



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2018 – 09:30 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)

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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

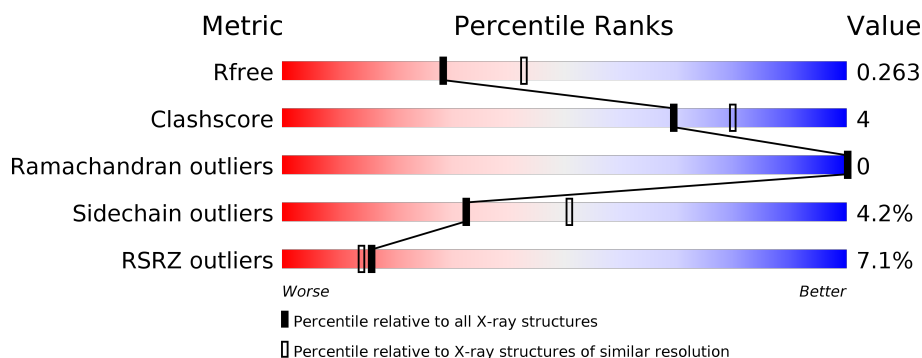
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	111664	3481 (2.40-2.40)
Clashscore	122126	3956 (2.40-2.40)
Ramachandran outliers	120053	3897 (2.40-2.40)
Sidechain outliers	120020	3898 (2.40-2.40)
RSRZ outliers	108989	3386 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	313	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>8%</div> <div>8%</div> </div> </div>
1	B	313	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>9%</div> <div>7%</div> </div> </div>
1	C	313	<div> <div>14%</div> <div> <div></div> <div>81%</div> <div>8%</div> <div>10%</div> </div> </div>
1	D	313	<div> <div>8%</div> <div> <div></div> <div>81%</div> <div>11%</div> <div>7%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9545 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.

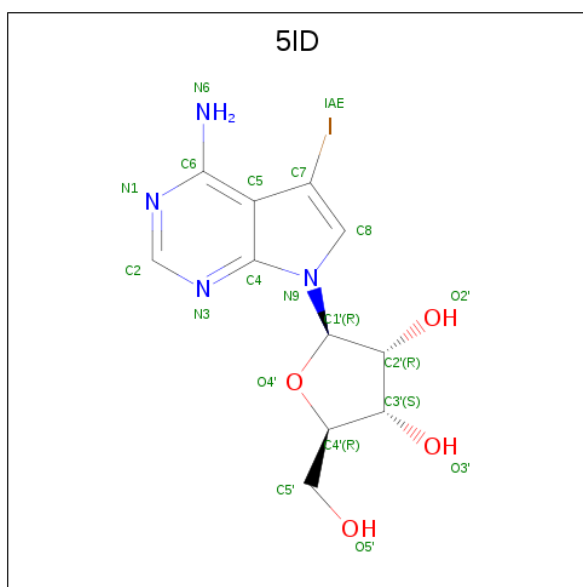
- Molecule 1 is a protein called CASEIN KINASE 1 GAMMA 2 ISOFORM.

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<sub>11</sub>H<sub>13</sub>IN<sub>4</sub>O<sub>4</sub>).



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

- 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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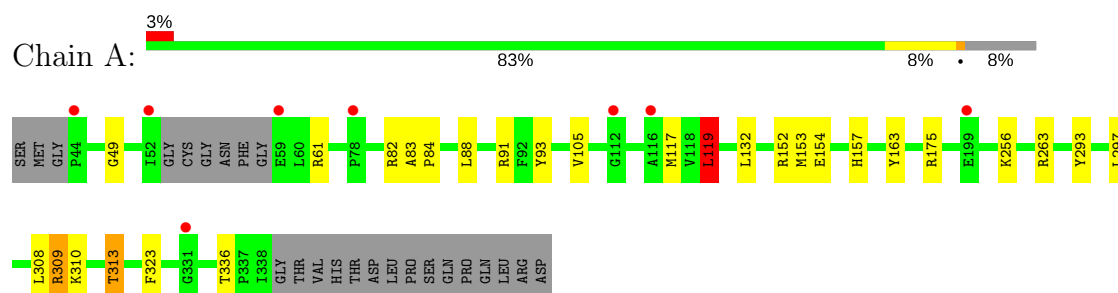
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	31	Total	O	0	0
			31	31		

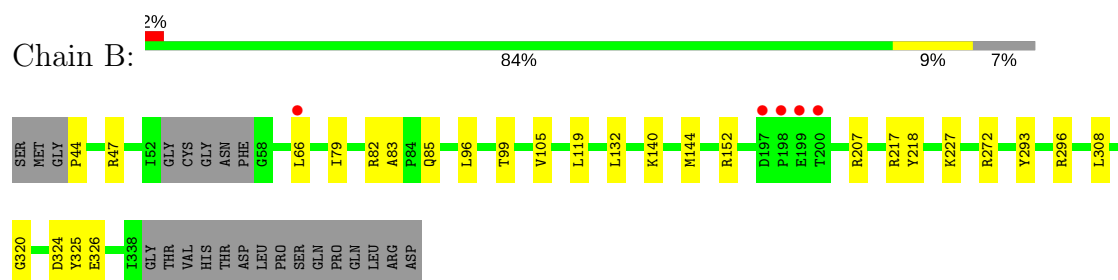
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

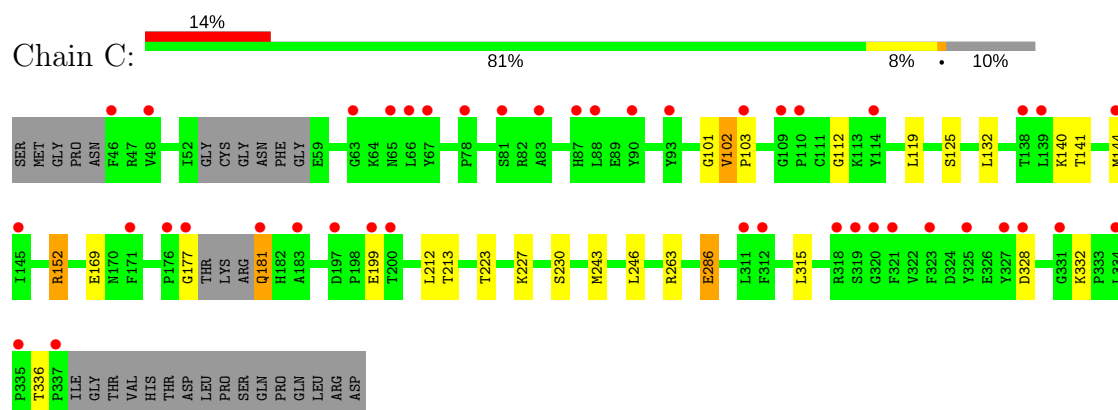
- Molecule 1: CASEIN KINASE 1 GAMMA 2 ISOFORM



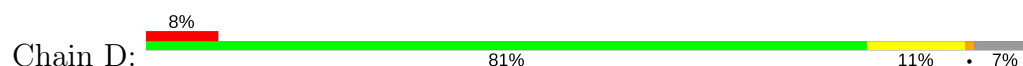
- Molecule 1: CASEIN KINASE 1 GAMMA 2 ISOFORM

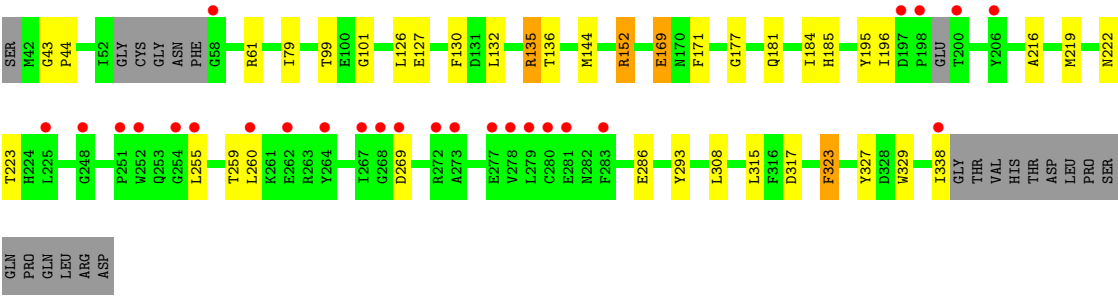


- Molecule 1: CASEIN KINASE 1 GAMMA 2 ISOFORM



- Molecule 1: CASEIN KINASE 1 GAMMA 2 ISOFORM





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.1	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 65.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9545	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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(°)	Ideal(°)
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 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	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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (73) 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: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	Interatomic distance (Å)	Clash overlap (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:A:93:TYR:HD1	1:A:117:MET:HE1	1.82	0.45
1:D:126:LEU:HD21	1:D:184:ILE:HD12	1.99	0.45
1:A:256:LYS:NZ	4:A:2046:HOH:O	2.50	0.45
1:D:216:ALA:HA	1:D:219:MET:SD	2.57	0.44
1:D:43:GLY:N	1:D:44:PRO:CD	2.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:VAL:HG11	1:A:117:MET:CE	2.51	0.41
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:B:119:LEU:HD13	2:B:1300:5ID:IAE	2.91	0.41
1:D:127:GLU:HG2	1:D:169:GLU:OE1	2.21	0.41
1:D:219:MET:HE2	1:D:223:THR:HG22	2.03	0.41
1:B:293:TYR:CD1	1:B:308:LEU:HD21	2.56	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: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%)	45	66
1	B	248/277 (90%)	238 (96%)	10 (4%)	34	53
1	C	217/277 (78%)	207 (95%)	10 (5%)	29	46
1	D	224/277 (81%)	212 (95%)	12 (5%)	24	38
All	All	934/1108 (84%)	895 (96%)	39 (4%)	32	51

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

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Mol	Chain	Res	Type
1	C	286	GLU
1	C	332	LYS
1	C	336	THR
1	D	61	ARG
1	D	79	ILE
1	D	99	THR
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 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	CSD	A	111	1	4,7,8	2.21	1 (25%)	2,8,10	6.59	1 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	CSD	B	111	1	4,7,8	1.68	1 (25%)	2,8,10	5.89	1 (50%)
1	CSD	C	111	1	4,7,8	0.71	0	2,8,10	2.74	1 (50%)
1	CSD	D	111	1	4,7,8	2.08	1 (25%)	2,8,10	3.31	1 (50%)

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	-	0/2/6/8	0/0/0/0
1	CSD	B	111	1	-	0/2/6/8	0/0/0/0
1	CSD	C	111	1	-	1/2/6/8	0/0/0/0
1	CSD	D	111	1	-	1/2/6/8	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	111	CSD	CA-C	2.87	1.54	1.50
1	D	111	CSD	CA-C	3.44	1.54	1.50
1	A	111	CSD	CA-C	4.07	1.55	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	111	CSD	OD1-SG-CB	3.43	112.06	105.54
1	D	111	CSD	OD1-SG-CB	4.32	113.75	105.54
1	B	111	CSD	OD1-SG-CB	8.14	121.03	105.54
1	A	111	CSD	OD1-SG-CB	9.17	122.98	105.54

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

## 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	-	19,22,22	1.64	2 (10%)	18,33,33	2.11	2 (11%)
2	5ID	B	1300	-	19,22,22	1.32	2 (10%)	18,33,33	2.34	5 (27%)
2	5ID	C	1300	-	19,22,22	1.83	2 (10%)	18,33,33	3.13	7 (38%)
2	5ID	D	1300	-	19,22,22	1.51	2 (10%)	18,33,33	1.94	4 (22%)

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1300	5ID	C8-N9	-3.05	1.33	1.38
2	A	1300	5ID	C8-N9	-3.04	1.33	1.38
2	D	1300	5ID	C8-N9	-2.16	1.34	1.38
2	B	1300	5ID	C5'-C4'	2.26	1.59	1.51
2	B	1300	5ID	O4'-C1'	3.37	1.46	1.41
2	D	1300	5ID	O4'-C1'	4.86	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1300	5ID	O4'-C1'	4.91	1.48	1.41
2	C	1300	5ID	O4'-C1'	6.48	1.50	1.41

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1300	5ID	N3-C2-N1	-8.22	121.83	128.86
2	A	1300	5ID	N3-C2-N1	-7.78	122.21	128.86
2	B	1300	5ID	N3-C2-N1	-7.18	122.72	128.86
2	D	1300	5ID	N3-C2-N1	-6.44	123.35	128.86
2	C	1300	5ID	C4'-O4'-C1'	-6.08	103.49	109.83
2	C	1300	5ID	C2'-C3'-C4'	-3.82	95.28	102.62
2	C	1300	5ID	C8-N9-C1'	-3.70	122.21	125.48
2	C	1300	5ID	O4'-C4'-C3'	-2.63	99.95	105.15
2	B	1300	5ID	C5'-C4'-C3'	-2.29	109.52	115.06
2	B	1300	5ID	C8-C7-IAE	-2.24	121.51	127.53
2	A	1300	5ID	C8-N9-C1'	-2.23	123.51	125.48
2	D	1300	5ID	C5'-C4'-C3'	-2.22	109.67	115.06
2	D	1300	5ID	C5-C6-N1	-2.15	117.09	122.65
2	B	1300	5ID	C5-C6-N1	-2.12	117.18	122.65
2	C	1300	5ID	C8-C7-IAE	-2.07	121.97	127.53
2	D	1300	5ID	O4'-C4'-C5'	2.19	113.86	109.18
2	B	1300	5ID	O4'-C4'-C5'	3.95	117.63	109.18
2	C	1300	5ID	O4'-C4'-C5'	4.67	119.16	109.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1300	5ID	3	0
2	C	1300	5ID	3	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	288/313 (92%)	0.40	8 (2%) 53 50	52, 61, 76, 91	0
1	B	289/313 (92%)	0.24	5 (1%) 70 67	49, 61, 76, 93	0
1	C	282/313 (90%)	0.75	43 (15%) 2 1	51, 61, 75, 80	0
1	D	290/313 (92%)	0.70	26 (8%) 9 8	51, 61, 74, 88	0
All	All	1149/1252 (91%)	0.52	82 (7%) 16 14	49, 61, 76, 93	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	319	SER	7.4
1	D	225	LEU	6.4
1	D	264	TYR	5.7
1	D	267	ILE	5.4
1	C	66	LEU	5.1
1	C	199	GLU	4.5
1	B	198	PRO	4.5
1	D	268	GLY	4.4
1	C	177	GLY	4.4
1	C	320	GLY	4.3
1	C	145	ILE	4.3
1	D	269	ASP	4.2
1	D	278	VAL	4.1
1	D	255	LEU	4.1
1	C	337	PRO	3.9
1	C	325	TYR	3.8
1	C	331	GLY	3.7
1	C	327	TYR	3.6
1	C	90	TYR	3.6
1	D	248	GLY	3.5
1	C	48	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	200	THR	3.4
1	C	88	LEU	3.4
1	D	279	LEU	3.4
1	C	323	PHE	3.3
1	C	93	TYR	3.3
1	C	46	PHE	3.3
1	C	83	ALA	3.3
1	C	81	SER	3.3
1	D	273	ALA	3.3
1	D	58	GLY	3.2
1	B	199	GLU	3.2
1	B	66	LEU	3.1
1	C	67	TYR	3.1
1	C	103	PRO	3.0
1	C	321	PHE	3.0
1	C	176	PRO	3.0
1	D	254	GLY	3.0
1	C	78	PRO	2.9
1	C	197	ASP	2.9
1	D	198	PRO	2.8
1	C	110	PRO	2.8
1	A	52	ILE	2.7
1	B	197	ASP	2.7
1	C	87	HIS	2.7
1	C	200	THR	2.7
1	C	335	PRO	2.7
1	D	272	ARG	2.6
1	D	338	ILE	2.6
1	C	334	LEU	2.6
1	D	260	LEU	2.6
1	C	65	ASN	2.6
1	C	114	TYR	2.5
1	D	252	TRP	2.5
1	C	138	THR	2.5
1	D	251	PRO	2.5
1	C	181	GLN	2.5
1	C	318	ARG	2.5
1	D	283	PHE	2.5
1	C	311	LEU	2.5
1	D	197	ASP	2.4
1	C	171	PHE	2.4
1	A	331	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	312	PHE	2.3
1	D	280	CYS	2.3
1	D	262	GLU	2.3
1	D	281	GLU	2.2
1	D	277	GLU	2.2
1	B	200	THR	2.2
1	C	109	GLY	2.2
1	C	139	LEU	2.2
1	D	206	TYR	2.1
1	C	183	ALA	2.1
1	A	78	PRO	2.1
1	C	144	MET	2.1
1	A	59	GLU	2.1
1	A	199	GLU	2.1
1	C	63	GLY	2.1
1	A	116	ALA	2.0
1	C	328	ASP	2.0
1	A	112	GLY	2.0
1	A	44	PRO	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	CSD	B	111	8/9	0.80	0.15	29,35,47,51	0
1	CSD	D	111	8/9	0.84	0.24	27,35,43,54	0
1	CSD	A	111	8/9	0.88	0.24	31,35,50,55	0
1	CSD	C	111	8/9	0.91	0.21	31,34,47,53	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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	5ID	C	1300	20/20	0.89	0.27	79,108,127,128	0
3	MG	C	1301	1/1	0.96	0.20	33,33,33,33	0
2	5ID	A	1300	20/20	0.98	0.09	41,49,64,70	0
2	5ID	B	1300	20/20	0.98	0.09	25,40,50,65	0
3	MG	B	1301	1/1	0.98	0.10	32,32,32,32	0
2	5ID	D	1300	20/20	0.98	0.08	32,55,75,83	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.