



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 26, 2022 – 04:07 pm BST

PDB ID : 6TV6
Title : Octameric McsB from *Bacillus subtilis*.
Authors : Suskiewicz, M.J.; Hajdusits, B.; Meinhart, A.; Clausen, T.
Deposited on : 2020-01-09
Resolution : 2.50 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	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

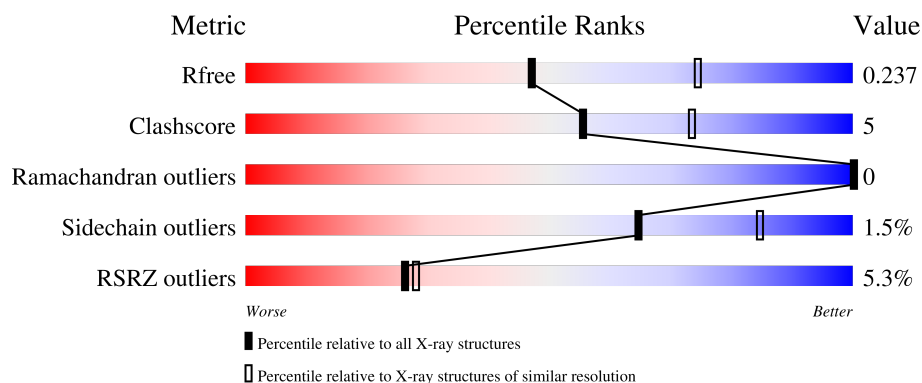
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	374	<div> <div>8%</div> <div>82%</div> <div>14%</div> <div>• •</div> </div>
1	B	374	<div> <div>4%</div> <div>84%</div> <div>10%</div> <div>6%</div> </div>
1	C	374	<div> <div>2%</div> <div>84%</div> <div>10%</div> <div>6%</div> </div>
1	D	374	<div> <div>6%</div> <div>80%</div> <div>12%</div> <div>• 6%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11404 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 Protein-arginine kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	P	S	0	0	0
			2880	1799	510	555	1	15			
1	B	353	Total	C	N	O	P	S	0	0	0
			2809	1758	496	539	1	15			
1	C	352	Total	C	N	O	P	S	0	0	0
			2798	1752	495	535	1	15			
1	D	351	Total	C	N	O	P	S	0	0	0
			2796	1751	494	535	1	15			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	initiating methionine	UNP P37570
A	-1	ALA	-	expression tag	UNP P37570
A	0	SER	-	expression tag	UNP P37570
A	364	LEU	-	expression tag	UNP P37570
A	365	GLU	-	expression tag	UNP P37570
A	366	HIS	-	expression tag	UNP P37570
A	367	HIS	-	expression tag	UNP P37570
A	368	HIS	-	expression tag	UNP P37570
A	369	HIS	-	expression tag	UNP P37570
A	370	HIS	-	expression tag	UNP P37570
A	371	HIS	-	expression tag	UNP P37570
B	-2	MET	-	initiating methionine	UNP P37570
B	-1	ALA	-	expression tag	UNP P37570
B	0	SER	-	expression tag	UNP P37570
B	364	LEU	-	expression tag	UNP P37570
B	365	GLU	-	expression tag	UNP P37570
B	366	HIS	-	expression tag	UNP P37570
B	367	HIS	-	expression tag	UNP P37570
B	368	HIS	-	expression tag	UNP P37570
B	369	HIS	-	expression tag	UNP P37570
B	370	HIS	-	expression tag	UNP P37570

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	371	HIS	-	expression tag	UNP P37570
C	-2	MET	-	initiating methionine	UNP P37570
C	-1	ALA	-	expression tag	UNP P37570
C	0	SER	-	expression tag	UNP P37570
C	364	LEU	-	expression tag	UNP P37570
C	365	GLU	-	expression tag	UNP P37570
C	366	HIS	-	expression tag	UNP P37570
C	367	HIS	-	expression tag	UNP P37570
C	368	HIS	-	expression tag	UNP P37570
C	369	HIS	-	expression tag	UNP P37570
C	370	HIS	-	expression tag	UNP P37570
C	371	HIS	-	expression tag	UNP P37570
D	-2	MET	-	initiating methionine	UNP P37570
D	-1	ALA	-	expression tag	UNP P37570
D	0	SER	-	expression tag	UNP P37570
D	364	LEU	-	expression tag	UNP P37570
D	365	GLU	-	expression tag	UNP P37570
D	366	HIS	-	expression tag	UNP P37570
D	367	HIS	-	expression tag	UNP P37570
D	368	HIS	-	expression tag	UNP P37570
D	369	HIS	-	expression tag	UNP P37570
D	370	HIS	-	expression tag	UNP P37570
D	371	HIS	-	expression tag	UNP P37570

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	25	Total O 25 25	0	0

Continued on next page...

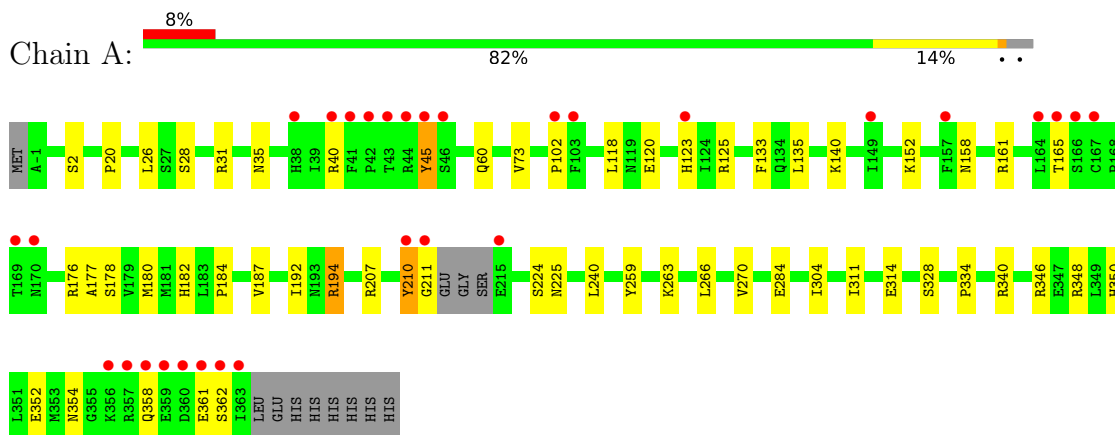
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	24	Total 24	O 24	0	0
3	C	40	Total 40	O 40	0	0
3	D	28	Total 28	O 28	0	0

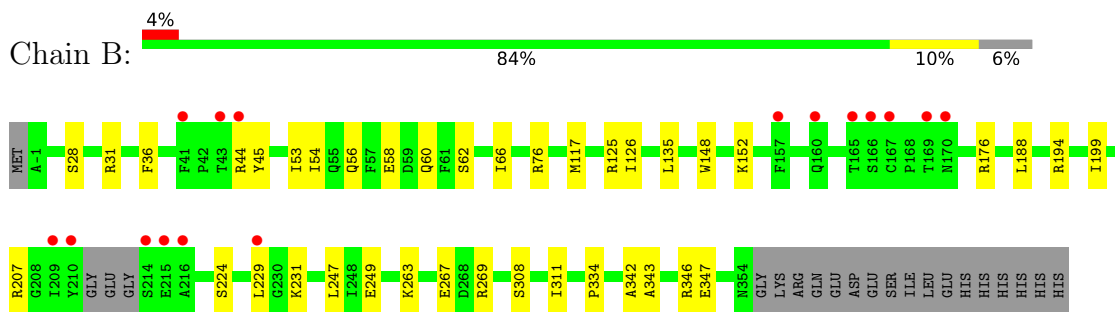
3 Residue-property plots [i](#)

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.

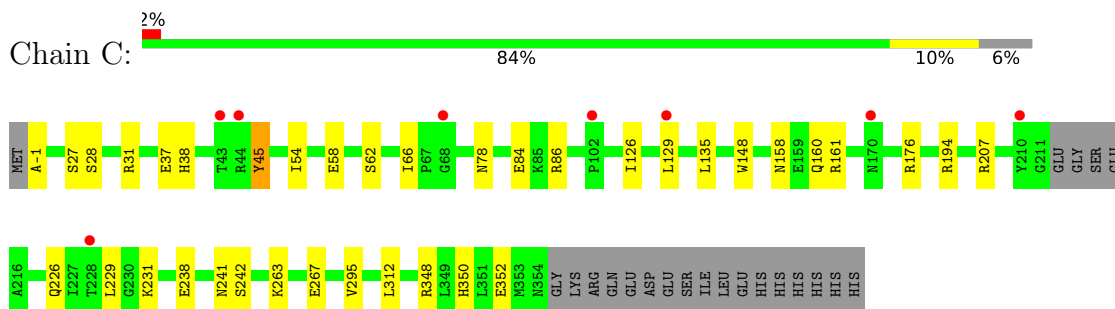
- Molecule 1: Protein-arginine kinase



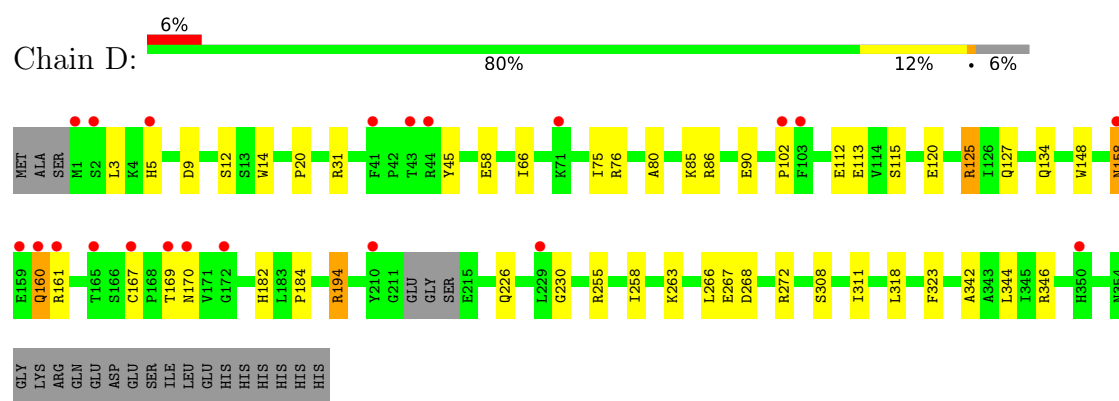
- Molecule 1: Protein-arginine kinase



- Molecule 1: Protein-arginine kinase



- Molecule 1: Protein-arginine kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	137.79Å 147.64Å 81.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.90 – 2.50 43.86 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (43.90-2.50) 99.8 (43.86-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.51Å)	Xtrriage
Refinement program	PHENIX 1.16	Depositor
R, R_{free}	0.195 , 0.237 0.193 , 0.237	Depositor DCC
R_{free} test set	2908 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	50.4	Xtrriage
Anisotropy	0.382	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11404	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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: RPI, MG

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	0/2904	0.62	0/3911
1	B	0.48	0/2833	0.64	0/3818
1	C	0.46	0/2822	0.61	0/3803
1	D	0.45	0/2820	0.61	0/3800
All	All	0.46	0/11379	0.62	0/15332

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	2880	0	2882	37	0
1	B	2809	0	2815	22	0
1	C	2798	0	2807	25	0
1	D	2796	0	2803	35	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	25	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	24	0	0	0	0
3	C	40	0	0	2	0
3	D	28	0	0	1	0
All	All	11404	0	11307	115	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 5.

All (115) 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:358:GLN:O	1:A:361:GLU:HG2	1.64	0.97
1:D:160:GLN:HE21	1:D:161:ARG:NH2	1.72	0.87
1:A:31:ARG:NH2	1:A:176:ARG:HD3	1.96	0.80
1:A:178:SER:HB3	1:A:224:SER:HB3	1.67	0.77
1:A:361:GLU:HG3	1:A:362:SER:N	2.02	0.73
1:A:259:TYR:CZ	1:A:263:LYS:HE2	2.23	0.73
1:D:80:ALA:O	1:D:85:LYS:HE2	1.89	0.72
1:A:102:PRO:HG3	1:D:230:GLY:HA3	1.71	0.72
1:B:176:ARG:HH12	1:B:207:ARG:HH12	1.37	0.71
1:D:31:ARG:NH2	1:D:170:ASN:HD21	1.87	0.71
1:D:120:GLU:OE2	1:D:125:ARG:NH1	2.24	0.71
1:A:210:TYR:HD1	1:A:210:TYR:H	1.41	0.69
1:D:31:ARG:HH22	1:D:170:ASN:HD21	1.41	0.68
1:D:160:GLN:NE2	1:D:161:ARG:NH2	2.42	0.67
1:A:31:ARG:HD3	1:A:125:ARG:HG2	1.78	0.66
1:B:343:ALA:O	1:B:347:GLU:HG2	1.99	0.63
1:D:5:HIS:CE1	1:D:9:ASP:OD2	2.54	0.60
1:A:20:PRO:HG2	1:A:133:PHE:O	2.01	0.60
1:C:176:ARG:HH22	1:C:207:ARG:HH22	1.48	0.60
1:D:258:ILE:HG22	1:D:266:LEU:HD22	1.84	0.60
1:C:160:GLN:HG3	1:C:161:ARG:HG3	1.85	0.59
1:D:167:CYS:HG	1:D:169:THR:HG1	1.51	0.58
1:D:3:LEU:HD13	1:D:75:ILE:HD12	1.86	0.57
1:C:348:ARG:O	1:C:352:GLU:HG2	2.04	0.57
1:B:54:ILE:HD11	1:B:76:ARG:HG2	1.87	0.57
1:A:187:VAL:HG22	1:A:192:ILE:HG21	1.87	0.56
1:B:176:ARG:NH1	1:B:207:ARG:HH12	2.03	0.56
1:D:160:GLN:HE21	1:D:161:ARG:HH21	1.52	0.56
1:C:-1:ALA:HB2	1:C:84:GLU:OE2	2.06	0.56
1:D:308:SER:HB3	1:D:311:ILE:HD12	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:GLN:NE2	1:B:152:LYS:HD3	2.21	0.55
1:A:350:HIS:CE1	1:A:354:ASN:ND2	2.75	0.55
1:A:178:SER:HB3	1:A:224:SER:CB	2.37	0.55
1:C:226:GLN:OE1	1:C:226:GLN:HA	2.05	0.55
1:B:188:LEU:HD21	1:B:269:ARG:CZ	2.38	0.53
1:A:210:TYR:CD1	1:A:210:TYR:N	2.73	0.53
1:D:20:PRO:HD2	1:D:134:GLN:HG2	1.90	0.52
1:C:231:LYS:NZ	3:C:601:HOH:O	2.40	0.52
1:D:115:SER:O	1:D:127:GLN:HG2	2.09	0.52
1:B:263:LYS:O	1:B:267:GLU:HG3	2.10	0.51
1:D:160:GLN:NE2	1:D:161:ARG:HH22	2.08	0.51
1:B:56:GLN:HG2	1:B:60:GLN:OE1	2.11	0.51
1:D:66:ILE:HD11	1:D:148:TRP:CE3	2.46	0.51
1:A:207:ARG:HD3	1:A:211:GLY:O	2.11	0.51
1:B:176:ARG:HH22	1:B:207:ARG:NH2	2.09	0.51
1:C:28:SER:HB3	1:C:135:LEU:HD23	1.92	0.51
1:D:5:HIS:HE1	1:D:9:ASP:OD2	1.94	0.50
1:B:58:GLU:HA	1:B:62:SER:HB2	1.93	0.50
1:C:45:TYR:HD1	1:C:45:TYR:O	1.92	0.50
1:A:28:SER:HB3	1:A:135:LEU:HD23	1.94	0.49
1:C:295:VAL:HG12	1:C:312:LEU:HD11	1.95	0.49
1:C:66:ILE:HD11	1:C:148:TRP:CE3	2.48	0.48
1:C:58:GLU:HA	1:C:62:SER:HB2	1.96	0.48
1:A:31:ARG:NH2	1:A:176:ARG:CD	2.71	0.48
1:D:31:ARG:HH22	1:D:170:ASN:ND2	2.11	0.48
1:A:2:SER:HB3	1:A:73:VAL:HG11	1.96	0.47
1:A:40:ARG:O	1:A:45:TYR:HB3	2.13	0.47
1:A:314:GLU:OE2	1:A:348:ARG:NH1	2.48	0.47
1:C:27:SER:HB2	1:C:129:LEU:HD11	1.96	0.47
1:C:176:ARG:HH22	1:C:207:ARG:NH2	2.12	0.47
1:C:31:ARG:HA	1:C:126:ILE:O	2.15	0.47
1:D:158:ASN:OD1	1:D:161:ARG:N	2.48	0.47
1:D:184:PRO:HD2	1:D:255:ARG:HH21	1.80	0.47
1:D:263:LYS:O	1:D:267:GLU:HG3	2.15	0.47
1:D:318:LEU:HD22	1:D:344:LEU:HD11	1.95	0.47
1:B:36:PHE:CE1	1:B:53:ILE:HG23	2.50	0.47
1:C:348:ARG:HD2	1:C:348:ARG:HA	1.74	0.47
1:A:266:LEU:O	1:A:270:VAL:HG13	2.14	0.46
1:A:118:LEU:HA	1:A:123:HIS:O	2.16	0.46
1:D:342:ALA:O	1:D:346:ARG:HB2	2.16	0.46
1:B:31:ARG:HA	1:B:126:ILE:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:GLN:CG	1:B:60:GLN:OE1	2.64	0.45
1:C:160:GLN:HG3	1:C:161:ARG:CG	2.45	0.45
1:A:177:ALA:O	1:A:240:LEU:HD22	2.16	0.45
1:A:194:RPI:CZ	1:B:334:PRO:HB3	2.47	0.45
1:A:334:PRO:HB3	1:D:194:RPI:CZ	2.47	0.45
1:D:182:HIS:CD2	1:D:184:PRO:HD3	2.52	0.45
1:A:284:GLU:HB3	3:D:601:HOH:O	2.16	0.45
1:A:361:GLU:CG	1:A:362:SER:N	2.75	0.45
1:C:263:LYS:O	1:C:267:GLU:HG3	2.17	0.45
1:A:178:SER:CB	1:A:224:SER:HB3	2.43	0.45
1:A:2:SER:CB	1:A:73:VAL:HG11	2.48	0.44
1:D:58:GLU:OE1	1:D:76:ARG:NH2	2.35	0.44
1:A:60:GLN:HB3	1:A:152:LYS:HD2	2.00	0.43
1:A:26:LEU:HD12	1:A:180:MET:HG2	2.00	0.43
1:D:90:GLU:OE1	1:D:323:PHE:N	2.48	0.43
1:D:226:GLN:HA	1:D:226:GLN:OE1	2.18	0.43
1:C:86:ARG:HD2	1:C:86:ARG:HA	1.83	0.43
1:C:238:GLU:OE2	1:C:242:SER:HB3	2.18	0.43
1:C:37:GLU:HG3	1:C:38:HIS:CE1	2.54	0.43
1:D:86:ARG:HD2	1:D:86:ARG:HA	1.87	0.42
1:A:350:HIS:CE1	1:A:354:ASN:HD21	2.37	0.42
1:C:350:HIS:HB2	3:C:634:HOH:O	2.19	0.42
1:D:268:ASP:OD1	1:D:272:ARG:HD2	2.19	0.42
1:B:342:ALA:O	1:B:346:ARG:HB2	2.20	0.42
1:B:28:SER:HB3	1:B:135:LEU:HD23	2.01	0.42
1:A:177:ALA:HB3	1:A:225:ASN:OD1	2.20	0.42
1:A:328:SER:HB3	1:A:340:ARG:NH1	2.35	0.42
1:B:229:LEU:HD12	1:B:229:LEU:HA	1.89	0.42
1:B:66:ILE:HD11	1:B:148:TRP:CE3	2.54	0.42
1:C:229:LEU:O	1:D:102:PRO:HG2	2.20	0.41
1:A:311:ILE:HG13	1:A:352:GLU:HG3	2.01	0.41
1:A:35:ASN:ND2	1:A:165:THR:HA	2.35	0.41
1:D:160:GLN:HG2	1:D:161:ARG:HG3	2.02	0.41
1:A:140:LYS:HE2	1:A:140:LYS:HB3	1.82	0.41
1:B:308:SER:H	1:B:311:ILE:HD12	1.85	0.41
1:B:117:MET:HB2	1:B:125:ARG:HB3	2.02	0.41
1:D:14:TRP:CE2	1:D:113:GLU:HB2	2.55	0.41
1:A:182:HIS:CD2	1:A:184:PRO:HD3	2.56	0.41
1:B:231:LYS:HB3	1:B:231:LYS:HE3	1.96	0.40
1:C:31:ARG:C	1:C:31:ARG:HD2	2.41	0.40
1:C:135:LEU:HD12	1:C:241:ASN:OD1	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:LYS:HB3	1:C:231:LYS:HE3	1.82	0.40
1:B:199:ILE:HD11	1:B:247:LEU:HD11	2.02	0.40
1:D:12:SER:HB3	1:D:112:GLU:OE1	2.21	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	357/374 (96%)	350 (98%)	7 (2%)	0	100	100
1	B	348/374 (93%)	342 (98%)	6 (2%)	0	100	100
1	C	347/374 (93%)	340 (98%)	7 (2%)	0	100	100
1	D	346/374 (92%)	334 (96%)	12 (4%)	0	100	100
All	All	1398/1496 (93%)	1366 (98%)	32 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	318/329 (97%)	311 (98%)	7 (2%)	52	77
1	B	311/329 (94%)	307 (99%)	4 (1%)	69	87

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	309/329 (94%)	305 (99%)	4 (1%)	69	87
1	D	309/329 (94%)	305 (99%)	4 (1%)	69	87
All	All	1247/1316 (95%)	1228 (98%)	19 (2%)	65	85

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	TYR
1	A	120	GLU
1	A	158	ASN
1	A	161	ARG
1	A	210	TYR
1	A	304	ILE
1	A	346	ARG
1	B	44	ARG
1	B	45	TYR
1	B	224	SER
1	B	249	GLU
1	C	45	TYR
1	C	54	ILE
1	C	78	ASN
1	C	158	ASN
1	D	45	TYR
1	D	125	ARG
1	D	158	ASN
1	D	160	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	170	ASN
1	D	5	HIS
1	D	160	GLN
1	D	170	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	RPI	D	194	1	12,14,15	2.81	5 (41%)	10,18,20	3.44	5 (50%)
1	RPI	B	194	1	12,14,15	2.80	6 (50%)	10,18,20	3.68	6 (60%)
1	RPI	A	194	1	12,14,15	2.99	5 (41%)	10,18,20	3.07	5 (50%)
1	RPI	C	194	1	12,14,15	3.03	6 (50%)	10,18,20	3.58	4 (40%)

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	RPI	D	194	1	-	3/9/14/16	-
1	RPI	B	194	1	-	3/9/14/16	-
1	RPI	A	194	1	-	2/9/14/16	-
1	RPI	C	194	1	-	3/9/14/16	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	194	RPI	CZ-NH2	6.47	1.45	1.36
1	A	194	RPI	CZ-NH1	6.11	1.46	1.29
1	A	194	RPI	CZ-NH2	5.95	1.45	1.36
1	D	194	RPI	CZ-NH2	5.71	1.44	1.36
1	C	194	RPI	CZ-NH1	5.67	1.45	1.29
1	D	194	RPI	CZ-NH1	5.60	1.45	1.29
1	B	194	RPI	CZ-NH1	5.57	1.45	1.29
1	B	194	RPI	CZ-NH2	5.26	1.44	1.36
1	B	194	RPI	P-NH2	4.35	1.71	1.63
1	C	194	RPI	P-NH2	3.74	1.70	1.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	194	RPI	P-O2P	3.49	1.51	1.46
1	D	194	RPI	P-O2P	3.41	1.51	1.46
1	D	194	RPI	P-NH2	3.35	1.70	1.63
1	A	194	RPI	P-NH2	3.25	1.69	1.63
1	C	194	RPI	P-O2P	3.10	1.51	1.46
1	A	194	RPI	P-O1P	-2.63	1.49	1.56
1	B	194	RPI	P-O2P	2.46	1.50	1.46
1	C	194	RPI	P-O3P	-2.43	1.50	1.56
1	B	194	RPI	P-O3P	-2.38	1.50	1.56
1	C	194	RPI	P-O1P	-2.15	1.51	1.56
1	D	194	RPI	P-O3P	-2.04	1.51	1.56
1	B	194	RPI	P-O1P	-2.00	1.51	1.56

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	194	RPI	CD-NE-CZ	-9.44	106.27	123.50
1	B	194	RPI	CD-NE-CZ	-8.97	107.12	123.50
1	D	194	RPI	CD-NE-CZ	-8.44	108.10	123.50
1	A	194	RPI	CD-NE-CZ	-7.69	109.47	123.50
1	B	194	RPI	NE-CZ-NH1	-5.26	110.41	120.26
1	C	194	RPI	NE-CZ-NH1	-5.10	110.70	120.26
1	D	194	RPI	NE-CZ-NH1	-4.57	111.69	120.26
1	A	194	RPI	NE-CZ-NH1	-3.90	112.95	120.26
1	D	194	RPI	O2P-P-NH2	-3.42	104.55	111.17
1	B	194	RPI	P-NH2-CZ	-2.81	120.10	128.34
1	B	194	RPI	NE-CZ-NH2	-2.81	110.02	117.84
1	A	194	RPI	NE-CZ-NH2	-2.79	110.08	117.84
1	D	194	RPI	NE-CZ-NH2	-2.72	110.27	117.84
1	B	194	RPI	O2P-P-NH2	-2.22	106.87	111.17
1	B	194	RPI	O3P-P-O2P	-2.14	108.06	113.45
1	A	194	RPI	P-NH2-CZ	-2.10	122.18	128.34
1	D	194	RPI	P-NH2-CZ	-2.10	122.19	128.34
1	C	194	RPI	O1P-P-O2P	-2.09	108.20	113.45
1	A	194	RPI	O1P-P-O2P	-2.08	108.22	113.45
1	C	194	RPI	P-NH2-CZ	-2.05	122.33	128.34

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	194	RPI	NH1-CZ-NE-CD

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	B	194	RPI	CZ-NH2-P-O2P
1	B	194	RPI	NH1-CZ-NE-CD
1	C	194	RPI	CZ-NH2-P-O2P
1	C	194	RPI	NH1-CZ-NE-CD
1	D	194	RPI	NH1-CZ-NE-CD
1	D	194	RPI	CZ-NH2-P-O2P
1	B	194	RPI	CG-CD-NE-CZ
1	C	194	RPI	CG-CD-NE-CZ
1	A	194	RPI	CG-CD-NE-CZ
1	D	194	RPI	CG-CD-NE-CZ

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	194	RPI	1	0
1	A	194	RPI	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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 ⓘ

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	361/374 (96%)	0.57	30 (8%)	11 11	37, 55, 86, 118	0
1	B	352/374 (94%)	0.28	16 (4%)	33 36	34, 51, 75, 98	0
1	C	351/374 (93%)	0.29	8 (2%)	60 63	35, 50, 73, 93	0
1	D	350/374 (93%)	0.44	21 (6%)	21 22	39, 53, 81, 120	0
All	All	1414/1496 (94%)	0.40	75 (5%)	26 28	34, 52, 79, 120	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	11.0
1	A	363	ILE	8.8
1	D	161	ARG	6.2
1	A	360	ASP	6.1
1	A	361	GLU	5.8
1	D	43	THR	5.3
1	B	209	ILE	4.9
1	A	362	SER	4.8
1	A	169	THR	4.7
1	B	170	ASN	4.7
1	A	358	GLN	4.5
1	B	43	THR	4.4
1	A	41	PHE	4.4
1	D	158	ASN	4.3
1	D	169	THR	4.2
1	D	210	TYR	4.2
1	D	159	GLU	3.9
1	D	160	GLN	3.9
1	A	357	ARG	3.9
1	A	103	PHE	3.8
1	B	167	CYS	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	214	SER	3.7
1	A	44	ARG	3.6
1	A	215	GLU	3.6
1	B	44	ARG	3.5
1	A	43	THR	3.5
1	A	210	TYR	3.4
1	B	215	GLU	3.4
1	A	211	GLY	3.4
1	D	170	ASN	3.3
1	A	170	ASN	3.3
1	D	165	THR	3.3
1	C	43	THR	3.2
1	A	166	SER	3.1
1	D	44	ARG	3.1
1	A	102	PRO	3.1
1	B	157	PHE	3.0
1	A	40	ARG	3.0
1	A	38	HIS	3.0
1	A	359	GLU	2.9
1	B	165	THR	2.9
1	D	2	SER	2.9
1	D	41	PHE	2.8
1	D	5	HIS	2.8
1	A	46	SER	2.8
1	B	166	SER	2.8
1	A	157	PHE	2.8
1	A	45	TYR	2.7
1	C	68	GLY	2.7
1	C	210	TYR	2.7
1	D	167	CYS	2.7
1	B	229	LEU	2.5
1	A	123	HIS	2.5
1	B	160	GLN	2.5
1	C	102	PRO	2.4
1	A	165	THR	2.4
1	C	44	ARG	2.4
1	A	164	LEU	2.3
1	D	102	PRO	2.3
1	A	167	CYS	2.3
1	B	41	PHE	2.2
1	C	228	THR	2.2
1	A	356	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	210	TYR	2.2
1	D	103	PHE	2.2
1	C	129	LEU	2.2
1	B	216	ALA	2.2
1	C	170	ASN	2.1
1	D	229	LEU	2.1
1	D	350	HIS	2.1
1	D	172	GLY	2.1
1	A	42	PRO	2.1
1	B	169	THR	2.0
1	A	149	ILE	2.0
1	D	71	LYS	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	RPI	A	194	15/16	0.97	0.14	34,45,53,56	0
1	RPI	B	194	15/16	0.97	0.15	35,41,49,55	0
1	RPI	D	194	15/16	0.97	0.15	41,46,53,59	0
1	RPI	C	194	15/16	0.98	0.16	37,47,58,58	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, 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	MG	D	500	1/1	0.88	0.06	58,58,58,58	0
2	MG	C	500	1/1	0.91	0.08	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	A	500	1/1	0.96	0.15	69,69,69,69	0
2	MG	B	500	1/1	0.97	0.09	55,55,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.