



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:19 AM UTC

PDB ID : 3ZRK / pdb_00003zrk
Title : Identification of 2-(4-pyridyl)thienopyridinones as GSK-3beta inhibitors
Authors : Gentile, G.; Bernasconi, G.; Pozzan, A.; Merlo, G.; Marzorati, P.; Bambrorough, 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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

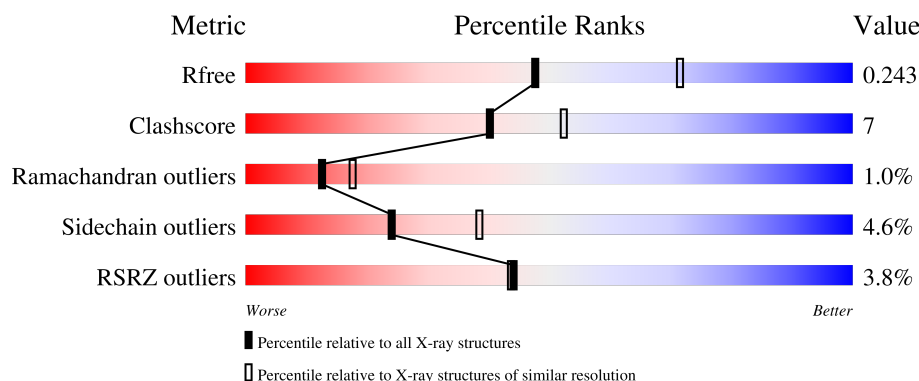
1 Overall quality at a glance

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}	180053	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (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 ≥ 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	4% 81% 10% 6%
1	B	371	2% 81% 11% 6%
2	X	32	12% 44% 25% 25%
2	Y	32	53% 12% 31%

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
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
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 (CCD ID: SO4) (formula: O₄S).



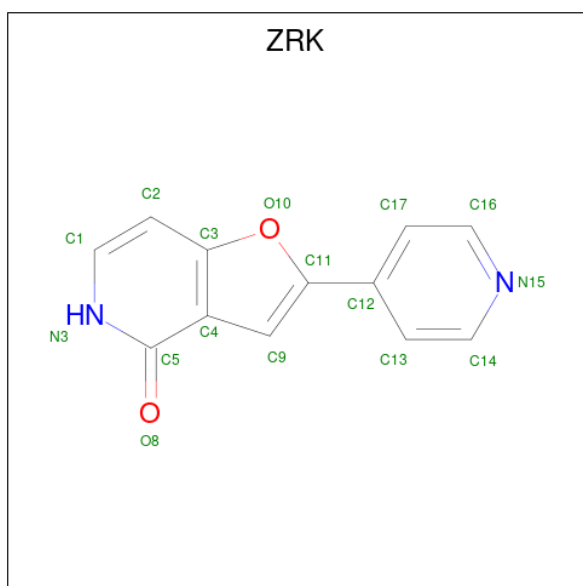
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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 (CCD ID: ZRK) (formula: C₁₂H₈N₂O₂).



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		

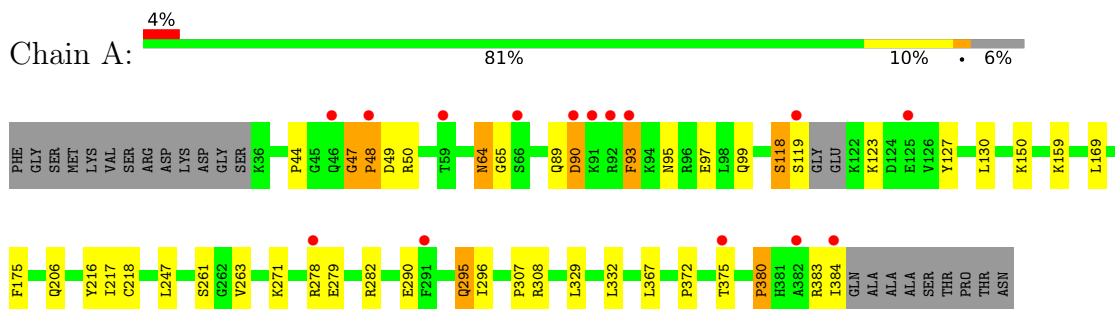
- Molecule 6 is water.

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		

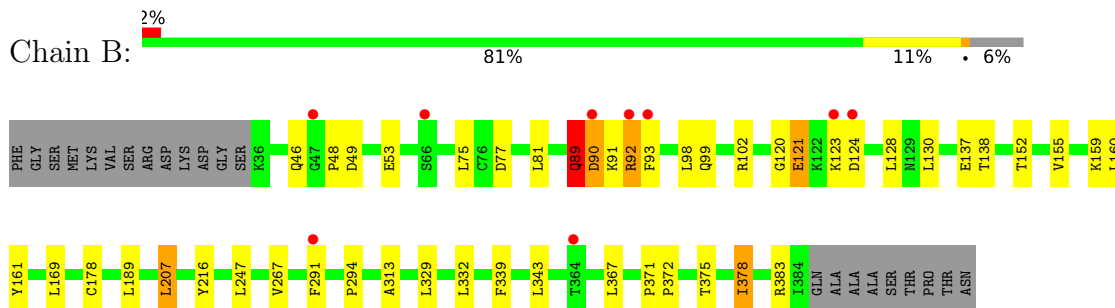
3 Residue-property plots [i](#)

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.

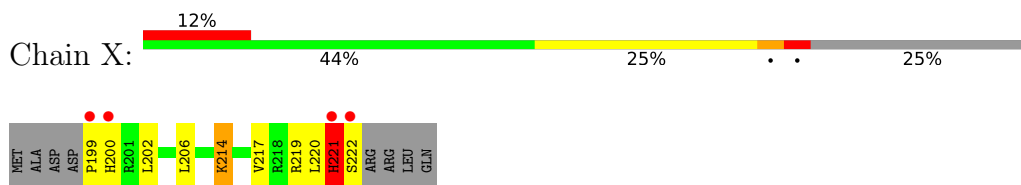
- Molecule 1: GLYCOGEN SYNTHASE KINASE-3 BETA



- 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, α , β , γ	151.90Å 151.90Å 201.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.37 20.00 – 2.37	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.37) 99.3 (20.00-2.37)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.72 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.3.0006	Depositor
R, R_{free}	0.198 , 0.243 (Not available) , 0.243	Depositor DCC
R_{free} test set	1825 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	39.8	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6350	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: SO4, PTR, GOL, ZRK

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	0.51	1/2882 (0.0%)	0.81	3/3924 (0.1%)
1	B	0.49	0/2920	0.79	3/3972 (0.1%)
2	X	0.43	0/197	0.97	1/263 (0.4%)
2	Y	0.42	0/172	0.87	0/230
All	All	0.50	1/6171 (0.0%)	0.81	7/8389 (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	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	7.67	1.64	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	GLY	N-CA-C	-5.75	100.60	112.34
1	B	371	PRO	N-CA-C	5.33	117.20	110.70
2	X	200	HIS	N-CA-C	-5.08	106.22	112.72
1	A	380	PRO	N-CA-C	5.08	122.93	112.47
1	B	378	ILE	CA-C-N	5.04	123.29	119.66
1	B	378	ILE	C-N-CA	5.04	123.29	119.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	380	PRO	CA-CB-CG	-5.02	94.96	104.50

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	42	0
1	B	2866	0	2849	33	0
2	X	195	0	214	13	0
2	Y	172	0	188	3	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	2	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	81	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 7.

All (81) 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
1:B:92:ARG:HD2	1:B:92:ARG:C	2.00	0.84
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: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
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:B:90:ASP:C	1:B:92:ARG:HA	2.21	0.66
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:A:90:ASP:OD1	1:A:90:ASP:N	2.33	0.61
2:Y:211:ASN:OD1	2:Y:214:LYS:HE3	2.01	0.61
1:B:90:ASP:CG	1:B:91:LYS:HA	2.25	0.60
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
2:X:221:HIS:N	2:X:222:SER:CA	2.60	0.55
1:B:53[B]:GLU:H	1:B:53[B]:GLU:CD	2.15	0.54
1:B:48:PRO:O	1:B:49:ASP:CB	2.56	0.53
1:B:48:PRO:O	1:B:49:ASP:HB2	2.08	0.52
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:279:GLU:CD	1:A:282:ARG:HH21	2.27	0.42
2:X:220:LEU:C	2:X:222:SER:HA	2.42	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:A:159:LYS:NZ	6:A:2018:HOH:O	2.53	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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	349/371 (94%)	340 (97%)	7 (2%)	2 (1%)	21	30
1	B	356/371 (96%)	338 (95%)	14 (4%)	4 (1%)	11	16
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%)	12	20

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

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%)	296 (96%)	14 (4%)	24	39
1	B	314/327 (96%)	302 (96%)	12 (4%)	29	46
2	X	22/29 (76%)	19 (86%)	3 (14%)	3	4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Y	19/29 (66%)	17 (90%)	2 (10%)	6	9
All	All	665/712 (93%)	634 (95%)	31 (5%)	24	37

All (31) 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
1	A	130	LEU
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	46	GLN
1	B	75	LEU
1	B	77	ASP
1	B	81	LEU
1	B	89	GLN
1	B	92	ARG
1	B	130	LEU
1	B	152	THR
1	B	169	LEU
1	B	207	LEU
1	B	247	LEU
1	B	329	LEU
2	X	206	LEU
2	X	214	LYS
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 (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	72	GLN
1	A	287	ASN
1	A	347	ASN
1	B	370	ASN
1	B	381	HIS
2	X	200	HIS
2	Y	221	HIS

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	PTR	A	216	1	15,16,17	1.91	1 (6%)	17,22,24	0.78	1 (5%)
1	PTR	B	216	1	15,16,17	1.95	1 (6%)	17,22,24	0.66	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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	216	PTR	OH-CZ	-7.07	1.24	1.40
1	A	216	PTR	OH-CZ	-7.02	1.24	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	PTR	O3P-P-OH	2.56	112.89	105.32
1	B	216	PTR	O3P-P-OH	2.32	112.18	105.32

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 oligosaccharides 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	B	1386	-	5,5,5	0.39	0	5,5,5	0.24	0
5	ZRK	B	1400	-	18,18,18	0.85	0	19,25,25	1.46	3 (15%)
3	SO4	B	1390	-	4,4,4	0.24	0	6,6,6	0.10	0
3	SO4	B	1384	-	4,4,4	0.21	0	6,6,6	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ZRK	A	1400	-	18,18,18	0.88	1 (5%)	19,25,25	1.44	3 (15%)
3	SO4	A	1386	-	4,4,4	0.25	0	6,6,6	0.21	0
4	GOL	A	1388	-	5,5,5	0.36	0	5,5,5	0.29	0
3	SO4	B	1391	-	4,4,4	0.24	0	6,6,6	0.12	0
3	SO4	A	1390	-	4,4,4	0.24	0	6,6,6	0.07	0
4	GOL	A	1387	-	5,5,5	0.36	0	5,5,5	0.27	0
3	SO4	B	1392	-	4,4,4	0.24	0	6,6,6	0.09	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	B	1386	-	-	2/4/4/4	-
5	ZRK	B	1400	-	-	0/4/4/4	0/3/3/3
5	ZRK	A	1400	-	-	0/4/4/4	0/3/3/3
4	GOL	A	1388	-	-	2/4/4/4	-
4	GOL	A	1387	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1400	ZRK	C9-C11	2.00	1.38	1.35

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1400	ZRK	C1-C2-C3	-3.99	114.56	118.59
5	B	1400	ZRK	C1-C2-C3	-3.94	114.61	118.59
5	B	1400	ZRK	C4-C9-C11	-2.82	104.95	107.47
5	A	1400	ZRK	O8-C5-N3	2.75	126.03	120.75
5	A	1400	ZRK	C4-C9-C11	-2.68	105.08	107.47
5	B	1400	ZRK	O8-C5-N3	2.60	125.73	120.75

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1387	GOL	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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

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, 95th 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 ²)	Q<0.9
1	A	346/371 (93%)	0.17	15 (4%) 40 39	18, 42, 71, 86	7 (2%)
1	B	348/371 (93%)	0.12	9 (2%) 57 56	17, 42, 67, 77	10 (2%)
2	X	24/32 (75%)	0.41	4 (16%) 4 4	36, 45, 71, 75	0
2	Y	22/32 (68%)	-0.01	0 100 100	41, 48, 64, 71	0
All	All	740/806 (91%)	0.15	28 (3%) 44 44	17, 42, 69, 86	17 (2%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	291[B]	PHE	6.1
1	B	124	ASP	5.2
1	B	291[A]	PHE	4.3
1	A	384	ILE	4.1
1	B	93	PHE	3.7
1	B	90	ASP	3.6
1	A	93	PHE	3.6
1	A	90	ASP	3.3
2	X	199	PRO	3.2
1	B	364	THR	3.0
1	A	125	GLU	3.0
1	B	123	LYS	2.6
1	A	91	LYS	2.6
1	A	92	ARG	2.6
1	A	46[A]	GLN	2.6
1	A	278[A]	ARG	2.6
1	A	48	PRO	2.5
1	A	382	ALA	2.3
1	A	119	SER	2.3
1	A	59	THR	2.3
2	X	221	HIS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	92	ARG	2.3
1	A	66	SER	2.3
2	X	200	HIS	2.3
2	X	222	SER	2.3
1	A	375	THR	2.2
1	B	47	GLY	2.1
1	B	66	SER	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, 95th 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 ²)	Q<0.9
1	PTR	B	216	16/17	0.90	0.13	45,52,54,55	0
1	PTR	A	216	16/17	0.92	0.13	42,49,52,53	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th 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 ²)	Q<0.9
3	SO4	B	1392	5/5	0.36	0.12	112,112,112,112	5
4	GOL	B	1386	6/6	0.49	0.19	92,93,93,93	0
4	GOL	A	1388	6/6	0.62	0.13	75,77,78,79	0
3	SO4	B	1390	5/5	0.71	0.09	117,117,117,117	0
3	SO4	A	1390	5/5	0.80	0.09	114,114,114,114	0
3	SO4	B	1391	5/5	0.83	0.18	85,85,86,86	0
4	GOL	A	1387	6/6	0.85	0.13	53,55,58,59	0
5	ZRK	A	1400	16/16	0.94	0.06	33,37,39,39	0
5	ZRK	B	1400	16/16	0.94	0.06	28,34,36,37	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	A	1386	5/5	0.97	0.06	36,37,43,43	0
3	SO4	B	1384	5/5	0.98	0.05	38,39,40,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.