA:HB1	2.32	0.50
1:A:482:THR:HG22	1:A:506:VAL:HG23	1.93	0.50
1:B:379:VAL:CG1	1:B:453:HIS:O	2.59	0.50
1:B:288:ASP:OD1	1:B:290:ARG:HB2	2.12	0.49
1:A:56:HIS:CD2	1:A:58:GLU:H	2.30	0.49
1:B:290:ARG:NE	1:B:296:GLY:O	2.39	0.48
1:B:201:ARG:O	1:B:565:TRP:HD1	1.96	0.48
1:A:163:GLU:OE1	1:A:165:PHE:HB3	2.13	0.48
1:A:390:ASN:HB2	1:A:391:PRO:HD2	1.96	0.48
1:B:40:THR:HA	1:B:43:GLU:H	1.79	0.47
1:B:160:GLY:C	1:B:162:VAL:H	2.17	0.47
1:B:34:LEU:O	1:B:37:GLY:HA2	2.14	0.47
1:A:328:LEU:HD11	1:A:349:LEU:HG	1.96	0.47
1:B:381:CYS:HB2	1:B:410:TRP:HB3	1.97	0.47
2:A:1569:ZKD:C6'	3:A:2021:HOH:O	2.54	0.47
1:A:23:PHE:HB2	1:A:52:LEU:HD13	1.96	0.47
1:A:367:SER:H	1:A:370:GLN:NE2	2.12	0.47
1:B:107:ALA:HB1	1:B:138:LEU:HD21	1.97	0.47
1:A:203:LYS:HD3	1:A:203:LYS:HA	1.60	0.47
1:A:211:VAL:HG13	1:A:301:PHE:CZ	2.50	0.47
1:A:223:LEU:O	1:A:355:PRO:HG2	2.16	0.46
2:A:1569:ZKD:S1'	2:A:1569:ZKD:O5B	2.73	0.46
1:B:213:ASN:H	1:B:213:ASN:ND2	2.02	0.46
1:B:206:LEU:HB3	1:B:238:LEU:CD2	2.46	0.46
1:B:375:GLU:HG2	3:B:2014:HOH:O	2.15	0.46
2:A:1569:ZKD:H4'	3:A:2022:HOH:O	2.15	0.46
1:A:385:ASN:HD21	2:A:1569:ZKD:H1'	1.81	0.46
1:A:259:GLN:HE21	1:A:259:GLN:HB2	1.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:ARG:HB3	1:A:538:ARG:NH2	2.31	0.45
1:A:39:THR:O	1:A:39:THR:OG1	2.31	0.45
1:B:313:LEU:CD1	1:B:355:PRO:HD2	2.47	0.45
1:B:160:GLY:CA	1:B:162:VAL:H	2.29	0.45
1:A:266:VAL:O	1:A:269:LEU:HB2	2.16	0.45
1:B:111:ALA:HB2	1:B:134:TRP:HD1	1.82	0.45
1:B:159:VAL:O	1:B:159:VAL:CG2	2.63	0.45
1:A:153:ALA:O	1:A:157:GLN:CG	2.65	0.45
1:A:172:ALA:HB1	1:A:176:GLU:HB2	1.98	0.45
1:A:380:LEU:HD22	1:A:458:LEU:HD11	1.98	0.45
1:A:233:ARG:HH11	1:A:233:ARG:HG2	1.82	0.44
1:A:213:ASN:N	1:A:213:ASN:ND2	2.56	0.44
1:B:482:THR:HG22	1:B:506:VAL:HG23	1.99	0.44
1:B:364:GLU:OE2	1:B:365:PRO:HD2	2.18	0.44
1:A:37:GLY:O	1:A:39:THR:HG23	2.18	0.44
1:A:124:GLU:OE1	1:A:126:TYR:HB3	2.18	0.44
1:A:290:ARG:NE	1:A:296:GLY:O	2.41	0.44
1:A:394:MET:O	1:A:395:ALA:C	2.54	0.43
1:B:495:LEU:O	1:B:499:LEU:HB2	2.18	0.43
1:A:377:GLY:HA2	1:A:406:ASP:HB3	2.00	0.43
1:A:495:LEU:O	1:A:499:LEU:HB2	2.18	0.43
1:A:24:VAL:O	1:A:28:MET:HB2	2.18	0.43
1:A:494:SER:O	1:A:498:HIS:ND1	2.46	0.43
1:A:255:THR:OG1	1:B:252:THR:HG21	2.19	0.43
1:A:313:LEU:CD1	1:A:355:PRO:HD2	2.49	0.43
1:B:121:LEU:HB3	1:B:124:GLU:HB2	2.00	0.43
1:A:48:ARG:HG3	1:A:48:ARG:NH1	2.15	0.43
1:B:100:ALA:O	1:B:103:ASP:N	2.51	0.43
1:B:397:MET:HE2	1:B:458:LEU:O	2.18	0.43
1:B:506:VAL:HG21	1:B:512:PHE:HA	2.01	0.43
1:A:64:GLY:N	1:A:79:LEU:HD13	2.33	0.42
1:A:163:GLU:HG2	1:A:184:ARG:HH21	1.83	0.42
1:B:48:ARG:HH11	1:B:48:ARG:CG	2.22	0.42
1:B:56:HIS:HD2	1:B:58:GLU:H	1.65	0.42
1:B:116:ARG:O	1:B:120:LEU:HG	2.19	0.42
1:A:404:VAL:HA	1:A:405:PRO:HD3	1.93	0.42
1:A:503:GLU:OE2	1:A:532:ARG:NH1	2.45	0.42
1:A:509:ASP:O	1:A:512:PHE:HB3	2.20	0.42
1:B:160:GLY:HA2	1:B:161:ALA:HB3	2.02	0.42
1:A:34:LEU:HD11	1:A:66:VAL:HG22	2.01	0.42
1:B:218:HIS:O	1:B:219:PRO:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:ASN:HB2	1:B:391:PRO:HD2	2.01	0.42
1:B:434:GLN:HA	1:B:434:GLN:NE2	2.32	0.42
1:A:218:HIS:O	1:A:219:PRO:C	2.55	0.42
1:A:367:SER:N	1:A:370:GLN:HE21	2.18	0.42
1:A:335:PRO:HD2	1:A:338:LEU:HB2	2.01	0.42
1:A:413:SER:HB2	1:A:439:MET:O	2.20	0.42
1:A:66:VAL:O	1:A:67:ARG:C	2.57	0.42
1:B:339:GLU:CG	1:B:348:ARG:HH22	2.32	0.41
1:A:126:TYR:CA	1:A:161:ALA:HB1	2.47	0.41
1:A:336:PRO:HA	1:A:339:GLU:HG3	2.01	0.41
1:B:50:LEU:HD11	1:B:63:LEU:HD22	2.03	0.41
1:A:46:VAL:O	1:A:49:GLY:N	2.54	0.41
1:B:36:MET:H	1:B:37:GLY:HA2	1.85	0.41
1:B:163:GLU:OE1	1:B:165:PHE:HB3	2.20	0.41
1:A:124:GLU:HA	1:A:125:PRO:HD3	1.86	0.41
1:A:379:VAL:CG1	1:A:453:HIS:O	2.69	0.41
1:B:419:ASP:OD1	1:B:419:ASP:N	2.54	0.41
1:A:27:LEU:H	1:A:27:LEU:HD12	1.87	0.40
1:A:321:ALA:HB1	1:A:323:TRP:CE2	2.57	0.40
1:A:324:MET:HB2	1:A:324:MET:HE2	1.94	0.40
1:A:367:SER:H	1:A:370:GLN:HE21	1.69	0.40
1:B:324:MET:HB2	1:B:324:MET:HE2	1.80	0.40
1:B:404:VAL:HA	1:B:405:PRO:HD3	1.95	0.40
1:A:48:ARG:CG	1:A:48:ARG:NH1	2.76	0.40
1:A:467:THR:O	1:A:470:SER:HB3	2.21	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	546/568 (96%)	501 (92%)	36 (7%)	9 (2%)	<b>9</b> <b>19</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	539/568 (95%)	495 (92%)	38 (7%)	6 (1%)	14	30
All	All	1085/1136 (96%)	996 (92%)	74 (7%)	15 (1%)	11	22

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	161	ALA
1	B	40	THR
1	B	41	ALA
1	B	161	ALA
1	A	40	THR
1	A	64	GLY
1	B	32	ALA
1	A	55	GLY
1	A	67	ARG
1	B	55	GLY
1	B	100	ALA
1	A	22	ASP
1	A	100	ALA
1	A	296	GLY
1	A	60	VAL

### 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	413/429 (96%)	379 (92%)	34 (8%)	11	22
1	B	406/429 (95%)	376 (93%)	30 (7%)	13	28
All	All	819/858 (96%)	755 (92%)	64 (8%)	12	25

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	22	ASP
1	A	23	PHE
1	A	24	VAL
1	A	29	LEU
1	A	33	GLU
1	A	34	LEU
1	A	47	GLN
1	A	48	ARG
1	A	53	HIS
1	A	69	THR
1	A	78	VAL
1	A	89	GLU
1	A	119	GLN
1	A	123	GLU
1	A	157	GLN
1	A	184	ARG
1	A	211	VAL
1	A	213	ASN
1	A	304	ARG
1	A	334	LEU
1	A	338	LEU
1	A	350	GLN
1	A	376	GLN
1	A	379	VAL
1	A	408	VAL
1	A	413	SER
1	A	434	GLN
1	A	447	TYR
1	A	463	TYR
1	A	466	HIS
1	A	467	THR
1	A	499	LEU
1	A	562	ARG
1	B	29	LEU
1	B	31	ASP
1	B	34	LEU
1	B	40	THR
1	B	47	GLN
1	B	48	ARG
1	B	53	HIS
1	B	89	GLU
1	B	119	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	123	GLU
1	B	124	GLU
1	B	157	GLN
1	B	159	VAL
1	B	184	ARG
1	B	213	ASN
1	B	304	ARG
1	B	334	LEU
1	B	338	LEU
1	B	350	GLN
1	B	376	GLN
1	B	379	VAL
1	B	380	LEU
1	B	408	VAL
1	B	413	SER
1	B	419	ASP
1	B	434	GLN
1	B	447	TYR
1	B	463	TYR
1	B	467	THR
1	B	499	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	21	GLN
1	A	47	GLN
1	A	56	HIS
1	A	81	GLN
1	A	177	GLN
1	A	213	ASN
1	A	259	GLN
1	A	370	GLN
1	A	385	ASN
1	A	392	GLN
1	A	434	GLN
1	B	47	GLN
1	B	56	HIS
1	B	119	GLN
1	B	177	GLN
1	B	213	ASN
1	B	259	GLN

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Mol	Chain	Res	Type
1	B	370	GLN
1	B	392	GLN
1	B	434	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides 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	ZKD	A	1569	-	35,41,41	1.65	6 (17%)	49,62,62	2.52	17 (34%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ZKD	A	1569	-	1/1/12/13	9/21/63/63	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1569	ZKD	C2'-N2'	-5.21	1.37	1.45
2	A	1569	ZKD	C2-N1	3.11	1.43	1.38
2	A	1569	ZKD	C2-N3	2.98	1.43	1.38
2	A	1569	ZKD	O5'-C1'	2.82	1.46	1.42
2	A	1569	ZKD	C6-C5	2.77	1.41	1.35
2	A	1569	ZKD	PB-O2B	-2.75	1.49	1.56

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1569	ZKD	C1'-C2'-N2'	7.76	125.60	111.17
2	A	1569	ZKD	C3'-C2'-N2'	7.20	124.22	110.62
2	A	1569	ZKD	C4-N3-C2	-4.97	120.03	126.58
2	A	1569	ZKD	C4'-C3'-C2'	-4.54	103.70	110.34
2	A	1569	ZKD	C2B-C1B-N1	4.22	125.18	113.22
2	A	1569	ZKD	O2B-PB-O1B	4.19	119.96	109.82
2	A	1569	ZKD	N3-C2-N1	3.87	120.02	114.89
2	A	1569	ZKD	C2'-N2'-C7'	3.50	131.70	123.18
2	A	1569	ZKD	C5B-C4B-C3B	-3.09	103.59	115.18
2	A	1569	ZKD	C5-C4-N3	3.02	119.35	114.84
2	A	1569	ZKD	O4-C4-C5	-2.57	120.65	125.16
2	A	1569	ZKD	O5'-C1'-S1'	-2.55	103.59	108.77
2	A	1569	ZKD	O7'-C7'-C8'	-2.49	117.43	122.06
2	A	1569	ZKD	C3B-C2B-C1B	-2.40	96.86	101.43
2	A	1569	ZKD	C8'-C7'-N2'	2.32	120.02	116.10
2	A	1569	ZKD	O2'-C2B-C3B	-2.15	104.86	111.82
2	A	1569	ZKD	O2-C2-N1	-2.15	119.93	122.79

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1569	ZKD	C2'

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1569	ZKD	C5B-O5B-PA-O2A
2	A	1569	ZKD	C5B-O5B-PA-O3A
2	A	1569	ZKD	C1'-C2'-N2'-C7'
2	A	1569	ZKD	C3B-C4B-C5B-O5B
2	A	1569	ZKD	O4B-C4B-C5B-O5B

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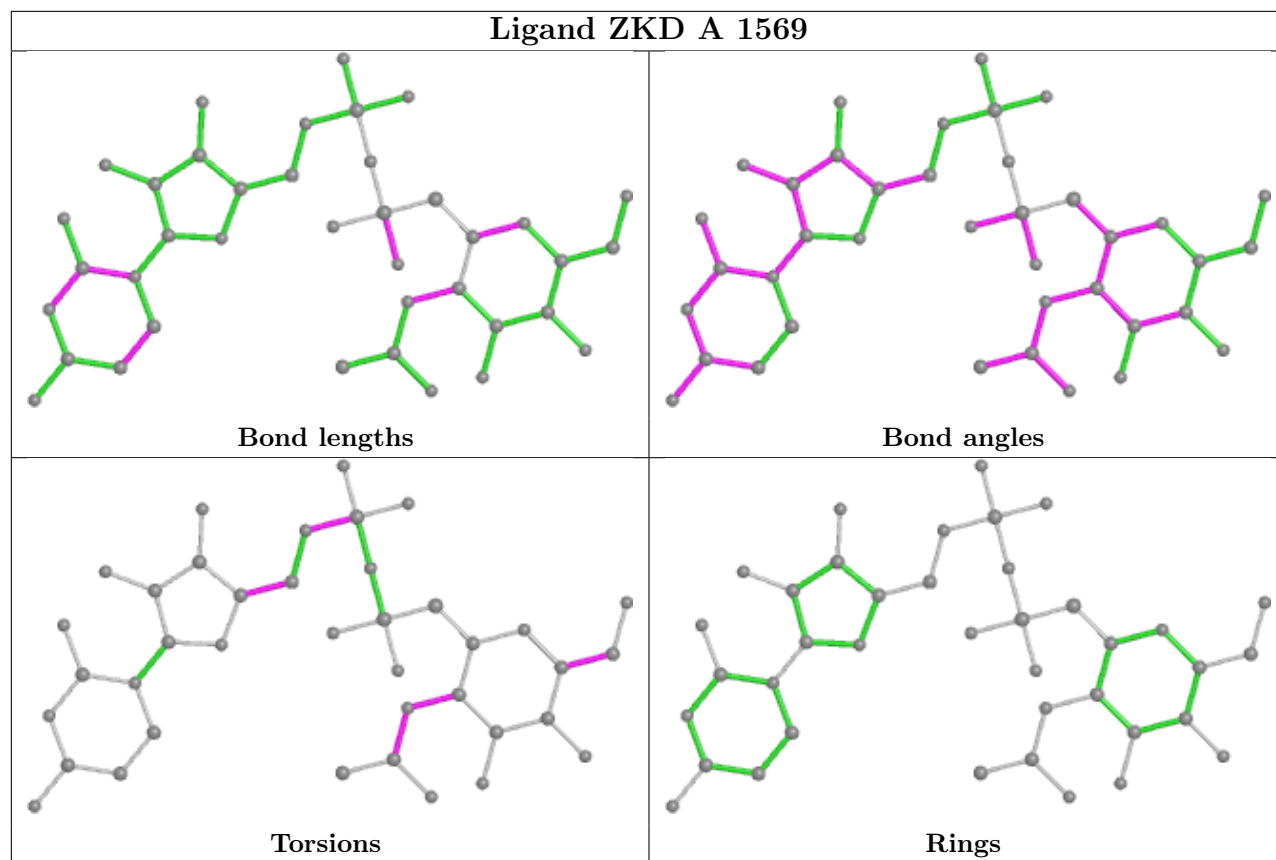
Mol	Chain	Res	Type	Atoms
2	A	1569	ZKD	O7'-C7'-N2'-C2'
2	A	1569	ZKD	C8'-C7'-N2'-C2'
2	A	1569	ZKD	C3'-C2'-N2'-C7'
2	A	1569	ZKD	O5'-C5'-C6'-O6'

There are no ring outliers.

1 monomer is involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1569	ZKD	14	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	548/568 (96%)	0.02	25 (4%) 32 26	44, 49, 54, 65	0
1	B	541/568 (95%)	0.34	44 (8%) 12 8	44, 49, 53, 65	0
All	All	1089/1136 (95%)	0.18	69 (6%) 20 15	44, 49, 54, 65	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	35	GLY	6.4
1	A	36	MET	6.3
1	A	32	ALA	5.9
1	B	37	GLY	5.6
1	B	78	VAL	5.4
1	B	36	MET	5.1
1	B	538	ARG	5.0
1	B	30	ALA	4.9
1	A	52	LEU	4.7
1	B	55	GLY	4.5
1	A	55	GLY	4.2
1	A	64	GLY	3.8
1	B	294	GLY	3.7
1	A	69	THR	3.7
1	B	190	ALA	3.7
1	B	434	GLN	3.6
1	B	68	TRP	3.6
1	B	70	GLN	3.5
1	B	62	ARG	3.4
1	A	31	ASP	3.3
1	B	377	GLY	3.2
1	B	54	PRO	3.1
1	B	35	GLY	3.1
1	A	22	ASP	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	293	GLY	3.0
1	A	26	TRP	3.0
1	B	89	GLU	2.9
1	A	37	GLY	2.9
1	A	28	MET	2.9
1	A	190	ALA	2.9
1	B	295	GLY	2.8
1	B	33	GLU	2.8
1	B	29	LEU	2.8
1	A	376	GLN	2.8
1	A	68	TRP	2.7
1	B	64	GLY	2.7
1	A	29	LEU	2.6
1	B	28	MET	2.5
1	B	39	THR	2.5
1	B	119	GLN	2.5
1	B	376	GLN	2.5
1	B	44	MET	2.4
1	B	34	LEU	2.4
1	B	286	LEU	2.4
1	B	566	LEU	2.4
1	B	406	ASP	2.4
1	B	56	HIS	2.4
1	B	47	GLN	2.3
1	B	40	THR	2.3
1	B	38	ASP	2.3
1	A	33	GLU	2.3
1	B	80	LEU	2.3
1	B	292	TRP	2.3
1	A	105	GLY	2.2
1	B	285	LEU	2.2
1	A	71	GLN	2.2
1	A	295	GLY	2.2
1	B	65	ARG	2.2
1	B	48	ARG	2.2
1	B	411	LEU	2.2
1	A	203	LYS	2.1
1	B	293	GLY	2.1
1	B	300	VAL	2.1
1	A	53	HIS	2.1
1	B	375	GLU	2.1
1	A	48	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	193	ARG	2.0
1	A	38	ASP	2.0
1	B	61	ALA	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](#)

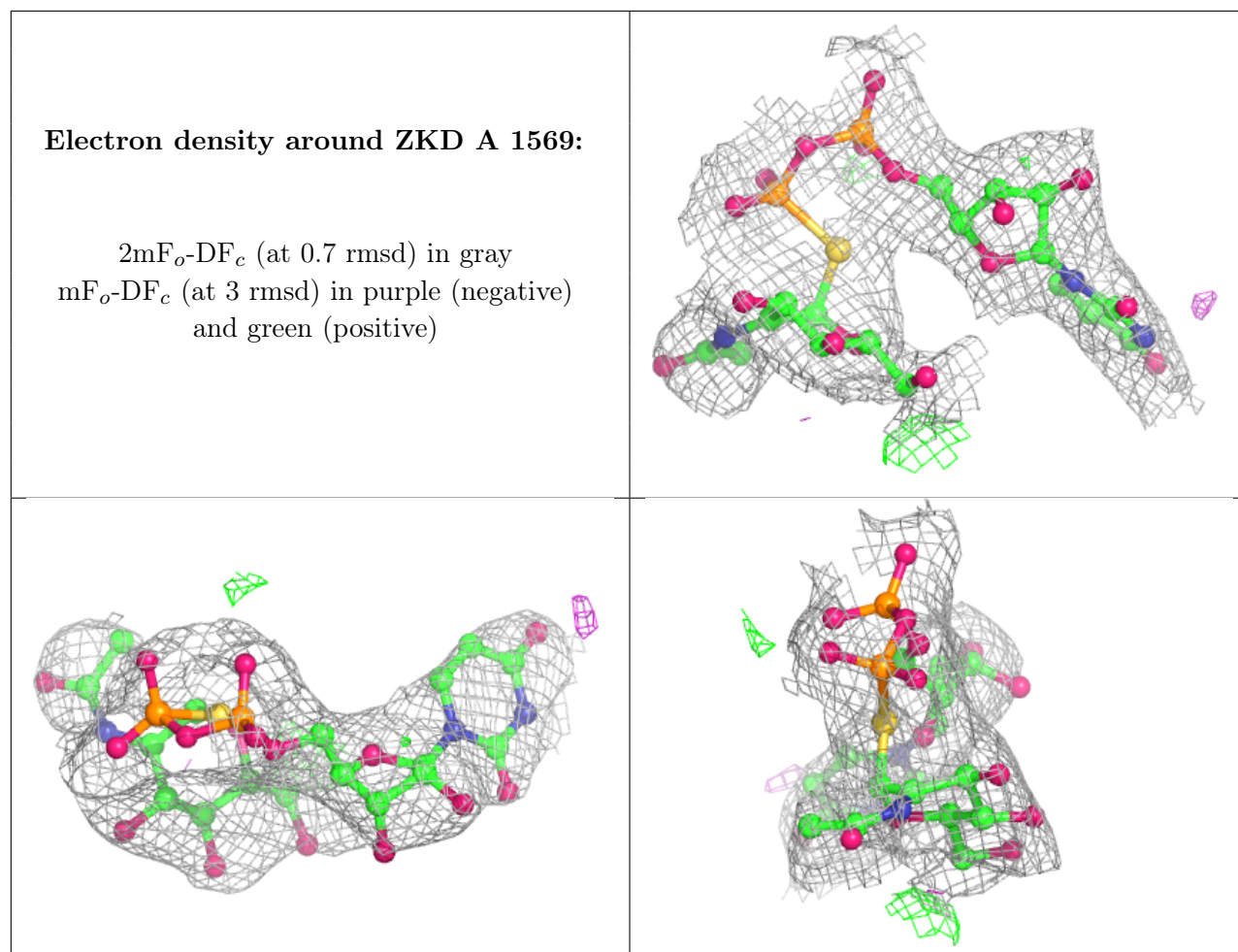
There are no monosaccharides in this entry.

## 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
2	ZKD	A	1569	39/39	0.91	0.18	34,48,57,61	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.