



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 24, 2017 – 02:08 AM EDT

PDB ID : 5BML
Title : ROCK 1 bound to a pyridine thiazole inhibitor
Authors : Jacobs, M.D.
Deposited on : unknown
Resolution : 2.95 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

<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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20030345

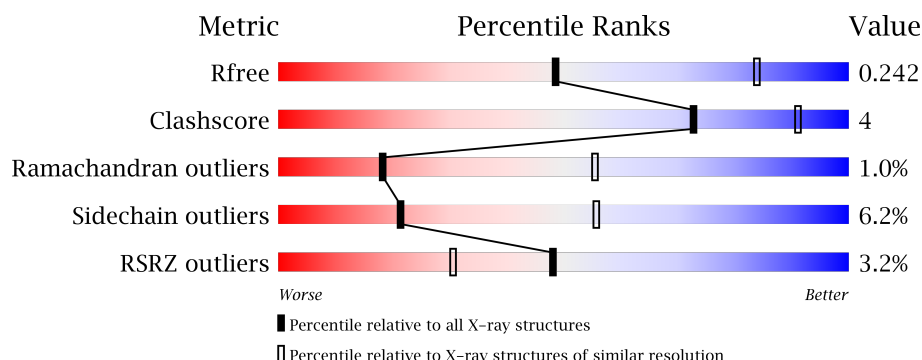
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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}	100719	2395 (3.00-2.92)
Clashscore	112137	2773 (3.00-2.92)
Ramachandran outliers	110173	2680 (3.00-2.92)
Sidechain outliers	110143	2683 (3.00-2.92)
RSRZ outliers	101464	2421 (3.00-2.92)

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 ≥ 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	415	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>12%</div> <div>5%</div> </div> </div>
1	B	415	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>13%</div> <div>5%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6506 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.

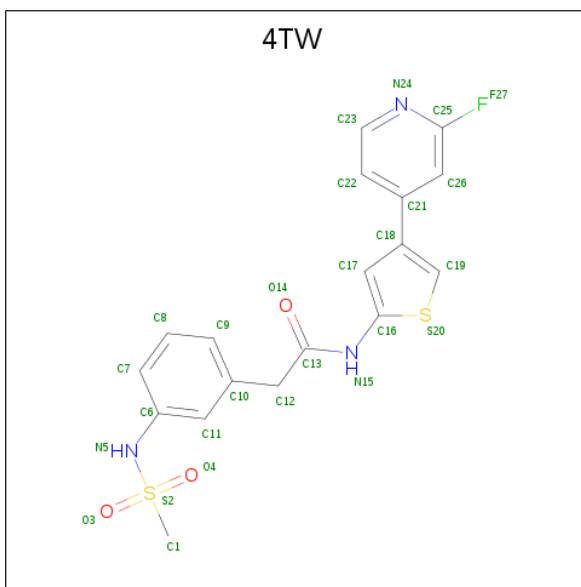
- Molecule 1 is a protein called Rho-associated protein kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	393	Total	C	N	O	S	0	0	0
			3195	2044	532	598	21			
1	B	395	Total	C	N	O	S	0	0	0
			3209	2052	530	606	21			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q13464
A	2	SER	-	expression tag	UNP Q13464
A	3	LEU	-	expression tag	UNP Q13464
A	4	HIS	-	expression tag	UNP Q13464
A	5	MET	-	expression tag	UNP Q13464
B	1	GLY	-	expression tag	UNP Q13464
B	2	SER	-	expression tag	UNP Q13464
B	3	LEU	-	expression tag	UNP Q13464
B	4	HIS	-	expression tag	UNP Q13464
B	5	MET	-	expression tag	UNP Q13464

- Molecule 2 is N-[4-(2-fluoropyridin-4-yl)thiophen-2-yl]-2-{3-[(methylsulfonyl)amino]phenyl} acetamide (three-letter code: 4TW) (formula: C₁₈H₁₆FN₃O₃S₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			27	18	1	3	3	2		
2	B	1	Total	C	F	N	O	S	0	0
			27	18	1	3	3	2		

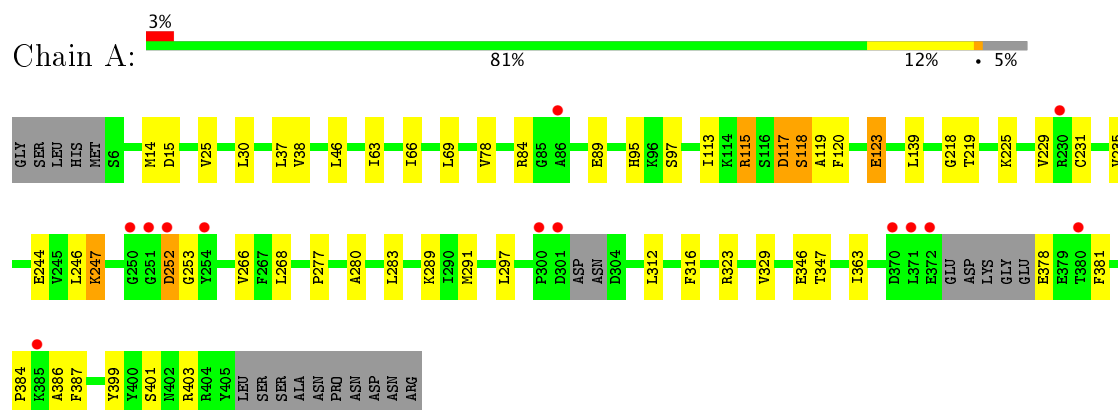
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	26	Total	O	0	0
			26	26		
3	B	22	Total	O	0	0
			22	22		

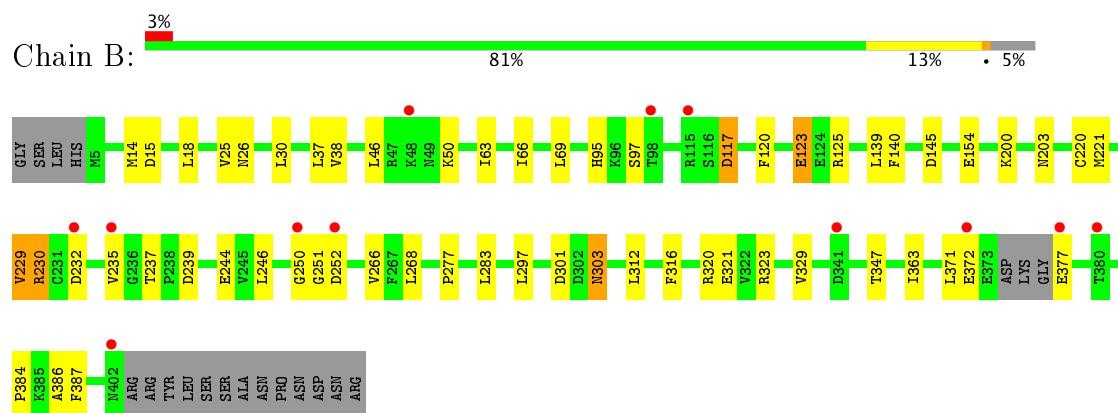
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Rho-associated protein kinase 1



• Molecule 1: Rho-associated protein kinase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	182.59 Å 182.59 Å 91.39 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.90 – 2.95 29.90 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.90-2.95) 99.6 (29.90-2.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 2.95 Å)	Xtriage
Refinement program	BUSTER-TNT 2.11.6, CNS	Depositor
R, R_{free}	0.205 , 0.235 0.210 , 0.242	Depositor DCC
R_{free} test set	1776 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	74.0	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 56.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.011 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6506	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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: 4TW

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	0.52	0/3270	0.70	1/4416 (0.0%)
1	B	0.51	0/3285	0.69	1/4438 (0.0%)
All	All	0.52	0/6555	0.70	2/8854 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	371	LEU	C-N-CA	5.41	135.22	121.70
1	A	118	SER	C-N-CA	5.05	134.32	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3195	0	3095	25	0
1	B	3209	0	3104	29	0
2	A	27	0	16	1	0
2	B	27	0	16	1	0
3	A	26	0	0	0	0
3	B	22	0	0	0	0
All	All	6506	0	6231	49	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 4.

All (49) 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:66:ILE:HD11	1:B:25:VAL:HG21	1.55	0.89
1:A:225:LYS:HD3	1:A:225:LYS:H	1.41	0.84
1:B:244:GLU:HG2	1:B:320:ARG:HD2	1.67	0.76
1:A:316:PHE:O	1:A:323:ARG:HD2	1.90	0.72
1:B:316:PHE:O	1:B:323:ARG:HD2	1.92	0.70
1:B:232:ASP:HA	1:B:250:GLY:H	1.63	0.64
1:B:221:MET:HB3	1:B:229:VAL:HG21	1.83	0.60
1:A:399:TYR:CE2	1:A:403:ARG:HG2	2.36	0.60
1:A:225:LYS:N	1:A:225:LYS:HD3	2.16	0.59
1:B:244:GLU:CG	1:B:320:ARG:HD2	2.33	0.58
1:B:200:LYS:HG2	1:B:203:ASN:ND2	2.20	0.57
1:B:200:LYS:H	1:B:203:ASN:HD22	1.50	0.57
1:A:30:LEU:HB3	1:B:30:LEU:HB3	1.87	0.56
1:B:38:VAL:HG11	1:B:63:ILE:HG21	1.90	0.53
1:A:38:VAL:HG11	1:A:63:ILE:HG21	1.92	0.52
1:A:25:VAL:HG21	1:B:66:ILE:HD11	1.92	0.51
1:A:14:MET:CE	1:B:69:LEU:HB2	2.42	0.50
1:A:225:LYS:H	1:A:225:LYS:CD	2.20	0.49
1:A:84:ARG:HD3	1:A:89:GLU:HB3	1.97	0.47
2:B:501:4TW:S20	2:B:501:4TW:O14	2.73	0.47
1:B:244:GLU:HG2	1:B:320:ARG:CD	2.41	0.47
1:A:69:LEU:HB2	1:B:14:MET:CE	2.45	0.46
1:A:266:VAL:HG13	1:A:277:PRO:HD2	1.98	0.46
1:A:46:LEU:HD21	1:A:387:PHE:N	2.31	0.46
1:B:244:GLU:CD	1:B:323:ARG:HH22	2.20	0.45
1:A:252:ASP:HB3	1:A:253:GLY:H	1.67	0.44
1:A:280:ALA:HB2	1:A:289:LYS:HD2	1.99	0.44
1:B:95:HIS:CE1	1:B:97:SER:HB3	2.53	0.44
1:B:266:VAL:HG13	1:B:277:PRO:HD2	1.99	0.43
1:B:50:LYS:HD3	1:B:50:LYS:HA	1.87	0.43
1:B:123:GLU:HG2	1:B:123:GLU:H	1.60	0.43
1:B:117:ASP:O	1:B:120:PHE:HD1	2.01	0.43
1:A:95:HIS:CE1	1:A:97:SER:HB3	2.54	0.43
1:B:140:PHE:HE2	1:B:154:GLU:HB3	1.83	0.42
1:B:18:LEU:HA	1:B:26:ASN:HA	2.01	0.42
1:A:89:GLU:HA	2:A:501:4TW:H6	2.01	0.42
1:A:346:GLU:CD	1:A:346:GLU:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:ARG:CZ	1:B:251:GLY:HA3	2.50	0.41
1:B:46:LEU:HD21	1:B:387:PHE:N	2.35	0.41
1:B:200:LYS:HG2	1:B:203:ASN:HD22	1.83	0.41
1:A:384:PRO:HB2	1:A:386:ALA:O	2.21	0.41
1:B:235:VAL:HG11	1:B:246:LEU:HD23	2.02	0.41
1:B:384:PRO:HB2	1:B:386:ALA:O	2.21	0.41
1:B:123:GLU:HG3	1:B:220:CYS:O	2.21	0.41
1:A:244:GLU:HA	1:A:247:LYS:HE2	2.01	0.41
1:A:246:LEU:HD23	1:A:291:MET:SD	2.61	0.41
1:A:37:LEU:HD13	1:B:37:LEU:HD13	2.03	0.40
1:A:123:GLU:HG2	1:A:123:GLU:H	1.59	0.40
1:A:120:PHE:HB2	1:A:218:GLY:O	2.21	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	387/415 (93%)	369 (95%)	13 (3%)	5 (1%)	14	48
1	B	391/415 (94%)	374 (96%)	14 (4%)	3 (1%)	22	61
All	All	778/830 (94%)	743 (96%)	27 (4%)	8 (1%)	18	55

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	303	ASN
1	B	372	GLU
1	A	119	ALA
1	A	115	ARG
1	A	117	ASP
1	A	252	ASP

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Mol	Chain	Res	Type
1	A	118	SER
1	B	237	THR

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	347/369 (94%)	325 (94%)	22 (6%)	21	55
1	B	350/369 (95%)	329 (94%)	21 (6%)	22	57
All	All	697/738 (94%)	654 (94%)	43 (6%)	21	56

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASP
1	A	78	VAL
1	A	113	ILE
1	A	115	ARG
1	A	117	ASP
1	A	123	GLU
1	A	139	LEU
1	A	219	THR
1	A	229	VAL
1	A	231	CYS
1	A	235	VAL
1	A	247	LYS
1	A	268	LEU
1	A	283	LEU
1	A	297	LEU
1	A	312	LEU
1	A	329	VAL
1	A	347	THR
1	A	363	ILE
1	A	378	GLU
1	A	381	PHE

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Mol	Chain	Res	Type
1	A	401	SER
1	B	15	ASP
1	B	117	ASP
1	B	123	GLU
1	B	125	ARG
1	B	139	LEU
1	B	145	ASP
1	B	229	VAL
1	B	230	ARG
1	B	239	ASP
1	B	252	ASP
1	B	268	LEU
1	B	283	LEU
1	B	297	LEU
1	B	301	ASP
1	B	303	ASN
1	B	312	LEU
1	B	321	GLU
1	B	329	VAL
1	B	347	THR
1	B	363	ILE
1	B	377	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	54	ASN
1	B	16	ASN
1	B	54	ASN
1	B	203	ASN
1	B	249	GLN
1	B	303	ASN
1	B	391	GLN

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 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$
2	4TW	A	501	-	26,29,29	1.46	7 (26%)	33,41,41	3.21	11 (33%)
2	4TW	B	501	-	26,29,29	1.45	5 (19%)	33,41,41	3.63	9 (27%)

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	4TW	A	501	-	-	0/15/17/17	0/3/3/3
2	4TW	B	501	-	-	0/15/17/17	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	4TW	C19-C18	-3.96	1.34	1.37
2	A	501	4TW	C19-C18	-2.95	1.35	1.37
2	A	501	4TW	C6-N5	-2.02	1.39	1.43
2	A	501	4TW	S2-N5	2.09	1.66	1.63
2	B	501	4TW	S2-N5	2.12	1.66	1.63
2	B	501	4TW	C1-S2	2.60	1.82	1.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	4TW	C1-S2	2.63	1.82	1.75
2	B	501	4TW	C19-S20	2.66	1.74	1.70
2	A	501	4TW	C19-S20	2.70	1.74	1.70
2	A	501	4TW	C25-N24	2.72	1.33	1.30
2	A	501	4TW	C16-S20	3.09	1.77	1.72
2	B	501	4TW	C25-N24	3.18	1.34	1.30

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	4TW	C26-C25-N24	-4.40	121.58	127.11
2	A	501	4TW	C19-C18-C21	-4.19	121.49	127.47
2	A	501	4TW	C26-C25-N24	-4.09	121.97	127.11
2	B	501	4TW	C22-C23-N24	-4.02	119.28	123.92
2	B	501	4TW	C19-C18-C21	-3.79	122.07	127.47
2	B	501	4TW	C1-S2-N5	-3.73	102.15	106.64
2	A	501	4TW	C22-C23-N24	-3.61	119.76	123.92
2	B	501	4TW	C18-C19-S20	-3.38	110.11	112.29
2	B	501	4TW	C16-N15-C13	-3.11	122.88	128.21
2	A	501	4TW	C18-C19-S20	-2.96	110.39	112.29
2	A	501	4TW	O4-S2-N5	-2.91	101.12	107.13
2	A	501	4TW	C16-N15-C13	-2.56	123.81	128.21
2	A	501	4TW	C12-C13-N15	2.04	120.06	114.94
2	A	501	4TW	C1-S2-N5	2.29	109.41	106.64
2	A	501	4TW	O3-S2-O4	3.64	124.29	118.78
2	B	501	4TW	O3-S2-C1	4.36	115.81	108.35
2	A	501	4TW	C23-N24-C25	8.16	121.57	115.64
2	B	501	4TW	C23-N24-C25	9.40	122.47	115.64
2	A	501	4TW	F27-C25-N24	12.66	119.43	114.79
2	B	501	4TW	F27-C25-N24	15.15	120.34	114.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	4TW	1	0
2	B	501	4TW	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	393/415 (94%)	0.01	13 (3%)	47 30	45, 71, 111, 151	0
1	B	395/415 (95%)	-0.03	12 (3%)	51 32	47, 74, 115, 139	0
All	All	788/830 (94%)	-0.01	25 (3%)	48 30	45, 73, 114, 151	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	341	ASP	4.0
1	A	372	GLU	3.6
1	B	372	GLU	3.3
1	B	402	ASN	3.2
1	B	98	THR	3.2
1	A	250	GLY	3.1
1	A	251	GLY	3.1
1	A	254	TYR	2.9
1	B	380	THR	2.9
1	B	252	ASP	2.8
1	A	380	THR	2.6
1	A	371	LEU	2.6
1	A	252	ASP	2.5
1	B	48	LYS	2.5
1	A	230	ARG	2.4
1	A	300	PRO	2.4
1	B	235	VAL	2.4
1	B	377	GLU	2.4
1	A	370	ASP	2.3
1	B	250	GLY	2.3
1	A	385	LYS	2.3
1	B	115	ARG	2.2
1	B	232	ASP	2.2
1	A	86	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	301	ASP	2.1

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 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, 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	LLDF	B-factors(Å ²)	Q<0.9
2	4TW	B	501	27/27	0.96	0.17	0.06	61,67,75,75	0
2	4TW	A	501	27/27	0.96	0.15	-0.85	55,64,79,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.