



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 16, 2023 – 07:00 pm GMT

PDB ID : 3ZRK  
Title : Identification of 2-(4-pyridyl)thienopyridinones as GSK-3beta inhibitors  
Authors : Gentile, G.; Bernasconi, G.; Pozzan, A.; Merlo, G.; Marzorati, P.; Bamborough, P.; Bax, B.; Bridges, A.; Brough, C.; Carter, P.; Cutler, G.; Neu, M.; Takada, M.  
Deposited on : 2011-06-16  
Resolution : 2.37 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  
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

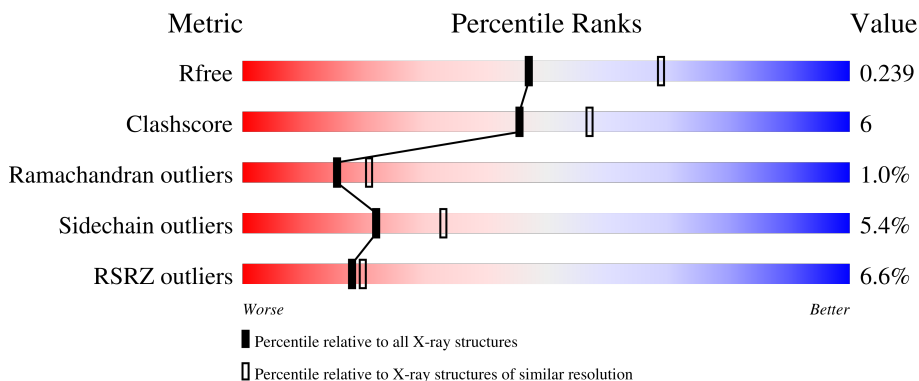
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.37 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	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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	371	
1	B	371	
2	X	32	
2	Y	32	

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	GOL	A	1387	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6350 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 GLYCOGEN SYNTHASE KINASE-3 BETA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	347	Total	C	N	O	P	S	0	7	0
			2828	1816	485	514	1	12			
1	B	349	Total	C	N	O	P	S	0	10	0
			2866	1838	492	523	1	12			

- Molecule 2 is a protein called PROTO-ONCOGENE FRAT1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	X	24	Total	C	N	O	0	0	0
			195	123	41	31			
2	Y	22	Total	C	N	O	0	0	0
			172	109	34	29			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	195	MET	-	expression tag	UNP Q92837
X	196	ALA	-	expression tag	UNP Q92837
Y	195	MET	-	expression tag	UNP Q92837
Y	196	ALA	-	expression tag	UNP Q92837

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



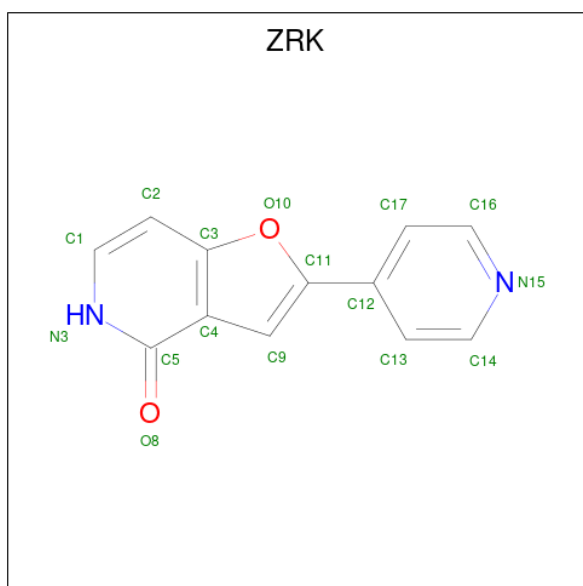
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is 2-(4-PYRIDINYL)FURO[3,2-C]PYRIDIN-4(5H)-ONE (three-letter code: ZRK) (formula: C<sub>12</sub>H<sub>8</sub>N<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			16	12	2	2		
5	B	1	Total	C	N	O	0	0
			16	12	2	2		

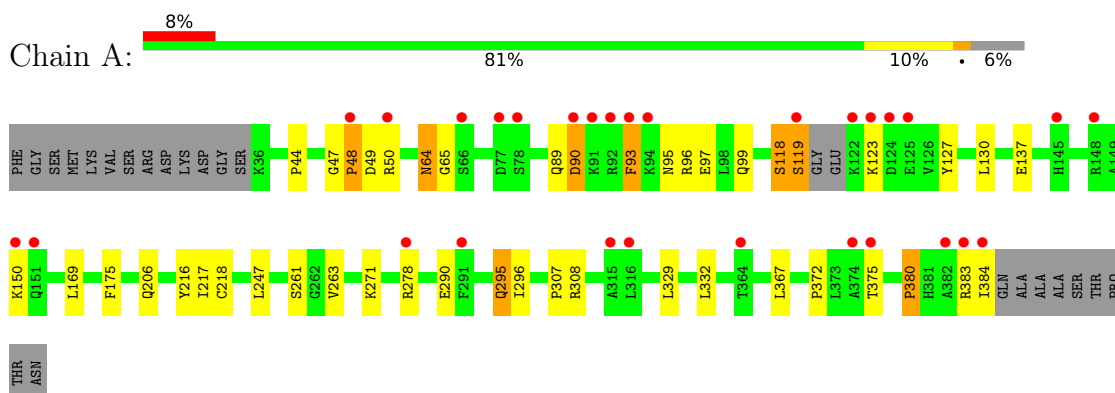
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	95	Total	O	0	0
			95	95		
6	B	108	Total	O	0	0
			108	108		
6	X	5	Total	O	0	0
			5	5		
6	Y	1	Total	O	0	0
			1	1		

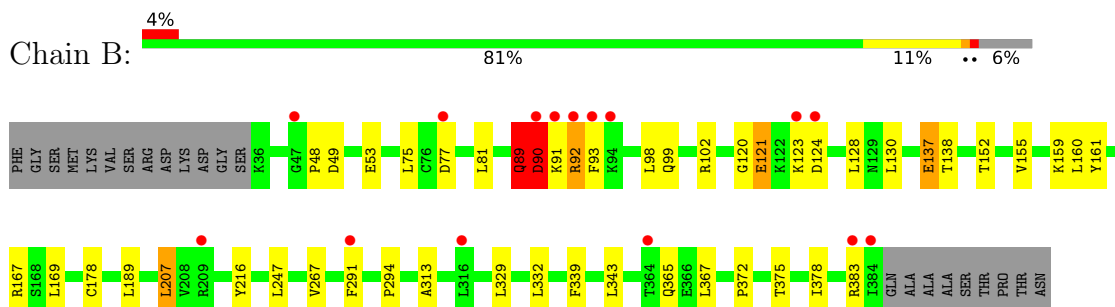
### 3 Residue-property plots [i](#)

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.

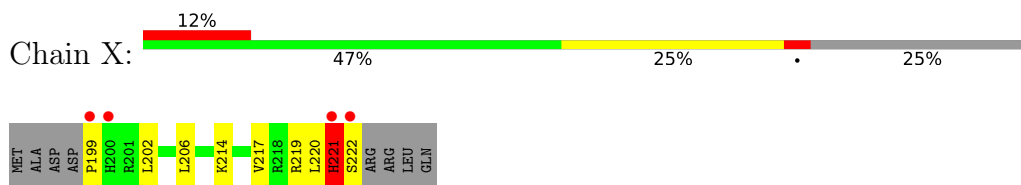
- Molecule 1: GLYCOGEN SYNTHASE KINASE-3 BETA



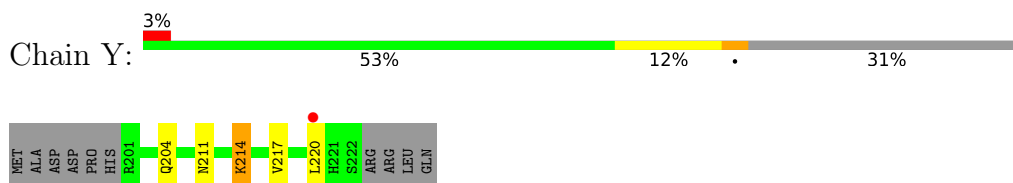
- Molecule 1: GLYCOGEN SYNTHASE KINASE-3 BETA



- Molecule 2: PROTO-ONCOGENE FRAT1



- Molecule 2: PROTO-ONCOGENE FRAT1





## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	151.90Å 151.90Å 201.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.37 37.97 – 2.37	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.37) 99.5 (37.97-2.37)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.72 (at 2.37Å)	Xtrriage
Refinement program	REFMAC 5.3.0006	Depositor
R, $R_{free}$	0.198 , 0.243 0.198 , 0.239	Depositor DCC
$R_{free}$ test set	1825 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.8	Xtrriage
Anisotropy	0.050	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 45.3	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	0.95	EDS
Total number of atoms	6350	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.76% 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: ZRK, SO4, PTR, GOL

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	0.41	1/2882 (0.0%)	0.56	0/3924
1	B	0.38	0/2920	0.55	0/3972
2	X	0.34	0/197	0.59	0/263
2	Y	0.34	0/172	0.57	0/230
All	All	0.39	1/6171 (0.0%)	0.56	0/8389

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	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	380	PRO	CA-CB	5.55	1.64	1.53

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	SER	Peptide
1	A	47	GLY	Peptide
1	B	89	GLN	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	2828	0	2807	40	0
1	B	2866	0	2849	34	0
2	X	195	0	214	12	0
2	Y	172	0	188	4	0
3	A	10	0	0	0	0
3	B	20	0	0	0	0
4	A	12	0	16	6	0
4	B	6	0	8	0	0
5	A	16	0	8	0	0
5	B	16	0	8	0	0
6	A	95	0	0	1	0
6	B	108	0	0	0	0
6	X	5	0	0	0	0
6	Y	1	0	0	0	0
All	All	6350	0	6098	79	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 6.

All (79) 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:X:221:HIS:N	2:X:222:SER:HA	1.77	0.99
1:A:48:PRO:HB2	1:A:49:ASP:HA	1.49	0.94
1:A:307:PRO:HB2	4:A:1387:GOL:H31	1.50	0.92
1:A:118:SER:HA	1:A:119:SER:HB2	1.48	0.92
1:A:48:PRO:CB	1:A:50:ARG:H	1.85	0.89
2:X:199:PRO:HA	2:X:202:LEU:HB3	1.60	0.83
1:A:308:ARG:H	4:A:1387:GOL:H12	1.44	0.83
1:A:48:PRO:HB3	1:A:50:ARG:H	1.43	0.82
1:B:92:ARG:HD2	1:B:92:ARG:C	2.00	0.80
1:B:90:ASP:OD1	1:B:91:LYS:HA	1.82	0.80
1:A:44:PRO:HG2	1:A:48:PRO:HG2	1.64	0.79
1:A:263:VAL:HG23	2:X:199:PRO:HB3	1.67	0.77
2:X:199:PRO:HG3	2:X:202:LEU:HD23	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:ASP:CB	1:B:91:LYS:HA	2.16	0.74
1:A:307:PRO:HB2	4:A:1387:GOL:C3	2.18	0.73
1:A:118:SER:CA	1:A:119:SER:HB2	2.18	0.73
1:A:90:ASP:HB2	1:A:93:PHE:CD1	2.25	0.71
1:A:48:PRO:HB2	1:A:50:ARG:H	1.57	0.68
1:B:91:LYS:H	1:B:93:PHE:H	1.41	0.68
1:B:91:LYS:N	1:B:93:PHE:H	1.93	0.67
1:A:48:PRO:HB3	1:A:50:ARG:N	2.09	0.64
1:A:48:PRO:CB	1:A:50:ARG:N	2.60	0.64
1:A:307:PRO:HD2	4:A:1387:GOL:H11	1.79	0.64
2:X:221:HIS:H	2:X:222:SER:HA	1.62	0.63
1:A:307:PRO:CB	4:A:1387:GOL:H31	2.29	0.62
1:A:118:SER:O	1:A:127:TYR:N	2.22	0.62
1:B:267:VAL:HG13	2:Y:220:LEU:HB3	1.82	0.61
1:A:48:PRO:HB2	1:A:49:ASP:CA	2.26	0.61
1:B:90:ASP:C	1:B:92:ARG:HA	2.21	0.61
1:A:90:ASP:N	1:A:90:ASP:OD1	2.33	0.61
2:Y:211:ASN:OD1	2:Y:214:LYS:HE3	2.01	0.61
1:A:375:THR:HA	1:A:383:ARG:HH22	1.69	0.58
1:B:91:LYS:N	1:B:92:ARG:HA	2.19	0.57
1:B:89:GLN:O	1:B:91:LYS:HG2	2.04	0.57
1:A:48:PRO:CB	1:A:49:ASP:HA	2.27	0.56
1:B:90:ASP:CG	1:B:91:LYS:HA	2.25	0.56
2:X:221:HIS:N	2:X:222:SER:CA	2.60	0.55
1:B:48:PRO:O	1:B:49:ASP:HB2	2.08	0.53
1:B:48:PRO:O	1:B:49:ASP:CB	2.56	0.53
1:A:175:PHE:O	1:A:206:GLN:NE2	2.43	0.51
1:B:155:VAL:HG12	1:B:159:LYS:HE3	1.93	0.51
1:B:291[B]:PHE:HE1	2:Y:214:LYS:HZ1	1.59	0.50
1:A:308:ARG:HG3	4:A:1387:GOL:H32	1.92	0.50
1:A:48:PRO:HB2	1:A:50:ARG:N	2.24	0.49
1:A:90:ASP:CB	1:A:93:PHE:CD1	2.94	0.49
1:B:53[B]:GLU:H	1:B:53[B]:GLU:CD	2.15	0.49
1:A:64:ASN:HD22	1:A:65:GLY:N	2.11	0.49
1:B:90:ASP:HB2	1:B:91:LYS:HA	1.93	0.49
1:A:271:LYS:HG3	2:X:220:LEU:HD11	1.95	0.48
1:A:48:PRO:CB	1:A:49:ASP:CA	2.88	0.48
1:A:375:THR:HB	1:B:372:PRO:HB3	1.95	0.48
1:B:89:GLN:HG3	1:B:128:LEU:HB2	1.95	0.47
1:B:378:ILE:HG22	1:B:383:ARG:HG3	1.96	0.47
1:A:372:PRO:HB2	1:B:375:THR:HG23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ILE:O	1:A:218[B]:CYS:HB2	2.15	0.47
1:B:178:CYS:HB2	1:B:207:LEU:HD22	1.98	0.46
1:B:91:LYS:HB2	1:B:93:PHE:CD1	2.51	0.45
1:A:332:LEU:HD11	1:A:367:LEU:HA	1.98	0.45
1:B:98[A]:LEU:CD2	1:B:102:ARG:HD2	2.46	0.45
1:A:93:PHE:CD1	1:A:93:PHE:N	2.83	0.45
1:A:261:SER:OG	2:X:199:PRO:HG2	2.17	0.45
1:B:120:GLY:O	1:B:121:GLU:HB3	2.16	0.45
1:B:161:TYR:CZ	1:B:189:LEU:HD21	2.52	0.45
1:B:91:LYS:N	1:B:92:ARG:CA	2.80	0.45
2:X:219:ARG:O	2:X:221:HIS:HB2	2.17	0.43
1:A:290:GLU:OE2	2:X:214:LYS:HB2	2.19	0.43
1:B:294:PRO:HB2	2:Y:217:VAL:HG11	2.01	0.43
1:A:97:GLU:OE2	6:A:2010:HOH:O	2.22	0.42
1:A:95:ASN:O	1:A:99[A]:GLN:HG2	2.19	0.42
1:B:160:LEU:HD13	1:B:343:LEU:HD22	2.01	0.42
1:A:295:GLN:O	1:A:295:GLN:HG3	2.20	0.42
1:A:296:ILE:HD11	2:X:217:VAL:HG13	2.01	0.41
1:B:98[A]:LEU:HD22	1:B:99[A]:GLN:NE2	2.36	0.41
1:B:313:ALA:HB2	1:B:339:PHE:CE1	2.56	0.41
1:B:137:GLU:HG3	1:B:138:THR:H	1.86	0.40
1:B:332:LEU:HD11	1:B:367:LEU:HA	2.03	0.40
1:A:296:ILE:HD12	2:X:217:VAL:HG22	2.03	0.40
1:B:90:ASP:HB2	1:B:91:LYS:CA	2.50	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	349/371 (94%)	340 (97%)	7 (2%)	2 (1%)	25 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	356/371 (96%)	338 (95%)	14 (4%)	4 (1%)	14	18
2	X	22/32 (69%)	20 (91%)	1 (4%)	1 (4%)	2	1
2	Y	20/32 (62%)	20 (100%)	0	0	100	100
All	All	747/806 (93%)	718 (96%)	22 (3%)	7 (1%)	15	23

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	PRO
1	B	121	GLU
1	B	90	ASP
1	B	124	ASP
1	B	123	LYS
2	X	221	HIS
1	A	123	LYS

### 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	310/327 (95%)	293 (94%)	17 (6%)	21	32
1	B	314/327 (96%)	299 (95%)	15 (5%)	25	39
2	X	22/29 (76%)	20 (91%)	2 (9%)	9	12
2	Y	19/29 (66%)	17 (90%)	2 (10%)	7	8
All	All	665/712 (93%)	629 (95%)	36 (5%)	22	33

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	89	GLN
1	A	90	ASP
1	A	93	PHE

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Mol	Chain	Res	Type
1	A	96	ARG
1	A	119	SER
1	A	130	LEU
1	A	137	GLU
1	A	150	LYS
1	A	169	LEU
1	A	247	LEU
1	A	278[A]	ARG
1	A	278[B]	ARG
1	A	295	GLN
1	A	329	LEU
1	A	380	PRO
1	A	384	ILE
1	B	75	LEU
1	B	77	ASP
1	B	81	LEU
1	B	89	GLN
1	B	90	ASP
1	B	92	ARG
1	B	130	LEU
1	B	137	GLU
1	B	152	THR
1	B	167	ARG
1	B	169	LEU
1	B	207	LEU
1	B	247	LEU
1	B	329	LEU
1	B	365	GLN
2	X	206	LEU
2	X	221	HIS
2	Y	204	GLN
2	Y	214	LYS

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	64	ASN
1	A	287	ASN
1	B	381	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	PTR	A	216	1	15,16,17	1.94	2 (13%)	19,22,24	0.74	1 (5%)
1	PTR	B	216	1	15,16,17	1.98	2 (13%)	19,22,24	0.61	1 (5%)

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	PTR	A	216	1	-	1/10/11/13	0/1/1/1
1	PTR	B	216	1	-	1/10/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	216	PTR	OH-CZ	-7.00	1.24	1.40
1	A	216	PTR	OH-CZ	-6.95	1.24	1.40
1	B	216	PTR	P-OH	2.54	1.63	1.59
1	A	216	PTR	P-OH	2.21	1.62	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	PTR	O3P-P-OH	2.45	112.89	105.24
1	B	216	PTR	O3P-P-OH	2.22	112.18	105.24



There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	216	PTR	O-C-CA-CB
1	B	216	PTR	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

11 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	GOL	A	1387	-	5,5,5	0.35	0	5,5,5	0.24	0
5	ZRK	B	1400	-	14,18,18	0.82	1 (7%)	17,25,25	2.58	4 (23%)
3	SO4	A	1386	-	4,4,4	0.17	0	6,6,6	0.20	0
4	GOL	B	1386	-	5,5,5	0.38	0	5,5,5	0.24	0
5	ZRK	A	1400	-	14,18,18	0.87	1 (7%)	17,25,25	2.59	4 (23%)
3	SO4	B	1384	-	4,4,4	0.14	0	6,6,6	0.22	0
3	SO4	B	1390	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	B	1392	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	B	1391	-	4,4,4	0.14	0	6,6,6	0.09	0
4	GOL	A	1388	-	5,5,5	0.35	0	5,5,5	0.25	0
3	SO4	A	1390	-	4,4,4	0.14	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
4	GOL	A	1387	-	-	2/4/4/4	-
5	ZRK	B	1400	-	-	0/2/4/4	0/3/3/3
4	GOL	B	1386	-	-	2/4/4/4	-
5	ZRK	A	1400	-	-	0/2/4/4	0/3/3/3
4	GOL	A	1388	-	-	3/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1400	ZRK	C4-C5	-2.27	1.43	1.47
5	B	1400	ZRK	C4-C5	-2.08	1.43	1.47

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1400	ZRK	C3-C2-C1	-8.32	114.56	119.96
5	B	1400	ZRK	C3-C2-C1	-8.24	114.61	119.96
5	A	1400	ZRK	O8-C5-N3	4.69	126.03	120.32
5	B	1400	ZRK	O8-C5-N3	4.44	125.73	120.32
5	B	1400	ZRK	C4-C3-C2	3.11	124.56	119.83
5	A	1400	ZRK	C4-C3-C2	2.85	124.17	119.83
5	A	1400	ZRK	C4-C5-N3	-2.51	112.19	114.31
5	B	1400	ZRK	C4-C5-N3	-2.39	112.30	114.31

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1387	GOL	O1-C1-C2-C3
4	A	1388	GOL	O1-C1-C2-C3
4	B	1386	GOL	O1-C1-C2-C3
4	A	1387	GOL	O1-C1-C2-O2
4	A	1388	GOL	O1-C1-C2-O2
4	B	1386	GOL	O1-C1-C2-O2
4	A	1388	GOL	C1-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1387	GOL	6	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	346/371 (93%)	0.38	29 (8%) 11 12	26, 42, 71, 86	0
1	B	348/371 (93%)	0.28	15 (4%) 35 38	26, 42, 68, 77	0
2	X	24/32 (75%)	0.18	4 (16%) 1 1	36, 45, 71, 75	0
2	Y	22/32 (68%)	0.04	1 (4%) 33 36	41, 48, 64, 71	0
All	All	740/806 (91%)	0.32	49 (6%) 18 20	26, 43, 69, 86	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	291[B]	PHE	7.0
1	A	384	ILE	6.7
1	B	90	ASP	6.4
1	B	291[A]	PHE	6.3
1	B	123	LYS	5.4
1	B	124	ASP	5.3
1	A	93	PHE	5.1
1	B	93	PHE	5.0
1	A	90	ASP	4.8
1	A	124	ASP	4.6
1	A	92	ARG	4.6
1	A	91	LYS	4.2
1	B	77	ASP	4.2
1	B	92	ARG	4.0
1	B	47	GLY	3.8
1	B	91	LYS	3.8
1	A	77	ASP	3.8
1	A	382	ALA	3.8
1	A	150	LYS	3.7
1	A	148	ARG	3.6
1	B	384	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	125	GLU	3.0
2	X	221	HIS	2.9
1	A	48	PRO	2.9
1	A	50	ARG	2.9
1	A	374	ALA	2.9
1	A	123	LYS	2.7
2	X	199	PRO	2.7
1	A	78	SER	2.7
1	A	66	SER	2.7
2	X	222	SER	2.5
1	A	375	THR	2.5
1	B	94	LYS	2.5
1	B	364	THR	2.4
1	B	383	ARG	2.3
1	A	94	LYS	2.3
1	B	209[A]	ARG	2.3
2	Y	220	LEU	2.2
1	A	145	HIS	2.2
1	A	316	LEU	2.2
1	A	122	LYS	2.2
1	A	278[A]	ARG	2.2
1	A	315	ALA	2.1
1	A	151	GLN	2.1
1	A	119	SER	2.1
2	X	200	HIS	2.0
1	B	316	LEU	2.0
1	A	364	THR	2.0
1	A	383	ARG	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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	PTR	B	216	16/17	0.91	0.13	45,52,54,55	0
1	PTR	A	216	16/17	0.94	0.14	42,49,52,53	0

### 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
4	GOL	B	1386	6/6	0.57	0.23	92,93,93,93	0
4	GOL	A	1388	6/6	0.66	0.25	75,77,78,79	0
3	SO4	B	1392	5/5	0.88	0.37	112,112,112,112	5
4	GOL	A	1387	6/6	0.88	0.39	53,55,58,59	0
3	SO4	A	1390	5/5	0.88	0.29	114,114,114,114	0
3	SO4	B	1390	5/5	0.88	0.21	117,117,117,117	0
3	SO4	B	1391	5/5	0.93	0.27	85,85,86,86	0
5	ZRK	A	1400	16/16	0.97	0.10	33,37,39,39	0
5	ZRK	B	1400	16/16	0.97	0.10	28,34,36,37	0
3	SO4	A	1386	5/5	0.99	0.11	36,37,43,43	0
3	SO4	B	1384	5/5	0.99	0.10	38,39,40,42	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.