WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 28, 2014 – 01:03 PM GMT

PDB ID : 2C47
Title : Structure of casein kinase 1 gamma 2
Authors : Bunkoczi, G.; Rellos, P.; Das, S.; Ugochukwu, E.; Fedorov, O.; Sobott, F.; Eswaran, J.; Amos, A.; Ball, L.; Von Delft, F.; Bullock, A.; Debreczeni, J.; Turnbull, A.; Sundstrom, M.; Weigelt, J.; Arrowsmith, C.; Edwards, A.; Knapp, S.
Deposited on : 2005-10-16
Resolution : 2.40 Å(reported)

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1 Overall quality at a glance (i)

The reported resolution of this entry is 2.40 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		0.263
Clashscore		4
Ramachandran outliers		0
Sidechain outliers		4.2%
RSRZ outliers		5.9%

Worse — Better

- Percentile relative to all X-ray structures
- Percentile relative to X-ray structures of similar resolution
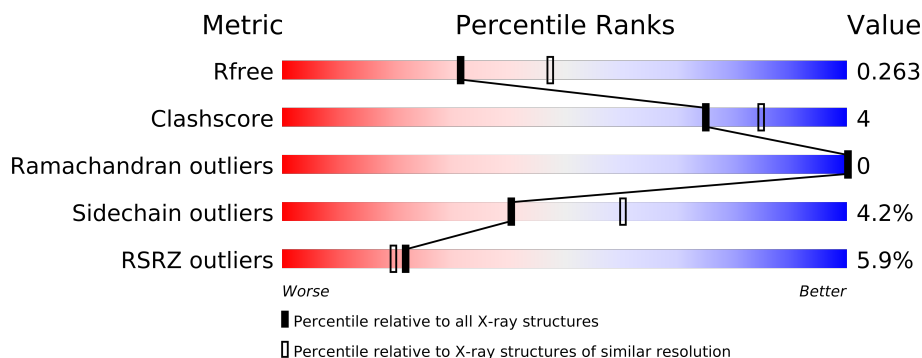
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	313	
1	B	313	
1	C	313	
1	D	313	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	MG	C	1301	-	X

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 9545 atoms, of which 0 are hydrogen and 0 are deuterium.

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.
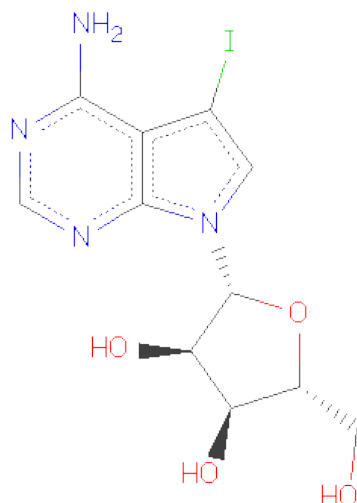
- Molecule 1 is a protein called CASEIN KINASE 1 GAMMA 2 ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	1	0
			2366	1539	392	425	10			
1	B	290	Total	C	N	O	S	0	1	0
			2376	1542	399	425	10			
1	C	283	Total	C	N	O	S	0	0	0
			2219	1440	366	403	10			
1	D	291	Total	C	N	O	S	0	0	0
			2295	1498	375	411	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	SER	-	EXPRESSION TAG	UNP P78368
A	42	MET	-	EXPRESSION TAG	UNP P78368
B	41	SER	-	EXPRESSION TAG	UNP P78368
B	42	MET	-	EXPRESSION TAG	UNP P78368
C	41	SER	-	EXPRESSION TAG	UNP P78368
C	42	MET	-	EXPRESSION TAG	UNP P78368
D	41	SER	-	EXPRESSION TAG	UNP P78368
D	42	MET	-	EXPRESSION TAG	UNP P78368

- Molecule 2 is (2R,3R,4S,5R)-2-(4-AMINO-5-IODO-7H-PYRROLO[2,3-D]PYRIMIDIN-7-YL)-5-(HYDROXYMETHYL)TETRAHYDROFURAN-3,4-DIOL (three-letter code: 5ID) (formula: $C_{11}H_{13}IN_4O_4$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	I	N	O	0	0
			20	11	1	4	4		
2	B	1	Total	C	I	N	O	0	0
			20	11	1	4	4		
2	C	1	Total	C	I	N	O	0	0
			20	11	1	4	4		
2	D	1	Total	C	I	N	O	0	0
			20	11	1	4	4		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	64	Total	O	0	0
			64	64		
4	B	81	Total	O	0	0
			81	81		
4	C	31	Total	O	0	0
			31	31		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	31	Total O 31 31		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 errors 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: CASEIN KINASE 1 GAMMA 2 ISOFORM

Chain A:
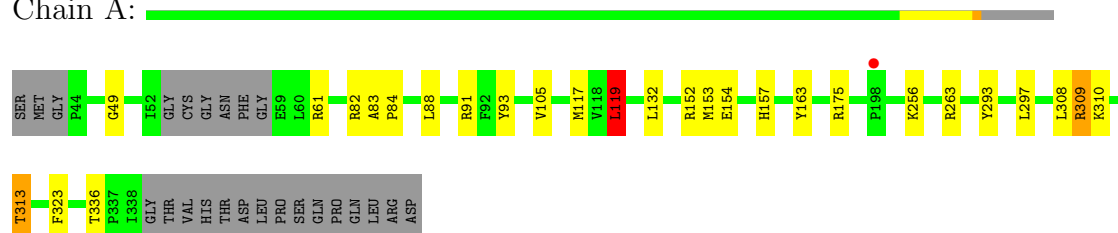
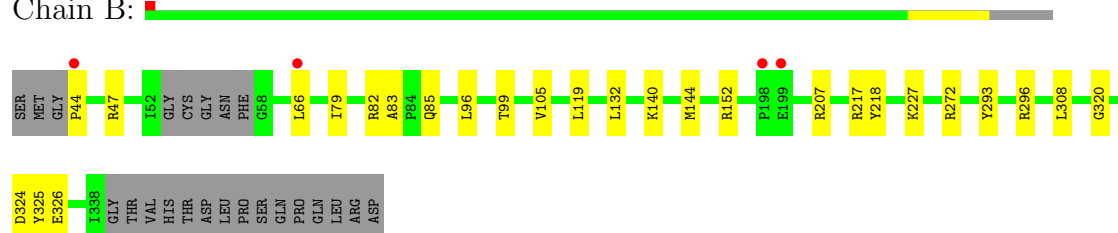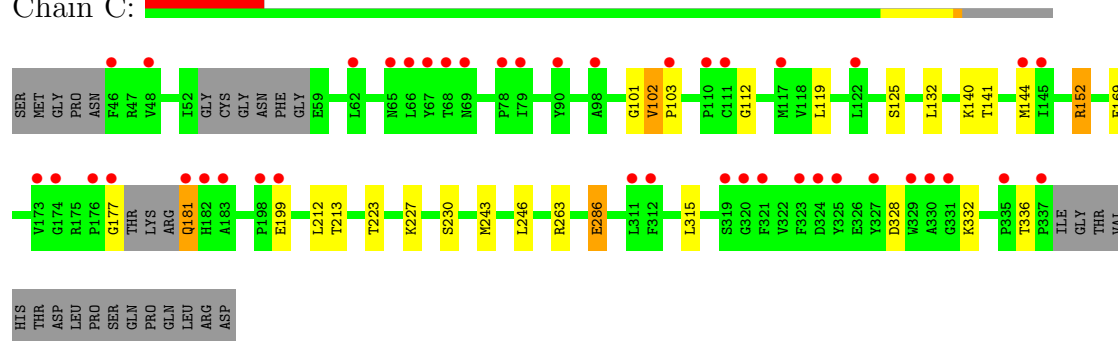- Molecule 1: CASEIN KINASE 1 GAMMA 2 ISOFORM

Chain B:
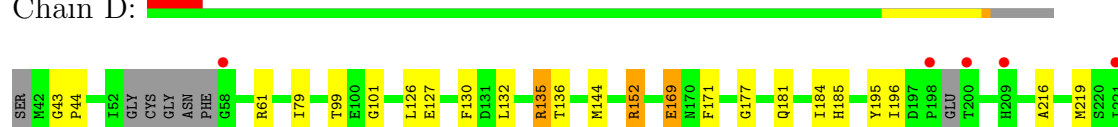
- Molecule 1: CASEIN KINASE 1 GAMMA 2 ISOFORM

Chain C:

- Molecule 1: CASEIN KINASE 1 GAMMA 2 ISOFORM

Chain D:
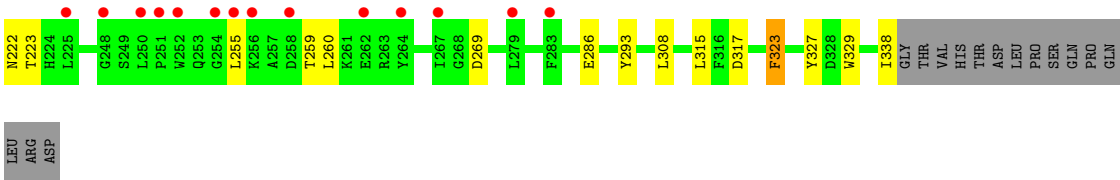
N222 T223 H224 L225 G248 S249 L250 P251 W252 Q253 G254 L255 K256 A257 D258 T259 L260 K261 E262 R263 Y264 I267 G268 D269 L279 F283 E286 Y293 L308 L315 F316 D317 F323 Y327 D328 W329 I338 GLY THR VAL HIS THR ASP LEU PRO SER GLN PRO GLN

LEU ARG ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	93.96Å 97.09Å 185.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 46.48 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-2.40) 99.3 (46.48-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.208 , 0.257 0.216 , 0.263	Depositor DCC
R_{free} test set	3383 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	44.1	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 44.4	EDS
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
L-test for twinning	$< |L| > = 0.47, < L^2 > = 0.31$	Xtriage
Outliers	2 of 66743 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9545	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CSD, MG, 5ID

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	0.59	0/2425	0.74	4/3284 (0.1%)
1	B	0.71	0/2434	0.80	1/3292 (0.0%)
1	C	0.52	0/2267	0.67	2/3074 (0.1%)
1	D	0.58	1/2349 (0.0%)	0.70	0/3189
All	All	0.60	1/9475 (0.0%)	0.73	7/12839 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	269	ASP	CG-OD2	7.73	1.43	1.25

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(º)	Ideal(º)
1	A	263	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	C	263	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	C	263	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	B	324	ASP	CB-CA-C	-5.85	98.70	110.40
1	A	309	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	263	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	A	119	LEU	CA-CB-CG	5.23	127.33	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens

added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2366	0	2307	16	0
1	B	2376	0	2337	13	0
1	C	2219	0	2099	18	0
1	D	2295	0	2172	26	0
2	A	20	0	13	0	0
2	B	20	0	13	3	0
2	C	20	0	13	3	0
2	D	20	0	13	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	64	0	0	2	0
4	B	81	0	0	3	0
4	C	31	0	0	1	0
4	D	31	0	0	1	0
All	All	9545	0	8967	73	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (73) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:127:GLU:OE2	1:D:135:ARG:NH1	2.10	0.85
1:D:152:ARG:NH1	1:D:184:ILE:O	2.14	0.80
1:D:222:ASN:CB	4:D:2017:HOH:O	2.32	0.77
1:B:105:VAL:HG12	1:B:119:LEU:HD23	1.70	0.73
1:D:152:ARG:HG2	1:D:152:ARG:HH11	1.58	0.69
1:A:297:LEU:O	4:A:2058:HOH:O	2.11	0.68
1:C:286:GLU:HG3	1:C:315:LEU:HD22	1.78	0.65
1:A:310:LYS:HA	1:A:313:THR:HG22	1.80	0.64
1:C:177:GLY:C	1:C:181:GLN:OE1	2.38	0.61
1:C:286:GLU:CG	1:C:315:LEU:HD22	2.32	0.60
1:C:112:GLY:HA3	1:D:259:THR:HG23	1.83	0.59
1:C:243:MET:HE1	1:C:246:LEU:HD12	1.85	0.57
2:B:1300:5ID:H5'2	4:B:2030:HOH:O	2.03	0.57
1:C:102:VAL:HG12	1:C:103:PRO:HD2	1.87	0.57
1:C:169:GLU:O	2:C:1300:5ID:H5'1	2.05	0.57
1:D:101:GLY:HA3	1:D:152:ARG:HD2	1.89	0.55
2:C:1300:5ID:N3	2:C:1300:5ID:H2'	2.21	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:141:THR:HG21	1:C:328:ASP:H	1.72	0.54
1:B:105:VAL:CG1	1:B:119:LEU:HD23	2.37	0.54
1:A:153:MET:HE1	1:A:163:TYR:HB3	1.91	0.53
1:D:195:TYR:CD2	1:D:196:ILE:HD12	2.44	0.52
1:C:140:LYS:O	1:C:144:MET:HG3	2.09	0.52
1:D:286:GLU:HG2	1:D:315:LEU:HD22	1.93	0.51
1:B:82:ARG:O	1:B:83:ALA:HB3	2.10	0.51
1:C:101:GLY:HA3	1:C:152:ARG:HD2	1.92	0.51
1:D:195:TYR:CE2	1:D:196:ILE:CD1	2.94	0.51
1:D:286:GLU:CG	1:D:315:LEU:HD22	2.42	0.50
1:D:259:THR:HG22	1:D:260:LEU:N	2.27	0.49
1:A:293:TYR:CD1	1:A:308:LEU:HD21	2.47	0.49
1:C:243:MET:CE	1:C:246:LEU:HD12	2.42	0.48
1:A:119:LEU:HD23	1:A:119:LEU:N	2.29	0.47
1:D:130:PHE:CE2	1:D:135:ARG:HG3	2.49	0.47
1:B:47:ARG:HG3	1:B:66:LEU:HD21	1.97	0.47
1:A:154:GLU:OE1	1:A:309:ARG:NH2	2.45	0.46
1:A:83:ALA:N	1:A:84:PRO:HD3	2.30	0.46
1:D:144:MET:CE	1:D:323:PHE:HA	2.45	0.46
1:C:141:THR:HG21	1:C:328:ASP:N	2.30	0.45
1:A:93:TYR:CD1	1:A:117:MET:HE1	2.51	0.45
1:D:293:TYR:CD1	1:D:308:LEU:HD21	2.52	0.45
1:D:126:LEU:HD21	1:D:184:ILE:HD12	1.99	0.45
1:A:93:TYR:HD1	1:A:117:MET:HE1	1.82	0.45
1:A:256:LYS:NZ	4:A:2046:HOH:O	2.50	0.45
1:D:43:GLY:N	1:D:44:PRO:CD	2.80	0.44
1:D:216:ALA:HA	1:D:219:MET:SD	2.57	0.44
1:A:153:MET:HE1	1:A:163:TYR:CB	2.47	0.44
1:C:230:SER:HB2	4:C:2011:HOH:O	2.19	0.43
1:B:217:ARG:HD2	1:B:218:TYR:CZ	2.54	0.43
1:C:125:SER:HB3	2:C:1300:5ID:H5'1	2.00	0.43
1:C:112:GLY:HA3	1:D:259:THR:CG2	2.48	0.42
1:B:144:MET:HE1	1:B:325:TYR:H	1.84	0.42
1:C:212:LEU:HD21	1:C:223:THR:O	2.19	0.42
4:B:2079:HOH:O	1:C:199:GLU:CB	2.67	0.42
1:A:49:GLY:O	1:A:61:ARG:HD2	2.20	0.42
1:B:96:LEU:O	1:B:99:THR:HG22	2.20	0.42
2:B:1300:5ID:C5'	4:B:2030:HOH:O	2.65	0.41
1:D:327:TYR:CD1	1:D:329:TRP:CZ2	3.08	0.41
1:A:153:MET:HE2	1:A:157:HIS:NE2	2.35	0.41
1:A:82:ARG:O	1:A:83:ALA:HB3	2.20	0.41
1:A:105:VAL:HG11	1:A:117:MET:CE	2.51	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:144:MET:CE	1:B:325:TYR:H	2.34	0.41
1:B:140:LYS:O	1:B:144:MET:HG3	2.21	0.41
1:D:259:THR:HG22	1:D:260:LEU:H	1.85	0.41
1:D:127:GLU:HG2	1:D:169:GLU:OE1	2.21	0.41
1:B:119:LEU:HD13	2:B:1300:5ID:IAE	2.91	0.41
1:D:219:MET:HE2	1:D:223:THR:HG22	2.03	0.41
1:B:47:ARG:CG	1:B:66:LEU:HD21	2.51	0.41
1:B:320:GLY:HA3	1:C:199:GLU:O	2.21	0.41
1:B:293:TYR:CD1	1:B:308:LEU:HD21	2.56	0.41
1:A:88:LEU:O	1:A:91:ARG:HB2	2.21	0.41
1:D:152:ARG:HA	1:D:152:ARG:HD3	1.84	0.41
1:D:177:GLY:H	1:D:181:GLN:NE2	2.19	0.41
1:D:327:TYR:CG	1:D:329:TRP:CZ2	3.09	0.40
1:D:171:PHE:HA	1:D:185:HIS: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	285/313 (91%)	277 (97%)	8 (3%)	0	100	100
1	B	286/313 (91%)	282 (99%)	4 (1%)	0	100	100
1	C	276/313 (88%)	273 (99%)	3 (1%)	0	100	100
1	D	284/313 (91%)	279 (98%)	5 (2%)	0	100	100
All	All	1131/1252 (90%)	1111 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	245/277 (88%)	238 (97%)	7 (3%)	55	76
1	B	248/277 (90%)	238 (96%)	10 (4%)	42	63
1	C	217/277 (78%)	207 (95%)	10 (5%)	37	55
1	D	224/277 (81%)	212 (95%)	12 (5%)	31	47
All	All	934/1108 (84%)	895 (96%)	39 (4%)	40	60

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	LEU
1	A	132	LEU
1	A	152	ARG
1	A	175	ARG
1	A	313	THR
1	A	323	PHE
1	A	336	THR
1	B	44	PRO
1	B	79	ILE
1	B	85	GLN
1	B	132	LEU
1	B	152	ARG
1	B	207	ARG
1	B	227	LYS
1	B	272	ARG
1	B	296	ARG
1	B	326	GLU
1	C	102	VAL
1	C	119	LEU
1	C	132	LEU
1	C	152	ARG
1	C	181	GLN
1	C	213	THR
1	C	227	LYS
1	C	286	GLU
1	C	332	LYS
1	C	336	THR
1	D	61	ARG
1	D	79	ILE
1	D	99	THR

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Mol	Chain	Res	Type
1	D	132	LEU
1	D	135	ARG
1	D	136	THR
1	D	152	ARG
1	D	169	GLU
1	D	255	LEU
1	D	317	ASP
1	D	323	PHE
1	D	338	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	D	181	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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	CSD	A	111	1	7,7,8	11.27	5 (71%)	6,8,10	8.83	6 (100%)
1	CSD	B	111	1	7,7,8	12.07	5 (71%)	6,8,10	6.76	6 (100%)
1	CSD	C	111	1	7,7,8	11.47	3 (42%)	6,8,10	5.28	6 (100%)
1	CSD	D	111	1	7,7,8	11.95	6 (85%)	6,8,10	8.03	6 (100%)

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	CSD	A	111	1	-	0/3/6/8	0/0/0/0
1	CSD	B	111	1	-	0/3/6/8	0/0/0/0
1	CSD	C	111	1	-	1/3/6/8	0/0/0/0
1	CSD	D	111	1	-	1/3/6/8	0/0/0/0

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	111	CSD	OD1-SG	23.99	1.81	1.47
1	C	111	CSD	OD1-SG	23.48	1.80	1.47
1	A	111	CSD	OD1-SG	22.64	1.79	1.47
1	D	111	CSD	OD1-SG	22.50	1.79	1.47
1	D	111	CSD	O-C	20.86	1.25	1.11
1	B	111	CSD	O-C	20.23	1.25	1.11
1	C	111	CSD	O-C	18.72	1.24	1.11
1	A	111	CSD	O-C	18.03	1.23	1.11
1	D	111	CSD	CB-CA	5.28	1.62	1.53
1	A	111	CSD	CB-CA	4.64	1.60	1.53
1	A	111	CSD	CA-C	3.83	1.55	1.48
1	C	111	CSD	OD2-SG	3.73	1.81	1.55
1	D	111	CSD	OD2-SG	3.52	1.80	1.55
1	B	111	CSD	CB-CA	3.47	1.59	1.53
1	D	111	CSD	CA-C	3.41	1.54	1.48
1	B	111	CSD	OD2-SG	3.40	1.79	1.55
1	A	111	CSD	OD2-SG	3.33	1.79	1.55
1	B	111	CSD	CA-C	3.04	1.54	1.48
1	D	111	CSD	CB-SG	2.45	1.88	1.80

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	111	CSD	C-CA-N	-14.41	99.43	113.83
1	D	111	CSD	C-CA-N	-13.20	100.65	113.83
1	A	111	CSD	OD2-SG-OD1	-11.40	90.46	109.39
1	D	111	CSD	OD2-SG-OD1	-11.33	90.57	109.39
1	C	111	CSD	C-CA-N	-11.31	102.53	113.83
1	B	111	CSD	C-CA-N	-10.82	103.02	113.83
1	B	111	CSD	OD2-SG-OD1	-8.90	94.61	109.39
1	A	111	CSD	CB-CA-N	6.91	121.27	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	111	CSD	OD1-SG-CB	6.69	122.98	105.25
1	D	111	CSD	CB-CA-N	6.45	120.53	110.16
1	B	111	CSD	OD1-SG-CB	5.95	121.03	105.25
1	A	111	CSD	OD2-SG-CB	4.90	117.14	97.42
1	B	111	CSD	CB-CA-N	4.65	117.64	110.16
1	D	111	CSD	OD2-SG-CB	4.46	115.38	97.42
1	B	111	CSD	CA-CB-SG	3.87	116.34	110.82
1	A	111	CSD	CA-CB-SG	3.74	116.16	110.82
1	D	111	CSD	CA-CB-SG	3.56	115.89	110.82
1	D	111	CSD	OD1-SG-CB	3.20	113.75	105.25
1	C	111	CSD	CA-CB-SG	3.13	115.29	110.82
1	C	111	CSD	CB-CA-N	3.13	115.19	110.16
1	C	111	CSD	OD2-SG-OD1	-2.87	104.63	109.39
1	C	111	CSD	OD1-SG-CB	2.57	112.06	105.25
1	B	111	CSD	OD2-SG-CB	2.38	107.02	97.42
1	C	111	CSD	OD2-SG-CB	2.13	105.99	97.42

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	111	CSD	CA-CB-SG-OD1
1	C	111	CSD	CA-CB-SG-OD1

There are no ring outliers.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	5ID	A	1300	-	22,22,22	1.56	2 (9%)	31,33,33	2.23	9 (29%)
2	5ID	B	1300	-	22,22,22	1.36	3 (13%)	31,33,33	2.64	11 (35%)
2	5ID	C	1300	-	22,22,22	1.66	3 (13%)	31,33,33	3.49	14 (45%)
2	5ID	D	1300	-	22,22,22	1.44	3 (13%)	31,33,33	2.00	8 (25%)

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	5ID	A	1300	-	-	0/6/22/22	0/1/3/3
2	5ID	B	1300	-	-	0/6/22/22	0/1/3/3
2	5ID	C	1300	-	-	2/6/22/22	0/1/3/3
2	5ID	D	1300	-	-	0/6/22/22	0/1/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1300	5ID	O4'-C1'	5.82	1.50	1.41
2	A	1300	5ID	O4'-C1'	4.40	1.48	1.41
2	D	1300	5ID	O4'-C1'	4.35	1.48	1.41
2	B	1300	5ID	O4'-C1'	3.00	1.46	1.41
2	C	1300	5ID	C8-N9	-2.88	1.33	1.38
2	A	1300	5ID	C8-N9	-2.87	1.33	1.38
2	D	1300	5ID	C8-C7	-2.55	1.33	1.37
2	C	1300	5ID	C8-C7	-2.33	1.34	1.37
2	B	1300	5ID	C2'-C1'	2.24	1.56	1.53
2	B	1300	5ID	C5'-C4'	2.15	1.59	1.52
2	D	1300	5ID	C8-N9	-2.01	1.34	1.38

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1300	5ID	O4'-C1'-N9	10.19	117.92	108.44
2	C	1300	5ID	N3-C2-N1	-8.23	121.83	128.71
2	A	1300	5ID	N3-C2-N1	-7.78	122.21	128.71
2	B	1300	5ID	N3-C2-N1	-7.16	122.72	128.71
2	B	1300	5ID	C5-C7-IAE	6.90	129.52	125.07
2	D	1300	5ID	N3-C2-N1	-6.41	123.35	128.71
2	C	1300	5ID	C5-C7-IAE	5.83	128.83	125.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1300	5ID	C4'-O4'-C1'	-5.76	103.49	109.75
2	C	1300	5ID	O4'-C4'-C5'	4.69	119.16	109.15
2	C	1300	5ID	N3-C4-N9	4.57	133.69	125.43
2	C	1300	5ID	C5-C4-N3	-4.22	117.35	125.71
2	B	1300	5ID	O4'-C4'-C5'	3.97	117.63	109.15
2	A	1300	5ID	C5-C7-IAE	3.87	127.56	125.07
2	B	1300	5ID	C3'-C2'-C1'	3.85	106.93	100.91
2	D	1300	5ID	N3-C4-N9	3.81	132.32	125.43
2	A	1300	5ID	N3-C4-N9	3.80	132.30	125.43
2	C	1300	5ID	C2'-C3'-C4'	-3.70	95.28	102.65
2	B	1300	5ID	C8-C7-IAE	-3.59	121.51	126.97
2	C	1300	5ID	C8-N9-C1'	-3.57	122.21	125.51
2	A	1300	5ID	C5-C4-N3	-3.57	118.65	125.71
2	B	1300	5ID	C5-C4-N3	-3.45	118.89	125.71
2	D	1300	5ID	C5-C4-N3	-3.45	118.89	125.71
2	B	1300	5ID	N3-C4-N9	3.33	131.45	125.43
2	C	1300	5ID	C8-C7-IAE	-3.29	121.97	126.97
2	B	1300	5ID	O4'-C1'-N9	3.29	111.50	108.44
2	D	1300	5ID	C3'-C2'-C1'	3.16	105.85	100.91
2	A	1300	5ID	O4'-C1'-N9	3.02	111.25	108.44
2	C	1300	5ID	C2-N3-C4	2.87	122.18	114.01
2	D	1300	5ID	C5-C7-IAE	2.79	126.87	125.07
2	A	1300	5ID	C8-C7-IAE	-2.61	123.00	126.97
2	C	1300	5ID	O4'-C4'-C3'	-2.58	99.95	105.17
2	A	1300	5ID	C2-N3-C4	2.35	120.71	114.01
2	B	1300	5ID	C5'-C4'-C3'	-2.26	109.52	115.06
2	D	1300	5ID	O4'-C4'-C5'	2.20	113.86	109.15
2	D	1300	5ID	C5'-C4'-C3'	-2.20	109.67	115.06
2	D	1300	5ID	C5-C6-N1	-2.18	117.09	122.89
2	A	1300	5ID	C2'-C1'-N9	-2.16	107.72	113.27
2	A	1300	5ID	C8-N9-C1'	-2.16	123.51	125.51
2	B	1300	5ID	C2-N3-C4	2.16	120.16	114.01
2	B	1300	5ID	C5-C6-N1	-2.15	117.18	122.89
2	C	1300	5ID	C3'-C2'-C1'	-2.13	97.58	100.91
2	C	1300	5ID	C2'-C1'-N9	-2.02	108.08	113.27

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1300	5ID	C2'-C1'-N9-C8
2	C	1300	5ID	C2'-C1'-N9-C4

There are no ring outliers.

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	289/313 (92%)	0.22	1 (0%)	91 92	41, 61, 76, 91	0
1	B	290/313 (92%)	0.26	4 (1%)	72 71	39, 61, 76, 93	0
1	C	283/313 (90%)	0.67	42 (14%)	3 2	39, 61, 75, 80	0
1	D	291/313 (92%)	0.44	19 (6%)	18 17	38, 61, 74, 88	0
All	All	1153/1252 (92%)	0.40	66 (5%)	22 21	38, 61, 76, 93	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	251	PRO	4.9
1	C	66	LEU	4.6
1	C	337	PRO	4.5
1	D	255	LEU	4.5
1	C	67	TYR	4.4
1	B	198	PRO	4.3
1	D	225	LEU	4.2
1	D	252	TRP	3.9
1	C	177	GLY	3.9
1	D	254	GLY	3.8
1	C	329	TRP	3.7
1	C	145	ILE	3.7
1	C	312	PHE	3.7
1	C	323	PHE	3.5
1	C	325	TYR	3.4
1	C	183	ALA	3.3
1	C	321	PHE	3.2
1	C	320	GLY	3.1
1	C	319	SER	3.1
1	C	48	VAL	3.1
1	C	335	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	66	LEU	3.0
1	D	283	PHE	2.9
1	D	264	TYR	2.9
1	C	173	VAL	2.9
1	C	69	ASN	2.9
1	A	198	PRO	2.9
1	D	58	GLY	2.9
1	D	267	ILE	2.9
1	D	209	HIS	2.8
1	B	44	PRO	2.8
1	D	279	LEU	2.6
1	C	327	TYR	2.6
1	D	248	GLY	2.6
1	C	331	GLY	2.6
1	D	221	ILE	2.6
1	C	111	CSD	2.6
1	C	68	THR	2.6
1	C	199	GLU	2.5
1	C	324	ASP	2.5
1	C	181	GLN	2.4
1	B	199	GLU	2.4
1	C	311	LEU	2.4
1	D	198	PRO	2.4
1	C	117	MET	2.3
1	C	78	PRO	2.3
1	D	250	LEU	2.3
1	C	176	PRO	2.3
1	D	200	THR	2.2
1	C	65	ASN	2.2
1	C	79	ILE	2.2
1	D	258	ASP	2.2
1	C	330	ALA	2.2
1	D	262	GLU	2.2
1	C	46	PHE	2.2
1	C	198	PRO	2.2
1	C	182	HIS	2.1
1	C	103	PRO	2.1
1	C	144	MET	2.1
1	D	256	LYS	2.1
1	C	98	ALA	2.1
1	C	62	LEU	2.1
1	C	174	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	122	LEU	2.1
1	C	110	PRO	2.1
1	C	90	TYR	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	RSR	LLDF	B-factors($\mathrm{\AA}^2$)	Q<0.9
1	CSD	D	111	8/9	0.17	0.95	27,35,43,54	0
1	CSD	A	111	8/9	0.18	-0.38	31,35,50,55	0
1	CSD	C	111	8/9	0.21	-0.67	31,34,47,53	0
1	CSD	B	111	8/9	0.12	-1.13	29,35,47,51	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	RSR	LLDF	B-factors($\mathrm{\AA}^2$)	Q<0.9
3	MG	C	1301	1/1	0.25	4.18	33,33,33,33	0
2	5ID	C	1300	20/20	0.26	1.38	79,108,127,128	0
2	5ID	D	1300	20/20	0.12	-1.33	32,55,75,83	0
2	5ID	A	1300	20/20	0.09	-2.33	41,49,64,70	0
3	MG	B	1301	1/1	0.11	-3.11	32,32,32,32	0
2	5ID	B	1300	20/20	0.09	-3.24	25,40,50,65	0

6.5 Other polymers (i)

There are no such residues in this entry.