



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 18, 2026 – 01:13 PM UTC

PDB ID : 2W2C / pdb\_00002w2c  
Title : STRUCTURE OF THE TETRADECAMERIC OLIGOMERISATION DOMAIN OF CALCIUM- CALMODULIN DEPENDENT PROTEIN KINASE II DELTA  
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Deposited on : 2008-10-28  
Resolution : 2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

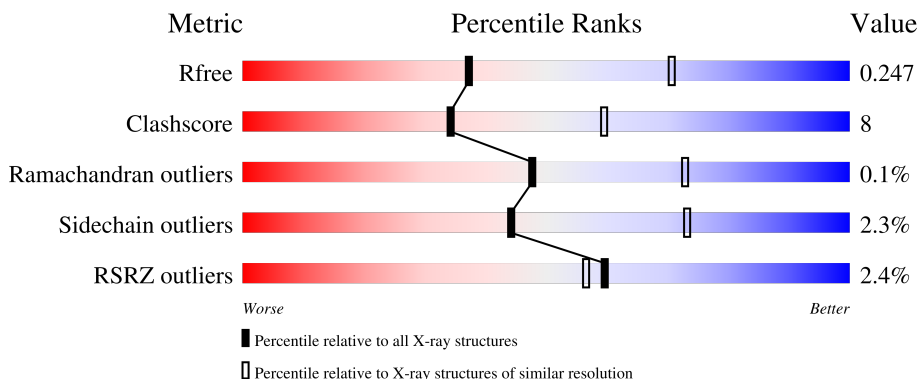
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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  $\geq 3$ , 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	144	 78% 10% 11%
1	B	144	 73% 15% 11%
1	C	144	 72% 15% 12%
1	D	144	 74% 12% 13%

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Mol	Chain	Length	Quality of chain
1	E	144	<p>% 78% 11% • 10%</p>
1	F	144	<p>% 76% 11% 12%</p>
1	G	144	<p>2% 74% 15% 12%</p>
1	H	144	<p>4% 75% 14% • 9%</p>
1	I	144	<p>4% 75% 13% • 11%</p>
1	J	144	<p>% 73% 12% • 13%</p>
1	K	144	<p>3% 79% 8% • 12%</p>
1	L	144	<p>3% 81% 9% • 10%</p>
1	M	144	<p>% 71% 15% • 13%</p>
1	N	144	<p>2% 74% 16% • 9%</p>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14067 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 CALCIUM/CALMODULIN-DEPENDENT PROTEIN KINASE TYPE II DELTA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	128	Total	C	N	O	S	0	0	0
			996	630	174	186	6			
1	B	128	Total	C	N	O	S	0	0	0
			1011	640	175	190	6			
1	C	127	Total	C	N	O	S	0	0	0
			992	628	174	184	6			
1	D	125	Total	C	N	O	S	0	0	0
			988	626	173	183	6			
1	E	129	Total	C	N	O	S	0	0	0
			994	627	175	187	5			
1	F	126	Total	C	N	O	S	0	0	0
			986	623	173	184	6			
1	G	127	Total	C	N	O	S	0	0	0
			991	625	175	186	5			
1	H	131	Total	C	N	O	S	0	0	0
			1010	636	178	191	5			
1	I	128	Total	C	N	O	S	0	0	0
			985	625	171	184	5			
1	J	125	Total	C	N	O	S	0	0	0
			972	617	168	181	6			
1	K	127	Total	C	N	O	S	0	0	0
			983	624	174	179	6			
1	L	130	Total	C	N	O	S	0	0	0
			1014	640	177	191	6			
1	M	125	Total	C	N	O	S	0	0	0
			975	620	171	179	5			
1	N	131	Total	C	N	O	S	0	0	0
			1015	644	175	190	6			

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0
2	I	1	Total C O 4 2 2	0	0
2	J	1	Total C O 4 2 2	0	0
2	K	1	Total C O 4 2 2	0	0
2	L	1	Total C O 4 2 2	0	0
2	M	1	Total C O 4 2 2	0	0
2	N	1	Total C O 4 2 2	0	0

- Molecule 3 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Cd 1	0	0
3	F	1	Total 1	Cd 1	0	0
3	H	1	Total 1	Cd 1	0	0
3	J	3	Total 3	Cd 3	0	0

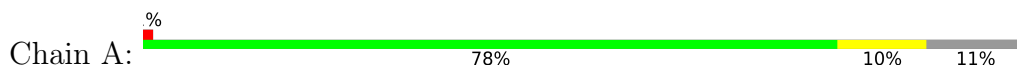
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total 7	O 7	0	0
4	B	10	Total 10	O 10	0	0
4	C	5	Total 5	O 5	0	0
4	D	8	Total 8	O 8	0	0
4	E	5	Total 5	O 5	0	0
4	F	5	Total 5	O 5	0	0
4	G	9	Total 9	O 9	0	0
4	H	6	Total 6	O 6	0	0
4	I	9	Total 9	O 9	0	0
4	J	8	Total 8	O 8	0	0
4	K	4	Total 4	O 4	0	0
4	L	5	Total 5	O 5	0	0
4	M	4	Total 4	O 4	0	0
4	N	8	Total 8	O 8	0	0

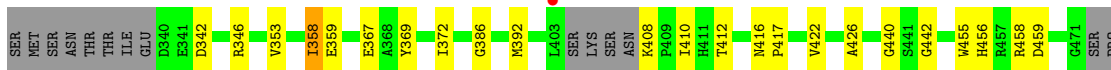
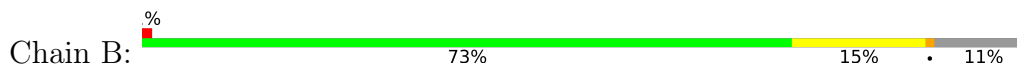
### 3 Residue-property plots [i](#)

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: CALCIUM/CALMODULIN-DEPENDENT PROTEIN KINASE TYPE II DELTA CHAIN



- Molecule 1: CALCIUM/CALMODULIN-DEPENDENT PROTEIN KINASE TYPE II DELTA CHAIN



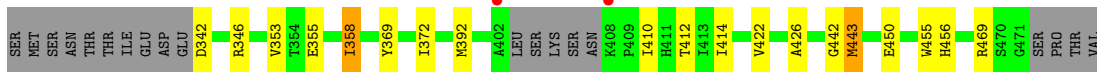
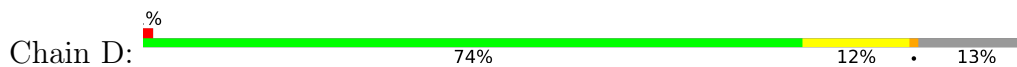
THR  
VAL

- Molecule 1: CALCIUM/CALMODULIN-DEPENDENT PROTEIN KINASE TYPE II DELTA CHAIN

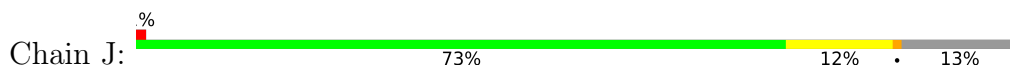


D459  
G471  
SER  
PRO  
THR  
THR  
VAL

- Molecule 1: CALCIUM/CALMODULIN-DEPENDENT PROTEIN KINASE TYPE II DELTA CHAIN

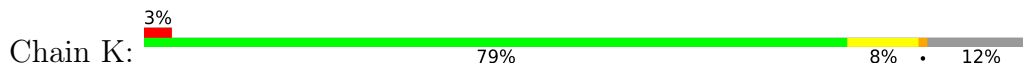




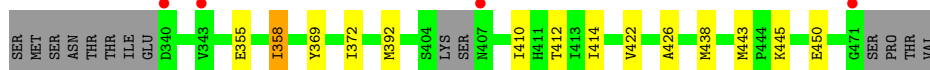
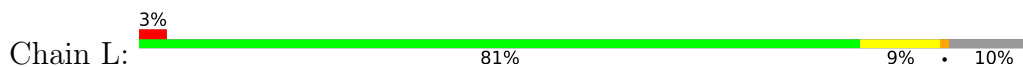


VAL

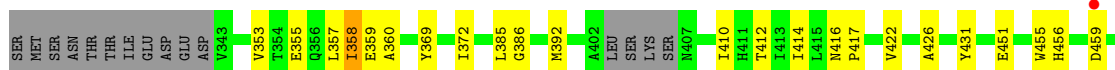
- Molecule 1: CALCIUM/CALMODULIN-DEPENDENT PROTEIN KINASE TYPE II DELTA CHAIN



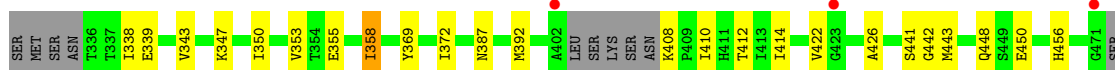
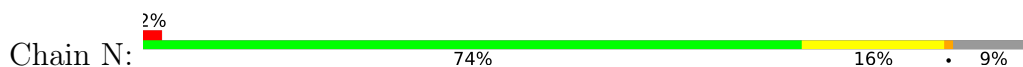
- Molecule 1: CALCIUM/CALMODULIN-DEPENDENT PROTEIN KINASE TYPE II DELTA CHAIN



- Molecule 1: CALCIUM/CALMODULIN-DEPENDENT PROTEIN KINASE TYPE II DELTA CHAIN

G471  
SER  
PRO  
THR  
VAL

- Molecule 1: CALCIUM/CALMODULIN-DEPENDENT PROTEIN KINASE TYPE II DELTA CHAIN

PRO  
THR  
VAL

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	149.55Å 117.80Å 160.76Å 90.00° 111.92° 90.00°	Depositor
Resolution (Å)	44.80 – 2.70 44.80 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (44.80-2.70) 99.5 (44.80-2.70)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.06 (at 2.69Å)	Xtrriage
Refinement program	REFMAC 5.5.0055	Depositor
R, $R_{free}$	0.211 , 0.245 0.218 , 0.247	Depositor DCC
$R_{free}$ test set	2134 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	70.9	Xtrriage
Anisotropy	0.050	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 62.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	14067	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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: ACT, CD

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	0.94	0/1020	0.93	2/1385 (0.1%)
1	B	1.08	0/1035	0.93	2/1403 (0.1%)
1	C	0.94	0/1016	0.90	0/1380
1	D	0.96	0/1012	0.90	0/1372
1	E	0.84	0/1018	0.88	2/1386 (0.1%)
1	F	0.82	0/1010	0.85	0/1371
1	G	0.85	0/1015	0.86	0/1379
1	H	0.85	0/1034	0.87	1/1407 (0.1%)
1	I	0.82	0/1009	0.87	0/1372
1	J	0.81	0/996	0.87	0/1354
1	K	0.83	0/1007	0.87	0/1368
1	L	0.91	0/1038	0.86	0/1409
1	M	0.91	0/999	0.87	0/1357
1	N	0.84	0/1039	0.92	2/1412 (0.1%)
All	All	0.89	0/14248	0.89	9/19355 (0.0%)

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	408	LYS	CA-C-N	6.77	127.16	119.92
1	A	408	LYS	C-N-CA	6.77	127.16	119.92
1	H	361	ILE	CB-CA-C	-5.93	104.38	111.97
1	N	408	LYS	CA-C-N	5.79	126.11	119.92
1	N	408	LYS	C-N-CA	5.79	126.11	119.92

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	996	0	903	15	0
1	B	1011	0	931	19	0
1	C	992	0	908	18	1
1	D	988	0	920	21	0
1	E	994	0	893	15	0
1	F	986	0	902	17	0
1	G	991	0	901	20	0
1	H	1010	0	908	18	1
1	I	985	0	889	18	1
1	J	972	0	887	18	0
1	K	983	0	903	13	1
1	L	1014	0	926	17	0
1	M	975	0	895	19	0
1	N	1015	0	928	22	0
2	A	4	0	3	1	0
2	B	4	0	3	0	0
2	C	4	0	3	0	0
2	D	4	0	3	1	0
2	E	4	0	3	1	0
2	F	4	0	3	1	0
2	G	4	0	3	1	0
2	H	4	0	3	1	0
2	I	4	0	3	1	0
2	J	4	0	3	0	0
2	K	4	0	3	0	0
2	L	4	0	3	0	0
2	M	4	0	3	0	0
2	N	4	0	3	0	0
3	B	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
3	J	3	0	0	0	0
4	A	7	0	0	0	0
4	B	10	0	0	0	0
4	C	5	0	0	0	0
4	D	8	0	0	0	0
4	E	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	5	0	0	2	0
4	G	9	0	0	0	0
4	H	6	0	0	0	0
4	I	9	0	0	3	0
4	J	8	0	0	0	0
4	K	4	0	0	0	0
4	L	5	0	0	0	0
4	M	4	0	0	0	0
4	N	8	0	0	0	0
All	All	14067	0	12736	202	2

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 8.

The worst 5 of 202 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:443:MET:HA	1:D:443:MET:HE2	1.37	1.01
1:G:411:HIS:CE1	4:I:2003:HOH:O	2.23	0.91
1:B:422:VAL:HG12	1:L:426:ALA:HB2	1.62	0.81
1:G:411:HIS:HE1	4:I:2003:HOH:O	1.62	0.81
1:J:443:MET:HE3	1:J:444:PRO:HD2	1.62	0.80

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:365:ASP:OD2	1:H:359:GLU:OE2[3_445]	2.11	0.09
1:I:400:GLU:O	1:K:371:LYS:NZ[3_545]	2.19	0.01

## 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	124/144 (86%)	120 (97%)	4 (3%)	0	100	100
1	B	124/144 (86%)	119 (96%)	5 (4%)	0	100	100
1	C	123/144 (85%)	119 (97%)	3 (2%)	1 (1%)	16	37
1	D	121/144 (84%)	118 (98%)	3 (2%)	0	100	100
1	E	125/144 (87%)	123 (98%)	2 (2%)	0	100	100
1	F	122/144 (85%)	117 (96%)	5 (4%)	0	100	100
1	G	123/144 (85%)	119 (97%)	4 (3%)	0	100	100
1	H	127/144 (88%)	123 (97%)	4 (3%)	0	100	100
1	I	124/144 (86%)	119 (96%)	5 (4%)	0	100	100
1	J	121/144 (84%)	118 (98%)	3 (2%)	0	100	100
1	K	123/144 (85%)	118 (96%)	5 (4%)	0	100	100
1	L	126/144 (88%)	120 (95%)	6 (5%)	0	100	100
1	M	121/144 (84%)	116 (96%)	4 (3%)	1 (1%)	16	37
1	N	127/144 (88%)	123 (97%)	4 (3%)	0	100	100
All	All	1731/2016 (86%)	1672 (97%)	57 (3%)	2 (0%)	48	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	459	ASP
1	C	459	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	97/126 (77%)	96 (99%)	1 (1%)	68	86
1	B	101/126 (80%)	98 (97%)	3 (3%)	36	66
1	C	98/126 (78%)	94 (96%)	4 (4%)	27	56
1	D	100/126 (79%)	97 (97%)	3 (3%)	36	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	97/126 (77%)	96 (99%)	1 (1%)	68	86
1	F	98/126 (78%)	97 (99%)	1 (1%)	68	86
1	G	98/126 (78%)	97 (99%)	1 (1%)	68	86
1	H	99/126 (79%)	96 (97%)	3 (3%)	36	66
1	I	95/126 (75%)	92 (97%)	3 (3%)	34	64
1	J	96/126 (76%)	94 (98%)	2 (2%)	47	75
1	K	96/126 (76%)	93 (97%)	3 (3%)	35	65
1	L	101/126 (80%)	99 (98%)	2 (2%)	48	76
1	M	95/126 (75%)	93 (98%)	2 (2%)	47	75
1	N	100/126 (79%)	97 (97%)	3 (3%)	36	66
All	All	1371/1764 (78%)	1339 (98%)	32 (2%)	44	73

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	410	ILE
1	N	338	ILE
1	F	410	ILE
1	E	410	ILE
1	N	358	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	456	HIS
1	L	456	HIS
1	N	411	HIS
1	E	448	GLN
1	F	436	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 6 are monoatomic - leaving 14 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	ACT	G	632	-	3,3,3	1.03	0	3,3,3	2.16	1 (33%)
2	ACT	I	632	-	3,3,3	1.02	0	3,3,3	2.47	2 (66%)
2	ACT	N	632	-	3,3,3	0.90	0	3,3,3	2.19	2 (66%)
2	ACT	C	632	-	3,3,3	1.31	0	3,3,3	2.34	2 (66%)
2	ACT	L	632	-	3,3,3	1.08	0	3,3,3	2.21	2 (66%)
2	ACT	E	632	-	3,3,3	0.92	0	3,3,3	2.36	2 (66%)
2	ACT	D	632	-	3,3,3	1.28	0	3,3,3	2.14	1 (33%)
2	ACT	J	632	-	3,3,3	1.12	0	3,3,3	2.69	2 (66%)
2	ACT	M	632	-	3,3,3	1.07	0	3,3,3	2.22	2 (66%)
2	ACT	H	632	-	3,3,3	1.21	0	3,3,3	3.16	2 (66%)
2	ACT	F	632	-	3,3,3	0.90	0	3,3,3	2.09	2 (66%)
2	ACT	A	632	-	3,3,3	0.89	0	3,3,3	2.56	2 (66%)
2	ACT	K	632	-	3,3,3	1.36	0	3,3,3	2.70	1 (33%)
2	ACT	B	632	-	3,3,3	1.42	0	3,3,3	2.26	2 (66%)

There are no bond length outliers.

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	632	ACT	OXT-C-O	-4.48	105.40	122.03
2	K	632	ACT	OXT-C-O	-3.92	107.48	122.03
2	J	632	ACT	OXT-C-O	-3.70	108.29	122.03
2	C	632	ACT	OXT-C-O	-3.35	109.61	122.03
2	A	632	ACT	OXT-C-O	-3.31	109.73	122.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	632	ACT	1	0
2	I	632	ACT	1	0
2	E	632	ACT	1	0
2	D	632	ACT	1	0
2	H	632	ACT	1	0
2	F	632	ACT	1	0
2	A	632	ACT	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [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, 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	128/144 (88%)	0.25	2 (1%) 70 68	36, 42, 52, 55	0
1	B	128/144 (88%)	0.07	1 (0%) 82 81	34, 41, 52, 66	0
1	C	127/144 (88%)	0.20	3 (2%) 59 56	33, 41, 50, 58	0
1	D	125/144 (86%)	0.20	2 (1%) 70 68	36, 42, 51, 55	0
1	E	129/144 (89%)	0.43	2 (1%) 70 68	38, 45, 52, 56	0
1	F	126/144 (87%)	0.17	2 (1%) 70 68	40, 45, 52, 56	0
1	G	127/144 (88%)	0.40	3 (2%) 59 56	38, 44, 52, 55	0
1	H	131/144 (90%)	0.49	6 (4%) 37 34	36, 44, 52, 59	0
1	I	128/144 (88%)	0.61	6 (4%) 36 33	37, 44, 52, 54	0
1	J	125/144 (86%)	0.22	1 (0%) 82 81	39, 45, 51, 53	0
1	K	127/144 (88%)	0.30	5 (3%) 43 39	35, 42, 51, 54	0
1	L	130/144 (90%)	0.31	4 (3%) 51 48	35, 42, 52, 57	0
1	M	125/144 (86%)	0.27	2 (1%) 70 68	36, 43, 51, 57	0
1	N	131/144 (90%)	0.23	3 (2%) 61 58	38, 45, 51, 55	0
All	All	1787/2016 (88%)	0.30	42 (2%) 59 56	33, 44, 52, 66	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	422	VAL	4.2
1	K	406	SER	3.8
1	D	402	ALA	3.4
1	A	363	ASN	3.3
1	F	459	ASP	3.3

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides 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	ACT	B	632	4/4	0.49	0.22	48,51,51,51	0
2	ACT	K	632	4/4	0.54	0.20	45,48,48,48	0
2	ACT	H	632	4/4	0.59	0.22	54,56,56,57	0
2	ACT	C	632	4/4	0.59	0.23	55,58,58,58	0
3	CD	F	1472	1/1	0.60	0.17	96,96,96,96	1
2	ACT	D	632	4/4	0.63	0.22	52,55,55,55	0
2	ACT	E	632	4/4	0.65	0.23	63,65,65,65	0
2	ACT	I	632	4/4	0.65	0.23	65,67,67,68	0
2	ACT	M	632	4/4	0.66	0.24	67,67,68,68	0
2	ACT	G	632	4/4	0.75	0.18	58,58,59,59	0
3	CD	J	1474	1/1	0.75	0.10	94,94,94,94	1
3	CD	J	1472	1/1	0.76	0.11	79,79,79,79	1
2	ACT	L	632	4/4	0.76	0.18	56,57,57,58	0
2	ACT	N	632	4/4	0.77	0.23	74,76,76,76	0
2	ACT	J	632	4/4	0.78	0.17	60,62,62,62	0
2	ACT	F	632	4/4	0.81	0.20	67,68,68,68	0
2	ACT	A	632	4/4	0.81	0.20	50,51,52,53	0
3	CD	H	1472	1/1	0.89	0.13	78,78,78,78	1
3	CD	B	1472	1/1	0.90	0.19	82,82,82,82	1
3	CD	J	1473	1/1	0.95	0.05	77,77,77,77	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.