



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:43 PM GMT

PDB ID : 4MD9
Title : Crystal Structure of symmetric CK2 holoenzyme with mutated alpha subunit (F121E truncated at aa 336)
Authors : Lolli, G.; Ranchio, A.; Battistutta, R.
Deposited on : 2013-08-22
Resolution : 3.50 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

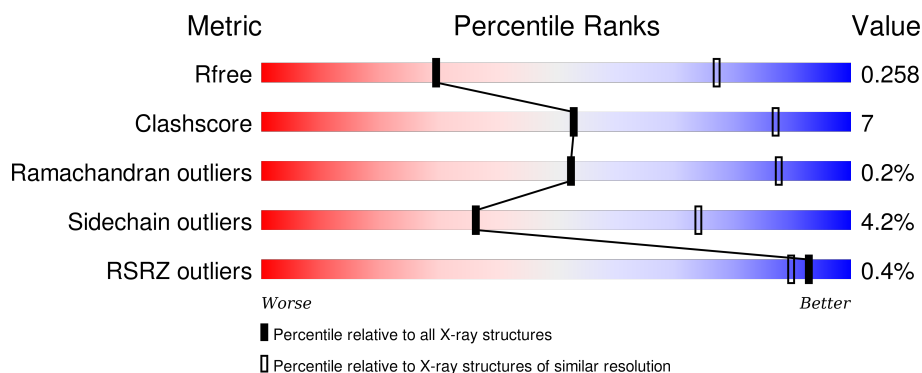
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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. 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	215	
1	B	215	
1	C	215	
1	D	215	
1	I	215	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	J	215	 76%13%10%
1	N	215	 76%13%8%
1	O	215	 2%77%14%8%
2	E	336	 81%16%..
2	F	336	 1%84%11%..
2	G	336	 79%16%..
2	H	336	 85%12%..
2	K	336	 1%82%14%..
2	L	336	 88%8%..
2	M	336	 78%20%..
2	P	336	 85%11%..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 35073 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 II subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	201	Total	C	N	O	S	0	0	0
			1643	1053	275	300	15			
1	B	195	Total	C	N	O	S	0	0	0
			1593	1025	268	285	15			
1	C	198	Total	C	N	O	S	0	0	0
			1619	1039	271	294	15			
1	D	196	Total	C	N	O	S	0	0	0
			1601	1029	270	287	15			
1	I	196	Total	C	N	O	S	0	0	0
			1601	1029	269	288	15			
1	J	194	Total	C	N	O	S	0	0	0
			1584	1020	267	282	15			
1	N	197	Total	C	N	O	S	0	0	0
			1610	1034	270	291	15			
1	O	198	Total	C	N	O	S	0	0	0
			1618	1038	272	293	15			

- Molecule 2 is a protein called Casein kinase II subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	329	Total	C	N	O	S	0	0	0
			2777	1777	488	501	11			
2	F	327	Total	C	N	O	S	0	0	0
			2767	1772	486	498	11			
2	G	329	Total	C	N	O	S	0	0	0
			2777	1777	488	501	11			
2	H	328	Total	C	N	O	S	0	0	0
			2771	1774	487	499	11			
2	K	328	Total	C	N	O	S	0	0	0
			2771	1774	487	499	11			
2	L	328	Total	C	N	O	S	0	0	0
			2771	1774	487	499	11			

Continued on next page...

Continued from previous page...

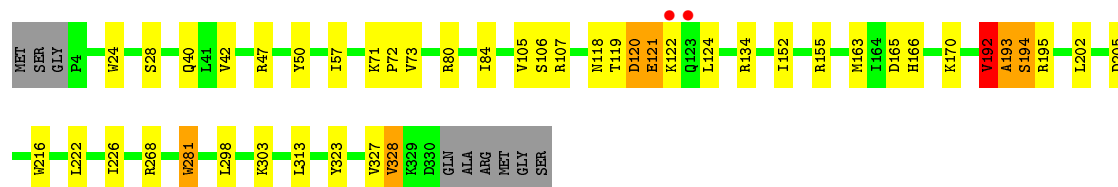
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	331	Total	C	N	O	S	0	0	0
			2791	1785	491	504	11			
2	P	328	Total	C	N	O	S	0	0	0
			2771	1774	487	499	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	121	GLU	PHE	ENGINEERED MUTATION	UNP P68400
F	121	GLU	PHE	ENGINEERED MUTATION	UNP P68400
G	121	GLU	PHE	ENGINEERED MUTATION	UNP P68400
H	121	GLU	PHE	ENGINEERED MUTATION	UNP P68400
K	121	GLU	PHE	ENGINEERED MUTATION	UNP P68400
L	121	GLU	PHE	ENGINEERED MUTATION	UNP P68400
M	121	GLU	PHE	ENGINEERED MUTATION	UNP P68400
P	121	GLU	PHE	ENGINEERED MUTATION	UNP P68400

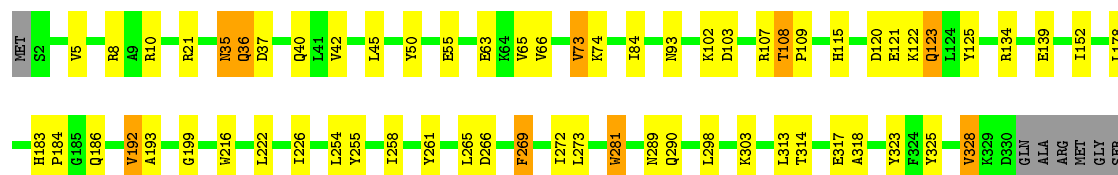
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	I	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		
3	N	1	Total	Zn	0	0
			1	1		
3	O	1	Total	Zn	0	0
			1	1		



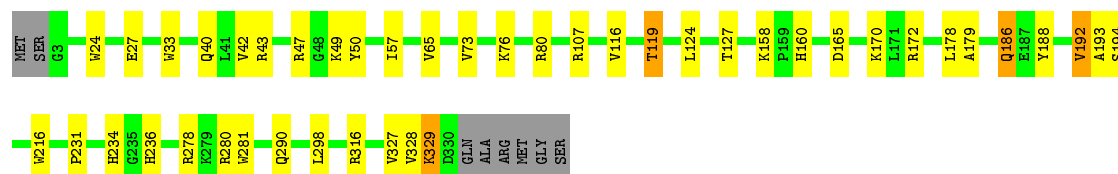
- Molecule 2: Casein kinase II subunit alpha

Chain G: 79% 16% ..



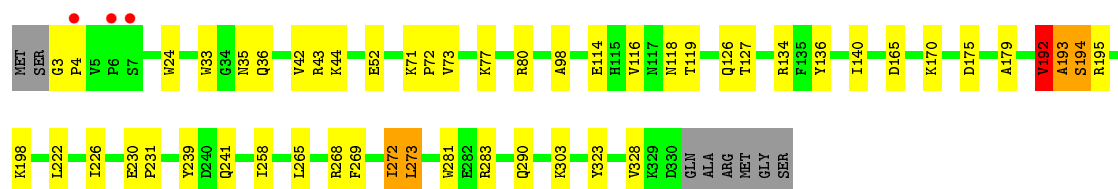
- Molecule 2: Casein kinase II subunit alpha

Chain H: 85% 12% ..



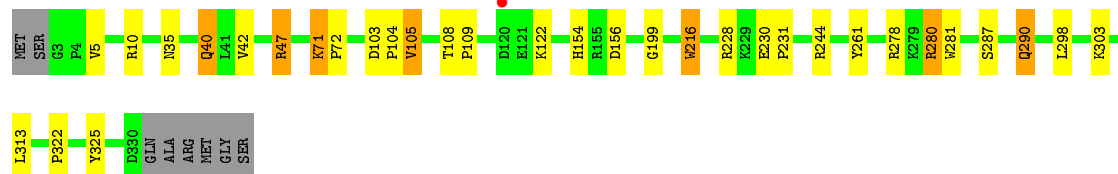
- Molecule 2: Casein kinase II subunit alpha

Chain K: 82% 14% ..



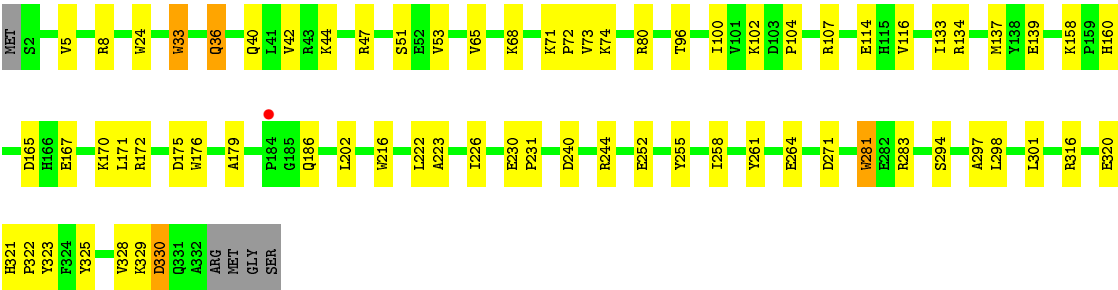
- Molecule 2: Casein kinase II subunit alpha

Chain L: 88% 8% ..

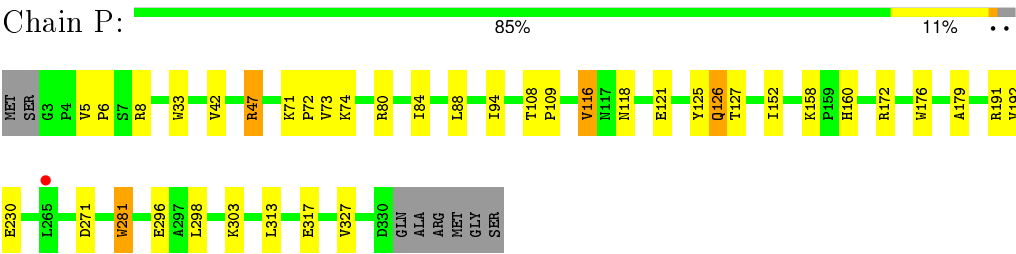


- Molecule 2: Casein kinase II subunit alpha

Chain M: 78% 20% ..



• Molecule 2: Casein kinase II subunit alpha



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	283.92Å 115.71Å 208.22Å 90.00° 119.22° 90.00°	Depositor
Resolution (Å)	181.72 – 3.50 48.31 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (181.72-3.50) 99.6 (48.31-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.229 , 0.259 0.228 , 0.258	Depositor DCC
R_{free} test set	3736 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	76.6	Xtriage
Anisotropy	0.490	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 45.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	2 of 74255 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	35073	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.83% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section:
ZN

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	0.62	0/1693	0.64	0/2296
1	B	0.62	1/1642 (0.1%)	0.64	0/2224
1	C	0.62	0/1668	0.62	0/2259
1	D	0.63	0/1650	0.62	0/2236
1	I	0.59	0/1650	0.61	1/2235 (0.0%)
1	J	0.59	1/1633 (0.1%)	0.61	0/2212
1	N	0.60	0/1659	0.62	0/2247
1	O	0.58	1/1667 (0.1%)	0.67	4/2259 (0.2%)
2	E	0.59	5/2851 (0.2%)	0.63	3/3856 (0.1%)
2	F	0.56	3/2841 (0.1%)	0.74	10/3842 (0.3%)
2	G	0.58	1/2851 (0.0%)	0.64	4/3856 (0.1%)
2	H	0.57	3/2845 (0.1%)	0.62	2/3848 (0.1%)
2	K	0.57	3/2845 (0.1%)	0.66	4/3848 (0.1%)
2	L	0.56	1/2845 (0.0%)	0.57	0/3848
2	M	0.57	5/2865 (0.2%)	0.58	0/3875
2	P	0.57	3/2845 (0.1%)	0.60	2/3848 (0.1%)
All	All	0.58	27/36050 (0.1%)	0.63	30/48789 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	M	0	1

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	9	TRP	CD2-CE2	6.28	1.48	1.41
2	P	176	TRP	CD2-CE2	6.21	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	281	TRP	CD2-CE2	5.88	1.48	1.41
2	E	281	TRP	CD2-CE2	5.60	1.48	1.41
1	J	9	TRP	CD2-CE2	5.55	1.48	1.41

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	120	ASP	N-CA-CB	-11.83	89.30	110.60
2	F	194	SER	N-CA-CB	-11.00	94.00	110.50
2	F	194	SER	CB-CA-C	10.41	129.88	110.10
2	G	192	VAL	N-CA-C	8.99	135.26	111.00
2	K	193	ALA	CB-CA-C	8.92	123.49	110.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	M	330	ASP	Peptide

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	1643	0	1556	32	0
1	B	1593	0	1519	29	0
1	C	1619	0	1535	50	0
1	D	1601	0	1524	44	0
1	I	1601	0	1523	45	0
1	J	1584	0	1513	39	0
1	N	1610	0	1529	43	0
1	O	1618	0	1534	51	0
2	E	2777	0	2719	24	0
2	F	2767	0	2712	23	0
2	G	2777	0	2719	34	0
2	H	2771	0	2714	21	0
2	K	2771	0	2714	25	0
2	L	2771	0	2714	36	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	M	2791	0	2732	30	0
2	P	2771	0	2714	21	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
All	All	35073	0	33971	453	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 7.

The worst 5 of 453 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:HIS:CD2	1:B:195:MET:HB3	1.61	1.34
1:C:193:HIS:CD2	1:C:195:MET:HB3	1.61	1.33
1:I:193:HIS:HD2	1:I:195:MET:HB3	1.06	1.17
1:D:193:HIS:HD2	1:D:195:MET:HB3	1.12	1.11
1:O:193:HIS:ND1	1:O:194:PRO:HD2	1.63	1.11

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	199/215 (93%)	194 (98%)	5 (2%)	0	100	100
1	B	191/215 (89%)	184 (96%)	7 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	194/215 (90%)	187 (96%)	7 (4%)	0	100	100
1	D	192/215 (89%)	184 (96%)	8 (4%)	0	100	100
1	I	192/215 (89%)	183 (95%)	8 (4%)	1 (0%)	34	78
1	J	190/215 (88%)	184 (97%)	5 (3%)	1 (0%)	34	78
1	N	193/215 (90%)	188 (97%)	5 (3%)	0	100	100
1	O	194/215 (90%)	191 (98%)	3 (2%)	0	100	100
2	E	327/336 (97%)	313 (96%)	13 (4%)	1 (0%)	46	84
2	F	325/336 (97%)	299 (92%)	24 (7%)	2 (1%)	30	75
2	G	327/336 (97%)	303 (93%)	23 (7%)	1 (0%)	46	84
2	H	326/336 (97%)	304 (93%)	21 (6%)	1 (0%)	46	84
2	K	326/336 (97%)	311 (95%)	14 (4%)	1 (0%)	46	84
2	L	326/336 (97%)	311 (95%)	15 (5%)	0	100	100
2	M	329/336 (98%)	309 (94%)	19 (6%)	1 (0%)	46	84
2	P	326/336 (97%)	307 (94%)	19 (6%)	0	100	100
All	All	4157/4408 (94%)	3952 (95%)	196 (5%)	9 (0%)	52	88

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	194	PRO
1	J	194	PRO
2	F	50	TYR
2	H	328	VAL
2	K	328	VAL

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	177/191 (93%)	170 (96%)	7 (4%)	38	75
1	B	171/191 (90%)	167 (98%)	4 (2%)	58	85

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	174/191 (91%)	164 (94%)	10 (6%)	25	66
1	D	172/191 (90%)	166 (96%)	6 (4%)	43	78
1	I	172/191 (90%)	163 (95%)	9 (5%)	29	68
1	J	170/191 (89%)	167 (98%)	3 (2%)	66	88
1	N	173/191 (91%)	162 (94%)	11 (6%)	22	62
1	O	174/191 (91%)	170 (98%)	4 (2%)	58	85
2	E	303/308 (98%)	290 (96%)	13 (4%)	35	74
2	F	302/308 (98%)	295 (98%)	7 (2%)	58	85
2	G	303/308 (98%)	290 (96%)	13 (4%)	35	74
2	H	302/308 (98%)	287 (95%)	15 (5%)	30	69
2	K	302/308 (98%)	285 (94%)	17 (6%)	26	66
2	L	302/308 (98%)	291 (96%)	11 (4%)	42	77
2	M	304/308 (99%)	288 (95%)	16 (5%)	28	67
2	P	302/308 (98%)	289 (96%)	13 (4%)	35	74
All	All	3803/3992 (95%)	3644 (96%)	159 (4%)	36	74

5 of 159 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	280	ARG
2	K	52	GLU
2	P	8	ARG
2	H	329	LYS
1	I	147	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	48	GLN
1	J	165	HIS
2	P	35	ASN
1	I	102	GLN
1	I	182	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 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 [i](#)

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	201/215 (93%)	-0.28	0 100 100	55, 81, 125, 152	0
1	B	195/215 (90%)	-0.24	1 (0%) 91 88	57, 77, 108, 135	0
1	C	198/215 (92%)	-0.28	0 100 100	55, 78, 124, 167	0
1	D	196/215 (91%)	-0.33	0 100 100	55, 76, 109, 142	0
1	I	196/215 (91%)	-0.20	1 (0%) 91 88	62, 86, 118, 135	0
1	J	194/215 (90%)	-0.15	0 100 100	58, 93, 122, 142	0
1	N	197/215 (91%)	-0.19	0 100 100	58, 92, 121, 140	0
1	O	198/215 (92%)	-0.02	5 (2%) 61 50	72, 102, 141, 178	0
2	E	329/336 (97%)	-0.17	1 (0%) 94 91	51, 92, 124, 153	0
2	F	327/336 (97%)	-0.19	2 (0%) 90 85	60, 87, 116, 134	0
2	G	329/336 (97%)	-0.32	0 100 100	59, 81, 109, 125	0
2	H	328/336 (97%)	-0.25	0 100 100	63, 90, 116, 126	0
2	K	328/336 (97%)	-0.21	3 (0%) 85 78	59, 84, 110, 148	0
2	L	328/336 (97%)	-0.13	1 (0%) 94 91	65, 94, 123, 154	0
2	M	331/336 (98%)	-0.09	1 (0%) 94 91	66, 89, 115, 129	0
2	P	328/336 (97%)	-0.20	1 (0%) 94 91	71, 93, 119, 148	0
All	All	4203/4408 (95%)	-0.20	16 (0%) 93 90	51, 88, 120, 178	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	68	GLN	4.8
2	L	120	ASP	3.1
1	O	56	LEU	2.8
2	K	6	PRO	2.6
2	M	184	PRO	2.5

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 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. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	ZN	C	301	1/1	1.00	0.16	-1.00	63,63,63,63	0
3	ZN	D	301	1/1	0.99	0.14	-1.04	63,63,63,63	0
3	ZN	I	301	1/1	0.99	0.12	-1.26	70,70,70,70	0
3	ZN	O	301	1/1	0.99	0.12	-1.30	59,59,59,59	0
3	ZN	N	301	1/1	0.98	0.13	-1.40	73,73,73,73	0
3	ZN	J	301	1/1	0.99	0.11	-1.62	77,77,77,77	0
3	ZN	A	301	1/1	1.00	0.10	-1.66	58,58,58,58	0
3	ZN	B	301	1/1	0.99	0.11	-1.74	66,66,66,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.