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

wwPDB X-ray Structure Validation Summary Report (i)

May 23, 2020 – 01:03 am BST

PDB ID	:	5UIQ
Title	:	Crystal structure of IRAK4 in complex with compound 9
Authors	:	Han, S.; Chang, J.S.
Deposited on	:	2017-01-14
Resolution	:	2.64 Å(reported)

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

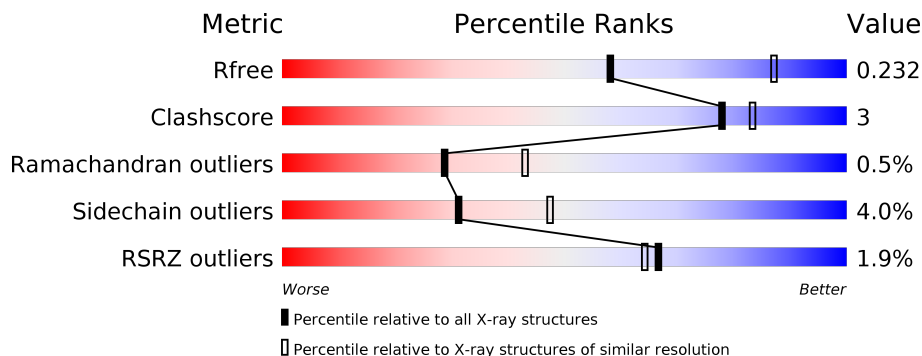|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 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		0.232
Clashscore		3
Ramachandran outliers		0.5%
Sidechain outliers		4.0%
RSRZ outliers		1.9%

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}	130704	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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 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 <=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	323	3% / 75% / 8% / 16%
1	B	323	% / 76% / 8% · 15%
1	C	323	2% / 75% / 12% · 12%
1	D	323	% / 76% / 9% / 15%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8759 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	271	Total	C	N	O	P	S	0	0	0
			2108	1322	351	418	3	14			
1	B	275	Total	C	N	O	P	S	0	1	0
			2155	1352	366	419	3	15			
1	C	283	Total	C	N	O	P	S	0	0	0
			2214	1387	374	436	3	14			
1	D	274	Total	C	N	O	P	S	0	0	0
			2167	1361	368	421	3	14			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	138	MET	-	initiating methionine	UNP Q9NWZ3
A	139	HIS	-	expression tag	UNP Q9NWZ3
A	140	HIS	-	expression tag	UNP Q9NWZ3
A	141	HIS	-	expression tag	UNP Q9NWZ3
A	142	HIS	-	expression tag	UNP Q9NWZ3
A	143	HIS	-	expression tag	UNP Q9NWZ3
A	144	HIS	-	expression tag	UNP Q9NWZ3
A	145	GLY	-	expression tag	UNP Q9NWZ3
A	146	GLY	-	expression tag	UNP Q9NWZ3
A	147	GLU	-	expression tag	UNP Q9NWZ3
A	148	ASN	-	expression tag	UNP Q9NWZ3
A	149	LEU	-	expression tag	UNP Q9NWZ3
A	150	TYR	-	expression tag	UNP Q9NWZ3
A	151	PHE	-	expression tag	UNP Q9NWZ3
A	152	GLN	-	expression tag	UNP Q9NWZ3
A	153	GLY	-	expression tag	UNP Q9NWZ3
B	138	MET	-	initiating methionine	UNP Q9NWZ3
B	139	HIS	-	expression tag	UNP Q9NWZ3
B	140	HIS	-	expression tag	UNP Q9NWZ3
B	141	HIS	-	expression tag	UNP Q9NWZ3
B	142	HIS	-	expression tag	UNP Q9NWZ3

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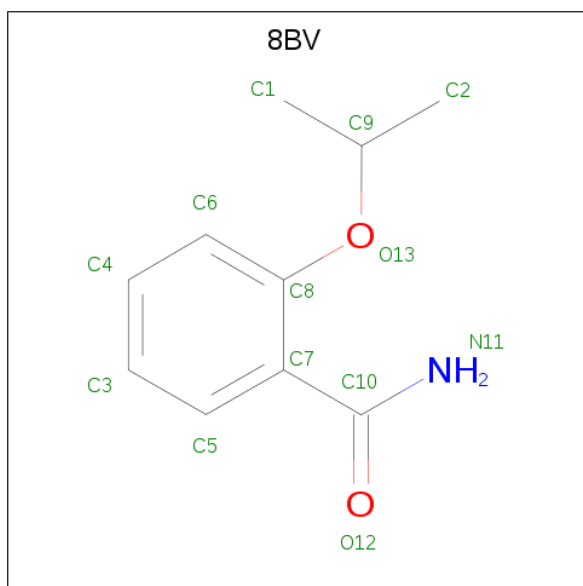
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Chain	Residue	Modelled	Actual	Comment	Reference
B	143	HIS	-	expression tag	UNP Q9NWZ3
B	144	HIS	-	expression tag	UNP Q9NWZ3
B	145	GLY	-	expression tag	UNP Q9NWZ3
B	146	GLY	-	expression tag	UNP Q9NWZ3
B	147	GLU	-	expression tag	UNP Q9NWZ3
B	148	ASN	-	expression tag	UNP Q9NWZ3
B	149	LEU	-	expression tag	UNP Q9NWZ3
B	150	TYR	-	expression tag	UNP Q9NWZ3
B	151	PHE	-	expression tag	UNP Q9NWZ3
B	152	GLN	-	expression tag	UNP Q9NWZ3
B	153	GLY	-	expression tag	UNP Q9NWZ3
C	138	MET	-	initiating methionine	UNP Q9NWZ3
C	139	HIS	-	expression tag	UNP Q9NWZ3
C	140	HIS	-	expression tag	UNP Q9NWZ3
C	141	HIS	-	expression tag	UNP Q9NWZ3
C	142	HIS	-	expression tag	UNP Q9NWZ3
C	143	HIS	-	expression tag	UNP Q9NWZ3
C	144	HIS	-	expression tag	UNP Q9NWZ3
C	145	GLY	-	expression tag	UNP Q9NWZ3
C	146	GLY	-	expression tag	UNP Q9NWZ3
C	147	GLU	-	expression tag	UNP Q9NWZ3
C	148	ASN	-	expression tag	UNP Q9NWZ3
C	149	LEU	-	expression tag	UNP Q9NWZ3
C	150	TYR	-	expression tag	UNP Q9NWZ3
C	151	PHE	-	expression tag	UNP Q9NWZ3
C	152	GLN	-	expression tag	UNP Q9NWZ3
C	153	GLY	-	expression tag	UNP Q9NWZ3
D	138	MET	-	initiating methionine	UNP Q9NWZ3
D	139	HIS	-	expression tag	UNP Q9NWZ3
D	140	HIS	-	expression tag	UNP Q9NWZ3
D	141	HIS	-	expression tag	UNP Q9NWZ3
D	142	HIS	-	expression tag	UNP Q9NWZ3
D	143	HIS	-	expression tag	UNP Q9NWZ3
D	144	HIS	-	expression tag	UNP Q9NWZ3
D	145	GLY	-	expression tag	UNP Q9NWZ3
D	146	GLY	-	expression tag	UNP Q9NWZ3
D	147	GLU	-	expression tag	UNP Q9NWZ3
D	148	ASN	-	expression tag	UNP Q9NWZ3
D	149	LEU	-	expression tag	UNP Q9NWZ3
D	150	TYR	-	expression tag	UNP Q9NWZ3
D	151	PHE	-	expression tag	UNP Q9NWZ3
D	152	GLN	-	expression tag	UNP Q9NWZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	153	GLY	-	expression tag	UNP Q9NWZ3

- Molecule 2 is 2-[(propan-2-yl)oxy]benzamide (three-letter code: 8BV) (formula: $C_{10}H_{13}NO_2$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 13	C 10	N 1	O 2	0	0
2	B	1	Total 13	C 10	N 1	O 2	0	0
2	C	1	Total 13	C 10	N 1	O 2	0	0
2	D	1	Total 13	C 10	N 1	O 2	0	0

- Molecule 3 is water.

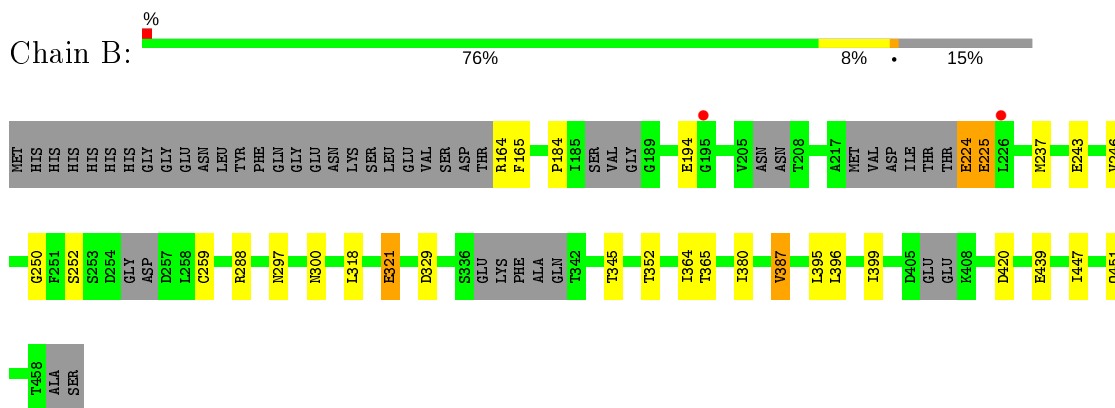| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	23	Total 23	O 23	0	0
3	B	13	Total 13	O 13	0	0
3	C	11	Total 11	O 11	0	0
3	D	16	Total 16	O 16	0	0

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.
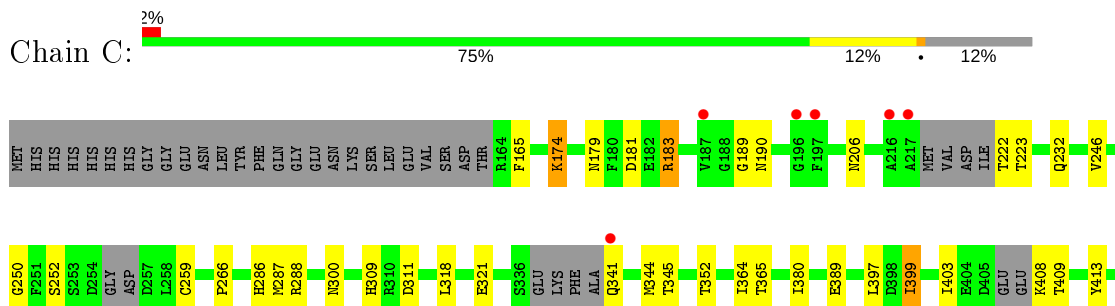
- Molecule 1: Interleukin-1 receptor-associated kinase 4
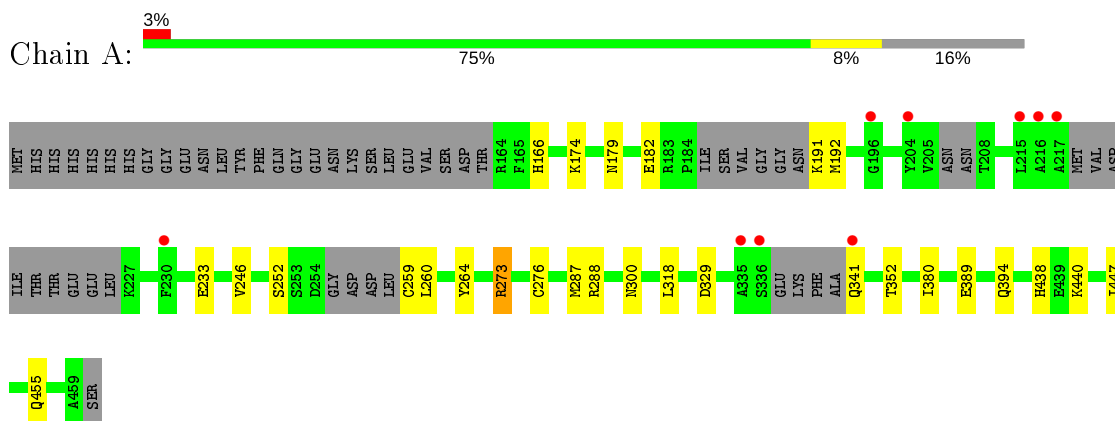
- Molecule 1: Interleukin-1 receptor-associated kinase 4

- Molecule 1: Interleukin-1 receptor-associated kinase 4

D420 I447 T458 ALA SER

• Molecule 1: Interleukin-1 receptor-associated kinase 4

Chain D:

%

76% 9% 15%

MET HIS HIS HIS HIS HIS GLY GLY GLU ASN LEU TYR PHE GLN GLY GLU ASN LYS SER LEU GLU VAL SER ASP THR R164 G193 GLU GLY G196 N206 N207 A216 ALA MET VAL ASP ILE THR THR GLU GLU L226 Q229 F230 E233 E243 V246 S252 S253 D254

GLY ASP D257 L258 C259 L260 P266 M287 R288 N300 E321 S328 D329 A335 SER GLU LYS PHE ALA GLN T342 T345 T352 I364 T365 I380 E389 Q394 L397 E402 D405 GLU GLU K408 K417 H438 I447 T458 ALA SER
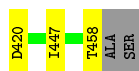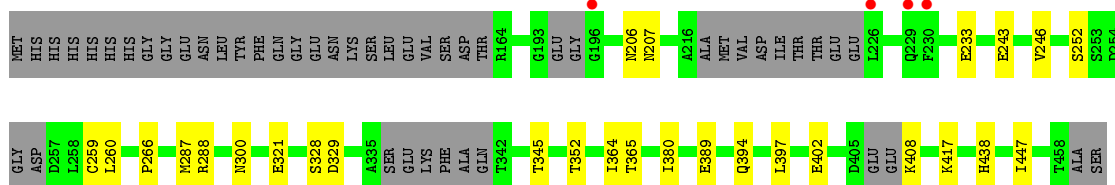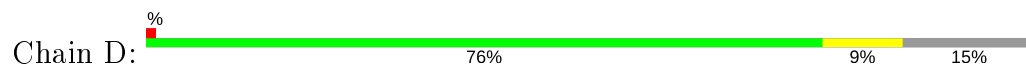
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	144.06Å 140.80Å 87.99Å 90.00° 124.90° 90.00°	Depositor
Resolution (Å)	19.86 – 2.64 19.86 – 2.64	Depositor EDS
% Data completeness (in resolution range)	94.7 (19.86-2.64) 94.9 (19.86-2.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.07 (at 2.63Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.198 , 0.226 0.202 , 0.232	Depositor DCC
R_{free} test set	1946 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å^2)	46.5	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 33.0	EDS
L-test for twinning[2]	$<|L|> = 0.49, <L^2> = 0.32$	Xtriage
Estimated twinning fraction	0.160 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8759	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.73% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, 8BV, 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	0.46	0/2107	0.65	0/2839
1	B	0.48	0/2158	0.65	0/2900
1	C	0.48	0/2215	0.66	0/2985
1	D	0.49	0/2167	0.66	0/2914
All	All	0.48	0/8647	0.66	0/11638

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 (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	2108	0	2025	12	0
1	B	2155	0	2118	15	0
1	C	2214	0	2153	14	0
1	D	2167	0	2147	12	0
2	A	13	0	0	0	0
2	B	13	0	0	0	0
2	C	13	0	0	0	0
2	D	13	0	0	0	0
3	A	23	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	13	0	0	0	0
3	C	11	0	0	0	0
3	D	16	0	0	0	0
All	All	8759	0	8443	50	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 3.

The worst 5 of 50 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:B:297:ASN:ND2	1:B:451:GLN:HE21	1.91	0.68
1:A:438:HIS:HD2	1:A:440:LYS:H	1.48	0.62
1:D:252:SER:HB3	1:D:259:CYS:HB2	1.82	0.61
1:B:321:GLU:O	1:D:243:GLU:HB2	2.01	0.61
1:B:387:VAL:HG13	1:B:395:LEU:HD23	1.85	0.59

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	256/323 (79%)	245 (96%)	10 (4%)	1 (0%)	34	48
1	B	260/323 (80%)	253 (97%)	5 (2%)	2 (1%)	19	28
1	C	270/323 (84%)	260 (96%)	9 (3%)	1 (0%)	34	48
1	D	260/323 (80%)	251 (96%)	8 (3%)	1 (0%)	34	48
All	All	1046/1292 (81%)	1009 (96%)	32 (3%)	5 (0%)	29	43

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	184	PRO
1	B	329	ASP
1	A	329	ASP
1	C	206	ASN
1	D	329	ASP

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	223/278 (80%)	217 (97%)	6 (3%)	44	63
1	B	231/278 (83%)	221 (96%)	10 (4%)	29	45
1	C	238/278 (86%)	223 (94%)	15 (6%)	18	27
1	D	236/278 (85%)	230 (98%)	6 (2%)	47	66
All	All	928/1112 (84%)	891 (96%)	37 (4%)	31	47

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	174	LYS
1	C	232	GLN
1	D	365	THR
1	C	183	ARG
1	C	222	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	190	ASN
1	C	232	GLN
1	D	207	ASN
1	B	394	GLN
1	C	175	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 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	SEP	A	346	1	8,9,10	0.81	0	8,12,14	2.18	2 (25%)
1	TPO	B	342	1	8,10,11	1.26	0	10,14,16	1.22	1 (10%)
1	SEP	B	346	1	8,9,10	0.91	0	8,12,14	1.49	3 (37%)
1	TPO	C	342	1	8,10,11	1.31	1 (12%)	10,14,16	2.19	2 (20%)
1	TPO	D	342	1	8,10,11	0.96	0	10,14,16	1.48	2 (20%)
1	TPO	B	345	1	8,10,11	0.84	0	10,14,16	1.42	1 (10%)
1	TPO	D	345	1	8,10,11	1.03	0	10,14,16	1.34	1 (10%)
1	SEP	C	346	1	8,9,10	0.89	0	8,12,14	2.24	2 (25%)
1	TPO	A	342	1	8,10,11	1.23	1 (12%)	10,14,16	2.52	3 (30%)
1	TPO	A	345	1	8,10,11	1.13	0	10,14,16	1.04	0
1	TPO	C	345	1	8,10,11	1.32	1 (12%)	10,14,16	0.94	0
1	SEP	D	346	1	8,9,10	0.92	0	8,12,14	2.30	1 (12%)

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	SEP	A	346	1	-	1/5/8/10	-
1	TPO	B	342	1	-	1/9/11/13	-
1	SEP	B	346	1	-	1/5/8/10	-
1	TPO	C	342	1	-	4/9/11/13	-
1	TPO	D	342	1	-	3/9/11/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	B	345	1	-	4/9/11/13	-
1	TPO	D	345	1	-	3/9/11/13	-
1	SEP	C	346	1	-	1/5/8/10	-
1	TPO	A	342	1	-	3/9/11/13	-
1	TPO	A	345	1	-	4/9/11/13	-
1	TPO	C	345	1	-	4/9/11/13	-
1	SEP	D	346	1	-	1/5/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	342	TPO	CG2-CB	2.33	1.57	1.51
1	A	342	TPO	CG2-CB	2.13	1.56	1.51
1	C	345	TPO	P-OG1	-2.05	1.55	1.59

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	346	SEP	OG-CB-CA	5.81	113.80	108.14
1	A	342	TPO	CG2-CB-CA	5.56	124.13	113.16
1	C	346	SEP	OG-CB-CA	5.25	113.26	108.14
1	A	346	SEP	OG-CB-CA	5.01	113.02	108.14
1	C	342	TPO	CG2-CB-CA	4.36	121.77	113.16

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	346	SEP	N-CA-CB-OG
1	B	342	TPO	CB-OG1-P-O3P
1	B	346	SEP	N-CA-CB-OG
1	C	342	TPO	N-CA-CB-OG1
1	C	342	TPO	C-CA-CB-CG2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

4 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	8BV	A	501	-	13,13,13	0.93	1 (7%)	17,17,17	1.17	2 (11%)
2	8BV	B	501	-	13,13,13	1.13	1 (7%)	17,17,17	1.41	3 (17%)
2	8BV	C	501	-	13,13,13	1.03	1 (7%)	17,17,17	1.29	3 (17%)
2	8BV	D	501	-	13,13,13	1.04	1 (7%)	17,17,17	1.47	3 (17%)

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	8BV	A	501	-	-	1/8/8/8	0/1/1/1
2	8BV	B	501	-	-	2/8/8/8	0/1/1/1
2	8BV	C	501	-	-	3/8/8/8	0/1/1/1
2	8BV	D	501	-	-	3/8/8/8	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	8BV	C10-N11	3.02	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	8BV	C10-N11	2.71	1.38	1.33
2	C	501	8BV	C10-N11	2.70	1.38	1.33
2	A	501	8BV	C10-N11	2.67	1.38	1.33

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	8BV	O13-C8-C7	3.14	121.81	116.57
2	A	501	8BV	C8-O13-C9	-2.97	113.80	119.53
2	B	501	8BV	C8-O13-C9	-2.91	113.93	119.53
2	B	501	8BV	C8-C7-C10	-2.75	123.20	125.10
2	D	501	8BV	O13-C9-C1	2.63	117.17	107.93

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	501	8BV	C7-C8-O13-C9
2	D	501	8BV	C6-C8-O13-C9
2	D	501	8BV	C1-C9-O13-C8
2	C	501	8BV	C2-C9-O13-C8
2	A	501	8BV	C2-C9-O13-C8

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	268/323 (82%)	-0.20	9 (3%)	45 41	31, 56, 116, 151	0
1	B	272/323 (84%)	-0.30	2 (0%)	87 86	30, 53, 97, 134	0
1	C	280/323 (86%)	-0.23	6 (2%)	63 60	28, 54, 105, 141	0
1	D	271/323 (83%)	-0.30	4 (1%)	73 71	30, 52, 94, 131	0
All	All	1091/1292 (84%)	-0.26	21 (1%)	66 64	28, 54, 104, 151	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	226	LEU	5.6
1	A	216	ALA	4.8
1	B	226	LEU	4.3
1	A	196	GLY	4.1
1	C	187	VAL	4.1

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	SEP	A	346	10/11	0.83	0.11	100,108,121,122	0
1	TPO	D	342	11/12	0.85	0.17	92,94,104,104	0
1	SEP	B	346	10/11	0.87	0.12	80,88,98,99	0
1	TPO	C	342	11/12	0.88	0.20	100,100,104,105	0
1	TPO	A	342	11/12	0.88	0.19	99,100,104,106	0
1	SEP	C	346	10/11	0.89	0.12	85,94,104,105	0
1	SEP	D	346	10/11	0.90	0.15	85,93,103,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
1	TPO	B	342	11/12	0.93	0.16	87,90,93,94	0
1	TPO	A	345	11/12	0.95	0.09	89,95,99,99	0
1	TPO	B	345	11/12	0.95	0.12	68,74,79,79	0
1	TPO	C	345	11/12	0.97	0.12	72,78,84,85	0
1	TPO	D	345	11/12	0.97	0.11	73,79,83,85	0

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. 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
2	8BV	D	501	13/13	0.94	0.17	46,46,49,50	0
2	8BV	B	501	13/13	0.97	0.14	39,41,44,46	0
2	8BV	C	501	13/13	0.97	0.17	54,56,59,60	0
2	8BV	A	501	13/13	0.97	0.14	47,49,51,52	0

6.5 Other polymers (i)

There are no such residues in this entry.