W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report (i)

Feb 13, 2017 – 06:01 pm GMT

PDB ID	:	4RMZ
Title	:	Crystal Structure of IRAK-4
Authors	:	Johnstone, S.; Sudom, A.; Liu, J.; Walker, N.P.; Wang, Z.
Deposited on	:	2014-10-22
Resolution	:	2.20 Å(reported)

The following versions of software and data (see references (i)) 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	:	trunk28620
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)	:	recalc28949

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 2.20 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	Percentile Ranks	Value
Rfree		0.297
Clashscore		6
Ramachandran outliers		0.2%
Sidechain outliers		5.5%
RSRZ outliers		9.4%

Worse ← → *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
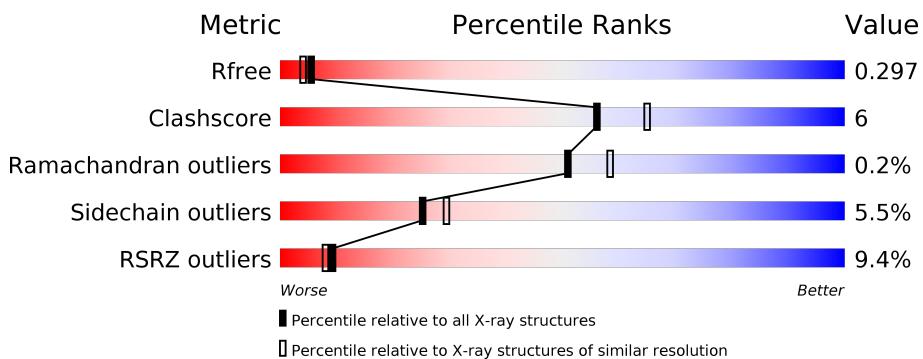
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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 <=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	307	9% / 79% 12% · 7%
1	B	307	8% / 82% 10% · 7%
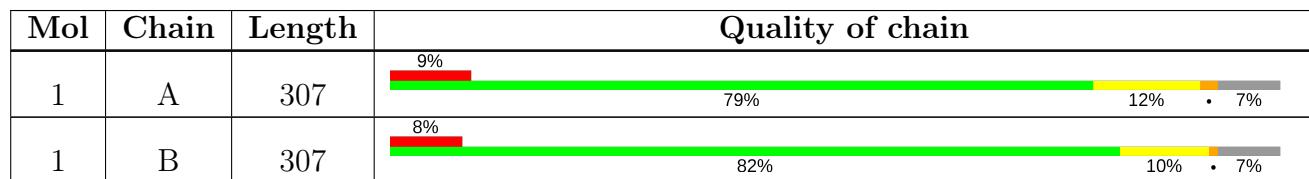
2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 4726 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 Interleukin-1 receptor-associated kinase 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	P	S	0	1	0
			2268	1421	379	451	3	14			
1	B	284	Total	C	N	O	P	S	0	0	0
			2240	1407	375	442	2	14			

- Molecule 2 is 3-NITRO-N-[1-PHENYL-5-(PIPERIDIN-1-YLMETHYL)-1H-BENZIMIDAZOL-2-YL]BENZAMIDE (three-letter code: T20) (formula: $C_{26}H_{25}N_5O_3$).
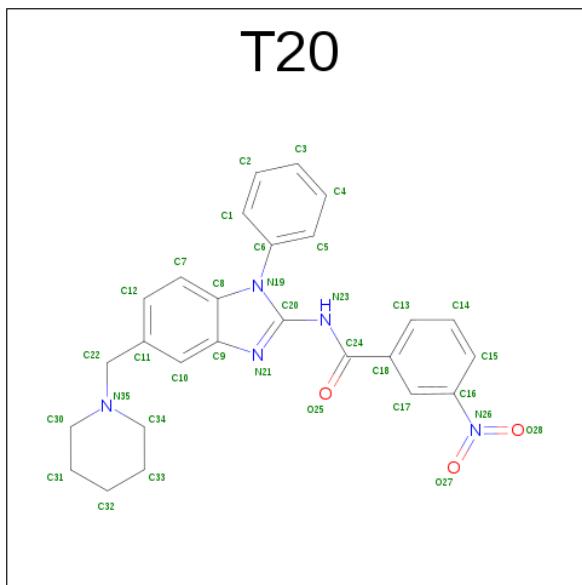
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			34	26	5	3		
2	B	1	Total	C	N	O	0	0
			34	26	5	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	72	Total O 72 72	0	0
3	B	78	Total O 78 78	0	0

3 Residue-property plots ⓘ

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: Interleukin-1 receptor-associated kinase 4
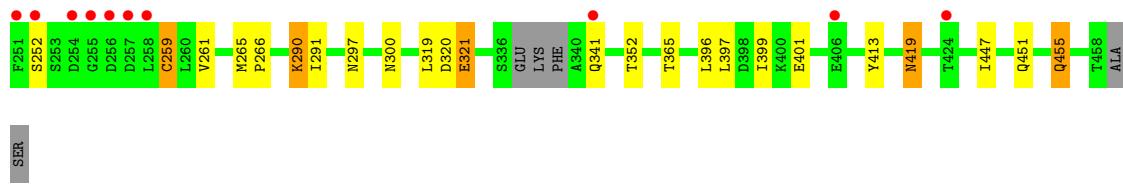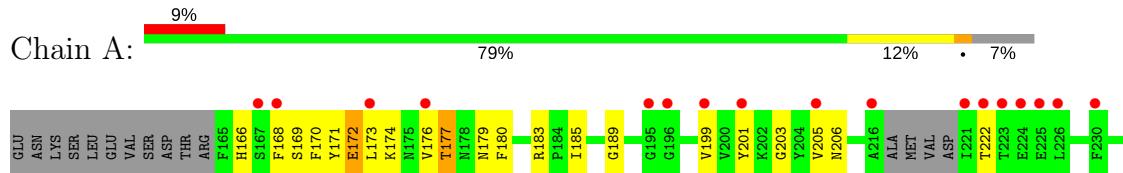
• Molecule 1: Interleukin-1 receptor-associated kinase 4
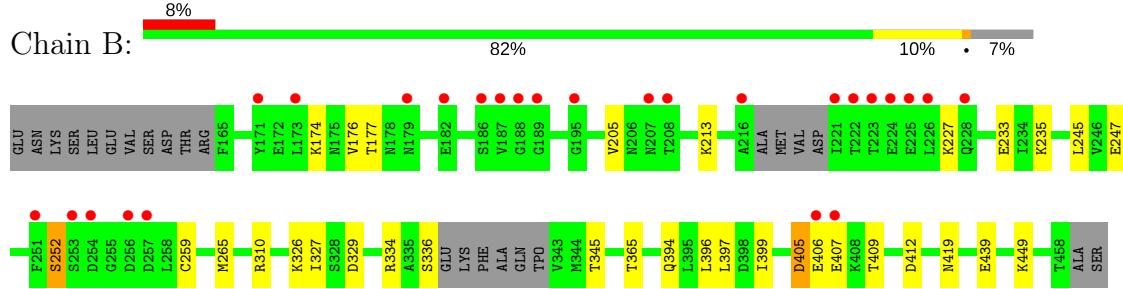
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	87.73Å 116.81Å 140.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 43.87 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-2.20) 99.6 (43.87-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.73 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.236 , 0.296 0.240 , 0.297	Depositor DCC
R_{free} test set	1862 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	30.6	Xtriage
Anisotropy	0.885	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 36.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4726	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.30% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< \|L\| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, T20, SEP

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	0.56	0/2274	0.74	0/3062
1	B	0.49	0/2255	0.66	0/3038
All	All	0.53	0/4529	0.70	0/6100

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2268	0	2230	40	0
1	B	2240	0	2205	12	0
2	A	34	0	0	2	0
2	B	34	0	0	1	0
3	A	72	0	0	6	1
3	B	78	0	0	2	0
All	All	4726	0	4435	52	1

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 (52) 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:199:VAL:HG12	3:A:615:HOH:O	1.72	0.89
1:A:174:LYS:HG2	1:A:179:ASN:HA	1.58	0.86
1:B:405:ASP:O	1:B:407:GLU:N	2.26	0.68
1:A:265:MET:CE	1:A:320:ASP:HB3	2.24	0.67
1:A:203:GLY:HA3	3:A:622:HOH:O	1.94	0.67
1:A:166:HIS:CD2	1:A:168:PHE:HE1	2.13	0.66
1:A:265:MET:HE1	1:A:320:ASP:HB3	1.79	0.64
1:A:172:GLU:O	1:A:176:VAL:HG22	1.97	0.64
1:A:171:TYR:HB2	3:A:619:HOH:O	2.03	0.57
1:A:199:VAL:HG13	1:A:201:TYR:HE1	1.70	0.57
1:A:205:VAL:O	1:A:205:VAL:HG12	2.04	0.55
1:B:334:ARG:NH2	1:B:345:TPO:O1P	2.40	0.55
1:A:419:ASN:C	1:A:419:ASN:HD22	2.11	0.54
1:B:245:LEU:HD23	1:B:327:ILE:HB	1.89	0.53
1:A:396:LEU:O	1:A:399:ILE:HB	2.09	0.52
1:A:166:HIS:CD2	1:A:168:PHE:CE1	2.96	0.52
1:B:310:ARG:HD2	3:B:633:HOH:O	2.10	0.51
1:B:409:THR:HG22	1:B:412:ASP:OD2	2.12	0.49
1:B:396:LEU:O	1:B:399:ILE:HB	2.12	0.49
1:A:174:LYS:HD2	1:A:179:ASN:HD22	1.79	0.48
1:B:213:LYS:HE3	2:B:501:T20:O28	2.14	0.48
1:A:300:ASN:HA	1:A:447:ILE:HG21	1.96	0.48
1:A:179:ASN:O	1:A:180:PHE:C	2.53	0.47
1:A:185:ILE:HD11	2:A:501:T20:C22	2.44	0.47
1:A:265:MET:HE3	1:A:320:ASP:N	2.30	0.47
1:B:176:VAL:HG23	1:B:177:THR:HG23	1.96	0.47
1:A:265:MET:HE3	1:A:320:ASP:CA	2.46	0.46
1:A:266:PRO:HD2	1:A:320:ASP:HA	1.96	0.46
1:A:169[A]:SER:OG	1:A:172:GLU:HG2	2.16	0.46
1:B:252:SER:HB3	1:B:259:CYS:HB2	1.97	0.46
1:A:321:GLU:CD	1:A:321:GLU:H	2.19	0.46
1:A:290:LYS:HG3	1:A:291:ILE:N	2.31	0.46
1:A:455:GLN:NE2	3:A:632:HOH:O	2.43	0.45
1:A:174:LYS:HD2	1:A:179:ASN:ND2	2.31	0.45
1:A:203:GLY:CA	3:A:622:HOH:O	2.60	0.45
1:A:168:PHE:CD2	1:A:261:VAL:HG21	2.51	0.45
1:A:169[B]:SER:HB3	3:A:603:HOH:O	2.17	0.44
1:B:176:VAL:HG11	1:B:205:VAL:HG12	1.99	0.44
1:A:252:SER:HB3	1:A:259:CYS:HB2	1.99	0.43
1:A:170:PHE:O	1:A:173:LEU:N	2.49	0.43
1:A:199:VAL:HG13	1:A:201:TYR:CE1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:GLU:HG3	3:B:654:HOH:O	2.18	0.43
1:A:185:ILE:HD11	2:A:501:T20:C11	2.49	0.42
1:B:265:MET:CE	1:B:326:LYS:HD2	2.50	0.42
1:A:419:ASN:C	1:A:419:ASN:ND2	2.73	0.41
1:A:297:ASN:ND2	1:A:451:GLN:OE1	2.52	0.41
1:A:399:ILE:HG13	1:A:413:TYR:CZ	2.55	0.41
1:A:265:MET:HE3	1:A:319:LEU:C	2.40	0.41
1:A:173:LEU:O	1:A:177:THR:HB	2.20	0.41
1:A:183:ARG:O	1:A:189:GLY:HA3	2.20	0.41
1:A:205:VAL:O	1:A:206:ASN:HB3	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:620:HOH:O	3:A:620:HOH:O[4_585]	2.12	0.08

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	279/307 (91%)	262 (94%)	17 (6%)	0	100	100
1	B	276/307 (90%)	264 (96%)	11 (4%)	1 (0%)	38	41
All	All	555/614 (90%)	526 (95%)	28 (5%)	1 (0%)	51	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	406	GLU

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	248/265 (94%)	235 (95%)	13 (5%)	27	32
1	B	246/265 (93%)	232 (94%)	14 (6%)	24	28
All	All	494/530 (93%)	467 (94%)	27 (6%)	25	29

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	GLU
1	A	177	THR
1	A	222	THR
1	A	259	CYS
1	A	290	LYS
1	A	321	GLU
1	A	341	GLN
1	A	352	THR
1	A	365	THR
1	A	397	LEU
1	A	401	GLU
1	A	419	ASN
1	A	455	GLN
1	B	174	LYS
1	B	227	LYS
1	B	233	GLU
1	B	235	LYS
1	B	252	SER
1	B	329	ASP
1	B	336	SER
1	B	365	THR
1	B	394	GLN
1	B	397	LEU
1	B	405	ASP
1	B	419	ASN
1	B	439	GLU
1	B	449	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	HIS
1	A	179	ASN
1	A	293	GLN
1	A	297	ASN
1	A	394	GLN
1	A	419	ASN
1	A	451	GLN
1	A	455	GLN
1	B	166	HIS
1	B	178	ASN
1	B	419	ASN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

5 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	TPO	A	342	1	9,10,11	0.63	0	10,14,16	1.30	1 (10%)
1	TPO	A	345	1	9,10,11	0.94	1 (11%)	10,14,16	1.13	0
1	SEP	A	346	1	9,9,10	0.57	0	9,12,14	1.31	0
1	TPO	B	345	1	9,10,11	0.77	0	10,14,16	1.12	1 (10%)
1	SEP	B	346	1	9,9,10	0.60	0	9,12,14	1.38	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
1	TPO	A	342	1	-	0/8/11/13	0/0/0/0
1	TPO	A	345	1	-	1/8/11/13	0/0/0/0
1	SEP	A	346	1	-	0/5/8/10	0/0/0/0
1	TPO	B	345	1	-	1/8/11/13	0/0/0/0
1	SEP	B	346	1	-	0/5/8/10	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	345	TPO	P-OG1	2.02	1.63	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	345	TPO	O3P-P-O2P	2.02	115.75	107.61
1	A	342	TPO	O3P-P-O2P	2.14	116.23	107.61

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	345	TPO	OG1-CB-CA-N
1	B	345	TPO	OG1-CB-CA-N

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	345	TPO	1	0

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	T20	A	501	-	37,38,38	2.37	10 (27%)	42,53,53	1.69	3 (7%)
2	T20	B	501	-	37,38,38	2.27	11 (29%)	42,53,53	1.73	7 (16%)

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	T20	A	501	-	-	0/18/28/28	0/5/5/5
2	T20	B	501	-	-	0/18/28/28	0/5/5/5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	T20	C22-C11	2.03	1.55	1.51
2	B	501	T20	C17-C16	2.08	1.41	1.38
2	B	501	T20	C2-C3	2.17	1.43	1.38
2	B	501	T20	C14-C13	2.20	1.43	1.38
2	B	501	T20	O25-C24	2.28	1.28	1.23
2	A	501	T20	O25-C24	2.43	1.28	1.23
2	B	501	T20	C22-C11	2.47	1.56	1.51
2	A	501	T20	C7-C8	2.75	1.46	1.41
2	A	501	T20	C17-C16	2.78	1.42	1.38
2	A	501	T20	C24-N23	3.44	1.44	1.35
2	B	501	T20	C12-C11	3.82	1.46	1.38
2	B	501	T20	C24-N23	3.89	1.45	1.35
2	A	501	T20	O27-N26	3.98	1.31	1.22
2	A	501	T20	C12-C11	4.31	1.47	1.38
2	B	501	T20	O28-N26	4.46	1.33	1.22
2	B	501	T20	O27-N26	4.64	1.33	1.22
2	A	501	T20	C5-C6	4.74	1.47	1.38
2	A	501	T20	O28-N26	4.94	1.34	1.22
2	B	501	T20	C5-C6	5.10	1.47	1.38
2	B	501	T20	C20-N23	6.72	1.46	1.35
2	A	501	T20	C20-N23	7.66	1.48	1.35

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	T20	C22-N35-C30	-3.88	102.87	111.08
2	A	501	T20	C22-N35-C30	-3.51	103.65	111.08
2	A	501	T20	O25-C24-N23	-2.35	118.32	123.69
2	B	501	T20	C17-C16-N26	-2.25	115.99	118.68
2	B	501	T20	C4-C5-C6	2.12	121.35	118.66
2	B	501	T20	C18-C17-C16	2.43	120.70	118.72
2	B	501	T20	C15-C16-N26	2.57	122.73	118.92
2	B	501	T20	C31-C30-N35	2.75	115.99	111.40
2	B	501	T20	C22-N35-C34	7.61	127.20	111.08
2	A	501	T20	C22-N35-C34	8.70	129.50	111.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	T20	2	0
2	B	501	T20	1	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(Å²)	Q<0.9
1	A	284/307 (92%)	0.39	27 (9%)	9	8	21, 38, 72, 96	0
1	B	282/307 (91%)	0.30	26 (9%)	10	8	19, 38, 76, 98	0
All	All	566/614 (92%)	0.35	53 (9%)	9	8	19, 38, 75, 98	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	195	GLY	7.0
1	A	257	ASP	6.4
1	B	254	ASP	6.4
1	B	256	ASP	6.2
1	A	255	GLY	5.6
1	B	188	GLY	4.2
1	A	221	ILE	4.2
1	A	252	SER	4.1
1	B	207	ASN	3.9
1	B	189	GLY	3.8
1	A	223	THR	3.8
1	A	254	ASP	3.6
1	A	168	PHE	3.5
1	B	223	THR	3.4
1	B	251	PHE	3.3
1	A	173	LEU	3.3
1	B	222	THR	3.3
1	B	253	SER	2.9
1	A	196	GLY	2.9
1	B	216	ALA	2.8
1	A	216	ALA	2.7
1	B	226	LEU	2.7
1	A	406	GLU	2.7
1	B	221	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	251	PHE	2.6
1	B	179	ASN	2.5
1	B	406	GLU	2.5
1	B	257	ASP	2.5
1	B	228	GLN	2.5
1	A	167	SER	2.5
1	B	208	THR	2.5
1	A	222	THR	2.4
1	A	258	LEU	2.4
1	B	187	VAL	2.3
1	A	201	TYR	2.3
1	A	256	ASP	2.3
1	B	225	GLU	2.3
1	B	186	SER	2.3
1	A	199	VAL	2.3
1	A	226	LEU	2.2
1	B	224	GLU	2.2
1	B	407	GLU	2.2
1	A	205	VAL	2.2
1	B	171	TYR	2.1
1	A	224	GLU	2.1
1	A	225	GLU	2.1
1	B	195	GLY	2.1
1	A	424	THR	2.1
1	B	173	LEU	2.1
1	A	230	PHE	2.1
1	A	341	GLN	2.0
1	A	176	VAL	2.0
1	B	182	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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
1	SEP	A	346	10/11	0.83	0.17	-	43,56,76,78	0
1	TPO	B	345	11/12	0.92	0.10	-	41,44,56,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
1	SEP	B	346	10/11	0.88	0.15	-	46,56,69,69	0
1	TPO	A	345	11/12	0.95	0.09	-	38,39,48,48	0
1	TPO	A	342	11/12	0.90	0.17	-	51,69,78,78	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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(Å²)	Q<0.9
2	T20	B	501	34/34	0.94	0.13	-0.17	27,34,46,56	0
2	T20	A	501	34/34	0.88	0.16	-0.41	40,43,51,56	0

6.5 Other polymers ⓘ

There are no such residues in this entry.

W O R L D W I D E
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PROTEIN DATA BANK