



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:29 PM UTC

PDB ID : 4DGL / pdb_00004dgl
Title : Crystal Structure of the CK2 Tetrameric Holoenzyme
Authors : Lolli, G.; Battistutta, R.
Deposited on : 2012-01-26
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
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)
Validation Pipeline (wwPDB-VP)	:	2.49

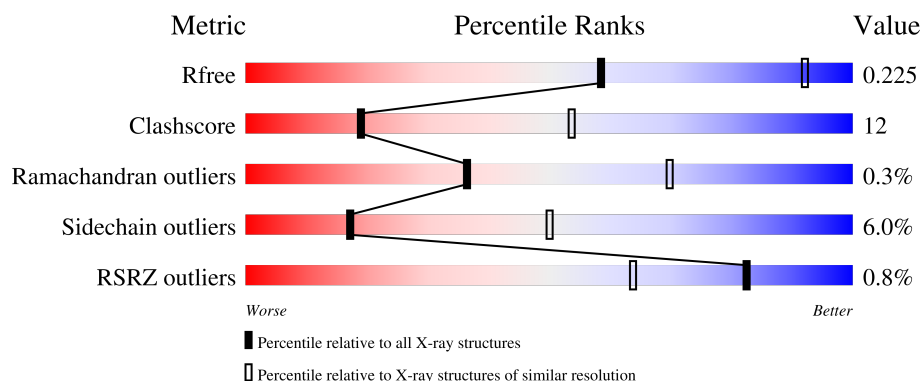
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	215	% 74% 16% • 7%
1	B	215	71% 19% • 7%
2	C	335	% 80% 16% • •
2	D	335	77% 19% • •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8877 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	200	Total	C	N	O	S	0	0	0
			1633	1050	279	289	15			
1	B	201	Total	C	N	O	S	0	0	0
			1643	1053	275	300	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	334	Total	C	N	O	S	0	0	0
			2815	1799	500	504	12			
2	D	328	Total	C	N	O	S	0	0	0
			2772	1775	490	496	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	125	ARG	TYR	engineered mutation	UNP P68400
D	125	ARG	TYR	engineered mutation	UNP P68400

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		

Continued on next page...

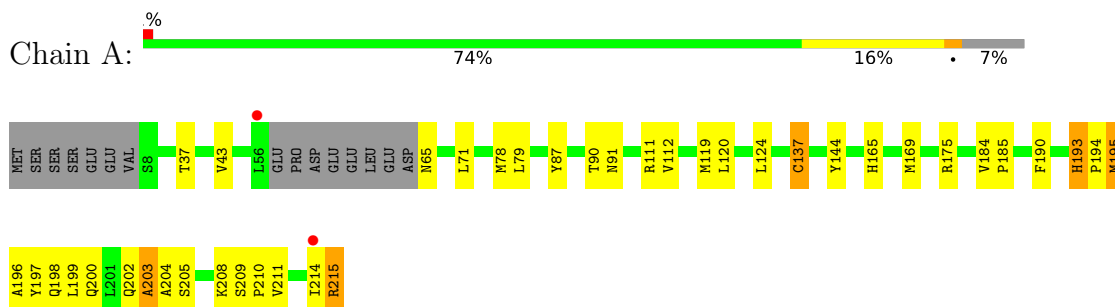
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	O	0	0
			2	2		
4	C	4	Total	O	0	0
			4	4		
4	D	5	Total	O	0	0
			5	5		

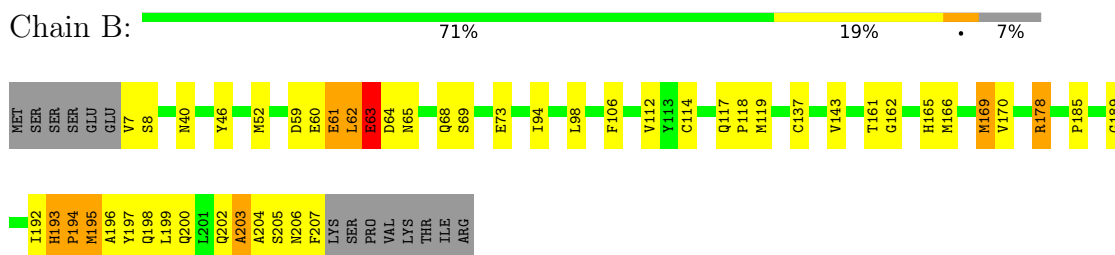
3 Residue-property plots

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.

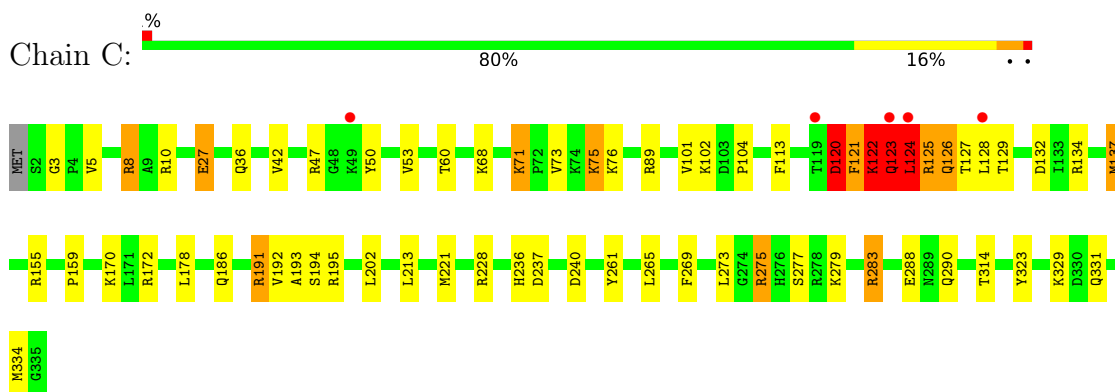
- Molecule 1: Casein kinase II subunit beta



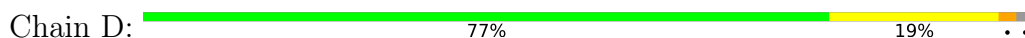
- Molecule 1: Casein kinase II subunit beta

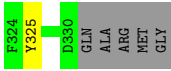
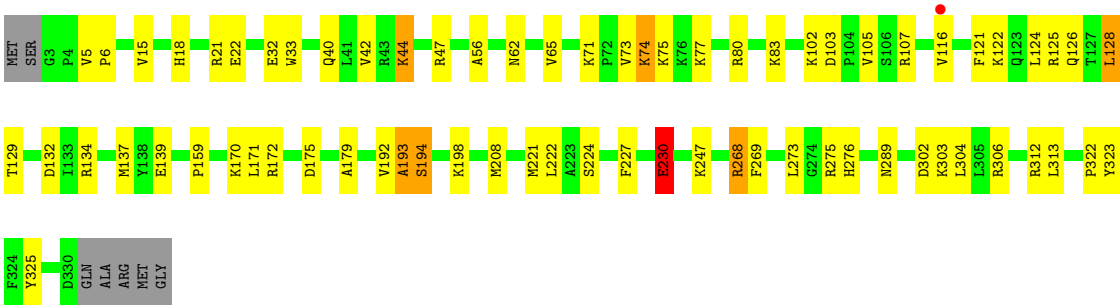


- Molecule 2: Casein kinase II subunit alpha



- Molecule 2: Casein kinase II subunit alpha





4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	175.65Å 175.65Å 96.26Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	152.12 – 3.00 152.12 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (152.12-3.00) 100.0 (152.12-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.94 (at 3.01Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.195 , 0.222 0.198 , 0.225	Depositor DCC
R_{free} test set	1726 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	70.3	Xtriage
Anisotropy	0.857	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.033 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8877	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.05	3/1682 (0.2%)	1.05	10/2277 (0.4%)
1	B	1.06	3/1693 (0.2%)	1.11	7/2296 (0.3%)
2	C	0.98	0/2889	1.12	10/3904 (0.3%)
2	D	0.98	1/2846 (0.0%)	1.00	4/3848 (0.1%)
All	All	1.01	7/9110 (0.1%)	1.07	31/12325 (0.3%)

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	C	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	178	ARG	CA-C	8.21	1.61	1.53
2	D	230	GLU	CA-C	-7.39	1.46	1.52
1	B	194	PRO	N-CA	-6.75	1.38	1.47
1	A	190	PHE	CA-C	-6.48	1.44	1.52
1	A	199	LEU	CA-C	-5.97	1.45	1.52
1	A	190	PHE	C-O	-5.81	1.16	1.24
1	B	199	LEU	CA-C	-5.12	1.45	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	124	LEU	N-CA-C	-16.86	92.25	113.16
2	C	121	PHE	N-CA-C	-13.14	95.33	113.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	GLY	N-CA-C	-11.69	88.48	112.34
2	C	122	LYS	N-CA-C	-10.77	89.79	108.52
1	B	62	LEU	N-CA-C	8.66	123.34	111.39
1	A	197	TYR	N-CA-C	-8.54	103.38	113.88
1	A	190	PHE	N-CA-C	-8.23	95.98	109.40
2	C	194	SER	N-CA-C	-7.97	95.64	108.55
1	B	61	GLU	CB-CA-C	-7.84	96.51	111.48
2	C	193	ALA	N-CA-C	7.76	119.48	108.00
1	B	197	TYR	N-CA-C	-7.75	104.35	113.88
2	C	124	LEU	CB-CA-C	7.72	123.91	110.01
1	A	193	HIS	CA-C-N	6.34	126.89	120.04
1	A	193	HIS	C-N-CA	6.34	126.89	120.04
1	B	63	GLU	CB-CA-C	-6.18	99.85	109.80
1	A	198	GLN	N-CA-C	-6.17	104.66	111.82
2	D	194	SER	N-CA-C	-6.08	98.71	108.55
2	D	193	ALA	N-CA-C	5.71	116.45	108.00
2	D	62	ASN	N-CA-C	5.67	120.01	113.38
1	B	195	MET	N-CA-C	-5.64	106.24	113.01
1	A	211	VAL	N-CA-C	-5.56	101.55	108.89
1	A	137	CYS	CA-C-N	5.50	125.17	119.56
1	A	137	CYS	C-N-CA	5.50	125.17	119.56
1	B	193	HIS	CA-C-O	5.38	126.78	120.87
1	B	198	GLN	N-CA-C	-5.21	105.77	111.82
2	D	175	ASP	N-CA-C	5.20	117.52	111.02
1	A	211	VAL	CB-CA-C	5.18	117.89	111.15
2	C	124	LEU	CA-C-O	5.17	125.54	119.28
2	C	120	ASP	CB-CA-C	5.16	118.25	109.53
1	A	195	MET	N-CA-C	-5.08	106.34	112.54
2	C	123	GLN	N-CA-C	5.02	121.48	110.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	71	LYS	Peptide

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	1633	0	1574	49	0
1	B	1643	0	1556	57	0
2	C	2815	0	2764	79	0
2	D	2772	0	2721	44	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	4	0	0	0	0
4	D	5	0	0	0	0
All	All	8877	0	8615	207	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 12.

All (207) 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:61:GLU:O	1:B:62:LEU:HG	1.39	1.21
2:C:124:LEU:HD23	2:C:124:LEU:N	1.58	1.15
2:D:268:ARG:HH11	2:D:268:ARG:HG2	1.15	1.11
1:B:193:HIS:CG	1:B:194:PRO:HD2	1.85	1.10
2:C:8:ARG:HG2	2:C:8:ARG:HH11	1.14	1.08
2:C:8:ARG:HH11	2:C:8:ARG:CG	1.65	1.07
1:B:61:GLU:HG2	1:B:62:LEU:H	1.19	0.99
2:C:236:HIS:CE1	2:C:240:ASP:HB2	1.99	0.98
1:B:61:GLU:HG2	1:B:62:LEU:N	1.70	0.96
2:C:124:LEU:N	2:C:124:LEU:CD2	2.27	0.96
1:A:208:LYS:O	1:A:208:LYS:HG3	1.63	0.95
2:D:303:LYS:HB3	2:D:313:LEU:CD1	1.97	0.95
1:A:193:HIS:HD2	1:A:195:MET:HB3	1.31	0.94
2:C:123:GLN:C	2:C:125:ARG:H	1.78	0.91
2:C:101:VAL:HG22	2:C:102:LYS:H	1.36	0.90
2:C:275:ARG:O	2:C:275:ARG:HG3	1.73	0.88
2:D:303:LYS:HD3	2:D:313:LEU:HD11	1.57	0.86
2:C:124:LEU:HB2	2:C:126:GLN:HB3	1.57	0.85
1:A:193:HIS:HD2	1:A:195:MET:CB	1.88	0.85
1:A:193:HIS:CD2	1:A:195:MET:HB3	2.11	0.85
1:A:91:ASN:N	2:C:47:ARG:HH12	1.74	0.85
2:C:236:HIS:CE1	2:C:240:ASP:CB	2.60	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:HIS:CD2	1:B:195:MET:H	1.95	0.84
2:D:47:ARG:HG2	2:D:47:ARG:HH11	1.42	0.84
2:C:120:ASP:C	2:C:122:LYS:H	1.84	0.82
1:A:193:HIS:CD2	1:A:195:MET:CB	2.62	0.82
1:A:91:ASN:H	2:C:47:ARG:NH1	1.78	0.82
1:A:193:HIS:CD2	1:A:195:MET:H	1.98	0.82
2:C:123:GLN:C	2:C:124:LEU:HD23	2.04	0.82
2:C:120:ASP:HB3	2:C:122:LYS:CB	2.10	0.81
2:D:303:LYS:HB3	2:D:313:LEU:HD11	1.63	0.81
2:C:121:PHE:CE1	2:C:128:LEU:HD21	2.16	0.80
2:C:8:ARG:HG2	2:C:8:ARG:NH1	1.84	0.80
2:C:120:ASP:HB3	2:C:122:LYS:HB3	1.63	0.80
1:B:189:GLY:HA3	2:C:36:GLN:HE22	1.49	0.78
1:B:193:HIS:HD2	1:B:195:MET:CB	1.97	0.78
2:D:268:ARG:HG2	2:D:268:ARG:NH1	1.95	0.77
1:B:193:HIS:CG	1:B:194:PRO:CD	2.68	0.76
2:D:303:LYS:HB3	2:D:313:LEU:HD12	1.67	0.76
1:A:91:ASN:H	2:C:47:ARG:HH12	1.30	0.76
2:C:121:PHE:CZ	2:C:128:LEU:HD21	2.21	0.76
1:B:193:HIS:HD2	1:B:195:MET:HB3	1.50	0.76
1:A:208:LYS:O	1:A:208:LYS:CG	2.33	0.76
2:C:101:VAL:HG22	2:C:102:LYS:N	2.01	0.75
2:C:124:LEU:HD23	2:C:124:LEU:H	1.49	0.75
2:C:121:PHE:CE1	2:C:128:LEU:CD2	2.70	0.74
2:C:120:ASP:C	2:C:122:LYS:N	2.44	0.74
1:B:60:GLU:HG3	1:B:61:GLU:H	1.53	0.74
2:D:303:LYS:CB	2:D:313:LEU:CD1	2.66	0.73
1:B:193:HIS:HD2	1:B:195:MET:H	1.35	0.73
1:A:193:HIS:CG	1:A:194:PRO:HD2	2.24	0.73
2:C:191:ARG:HH11	2:C:191:ARG:HG3	1.54	0.72
2:D:303:LYS:CB	2:D:313:LEU:HD11	2.20	0.71
2:C:191:ARG:HH11	2:C:191:ARG:CG	2.03	0.71
1:A:119:MET:HE1	1:A:144:TYR:CD1	2.26	0.71
2:C:236:HIS:CE1	2:C:240:ASP:CG	2.70	0.70
1:B:193:HIS:CD2	1:B:195:MET:HB3	2.27	0.69
1:B:193:HIS:CD2	1:B:194:PRO:HD2	2.28	0.69
2:D:47:ARG:HG2	2:D:47:ARG:NH1	2.06	0.69
2:D:268:ARG:HH11	2:D:268:ARG:CG	2.01	0.68
1:A:209:SER:HB2	1:A:210:PRO:HD2	1.73	0.67
1:B:52:MET:HE1	1:B:73:GLU:HG2	1.76	0.67
2:C:195:ARG:NH1	2:C:237:ASP:HA	2.09	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:LEU:HD12	1:B:62:LEU:O	1.93	0.67
2:C:8:ARG:CG	2:C:8:ARG:NH1	2.37	0.67
1:A:214:ILE:O	1:A:215:ARG:C	2.38	0.66
1:A:202:GLN:O	1:A:204:ALA:N	2.29	0.65
1:B:193:HIS:CD2	1:B:195:MET:CB	2.79	0.65
1:B:61:GLU:O	1:B:62:LEU:CG	2.31	0.65
1:A:43:VAL:HG21	1:A:79:LEU:HG	1.77	0.65
2:C:121:PHE:HE1	2:C:128:LEU:CD2	2.10	0.65
1:B:189:GLY:HA3	2:C:36:GLN:NE2	2.13	0.64
1:B:61:GLU:C	1:B:62:LEU:HG	2.20	0.64
2:D:159:PRO:HD3	2:D:221:MET:HG2	1.80	0.63
1:A:196:ALA:HB2	2:D:42:VAL:HA	1.81	0.62
1:B:61:GLU:CG	1:B:62:LEU:H	2.01	0.62
1:B:196:ALA:HB2	2:C:42:VAL:HA	1.81	0.62
1:B:7:VAL:HG22	1:B:8:SER:H	1.65	0.62
2:C:277:SER:OG	2:C:279:LYS:HE3	2.00	0.62
2:C:126:GLN:HG3	2:C:127:THR:N	2.13	0.61
2:C:8:ARG:HH11	2:C:8:ARG:HG3	1.60	0.61
1:A:193:HIS:CD2	1:A:195:MET:HB2	2.36	0.60
1:B:193:HIS:ND1	1:B:194:PRO:HD2	2.17	0.60
1:A:119:MET:CE	1:A:137:CYS:HB2	2.31	0.60
2:C:123:GLN:N	2:C:123:GLN:CD	2.59	0.60
2:C:120:ASP:HB3	2:C:122:LYS:HB2	1.84	0.59
2:C:101:VAL:CG2	2:C:102:LYS:H	2.12	0.59
2:C:123:GLN:C	2:C:125:ARG:N	2.52	0.58
2:C:128:LEU:HB3	2:C:132:ASP:CB	2.34	0.58
1:B:202:GLN:O	1:B:204:ALA:N	2.36	0.58
2:C:123:GLN:N	2:C:123:GLN:OE1	2.37	0.58
1:A:165:HIS:HB3	1:B:192:ILE:HD11	1.85	0.58
1:B:64:ASP:HA	1:B:68:GLN:H	1.68	0.57
2:D:73:VAL:HG12	2:D:74:LYS:N	2.19	0.57
1:B:206:ASN:O	1:B:207:PHE:C	2.46	0.57
1:A:193:HIS:HB2	2:D:40:GLN:HB2	1.85	0.57
2:D:303:LYS:CB	2:D:313:LEU:HD12	2.30	0.57
1:A:193:HIS:HD2	1:A:195:MET:H	1.50	0.57
2:C:10:ARG:HH12	2:C:314:THR:HG23	1.70	0.56
1:B:204:ALA:O	1:B:207:PHE:HB2	2.06	0.56
1:A:196:ALA:HB1	2:D:42:VAL:O	2.06	0.56
2:C:129:THR:H	2:C:132:ASP:HB2	1.71	0.55
1:A:202:GLN:C	1:A:204:ALA:N	2.62	0.55
2:D:124:LEU:HB2	2:D:128:LEU:HD13	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:10:ARG:NH1	2:C:314:THR:HG23	2.21	0.55
2:D:73:VAL:HG12	2:D:74:LYS:H	1.71	0.55
2:C:123:GLN:C	2:C:124:LEU:CD2	2.77	0.55
1:B:193:HIS:HD2	1:B:195:MET:N	2.03	0.54
2:C:236:HIS:ND1	2:C:240:ASP:CG	2.65	0.54
2:C:123:GLN:CA	2:C:125:ARG:H	2.21	0.54
2:C:128:LEU:HB3	2:C:132:ASP:HB2	1.89	0.54
2:D:73:VAL:HG11	2:D:77:LYS:HD3	1.90	0.54
1:A:175:ARG:HG3	1:B:200:GLN:HB3	1.90	0.54
2:D:194:SER:O	2:D:198:LYS:HG3	2.07	0.54
1:B:119:MET:HE3	1:B:137:CYS:HB2	1.90	0.53
2:C:123:GLN:HA	2:C:125:ARG:H	1.72	0.53
1:A:202:GLN:C	1:A:204:ALA:H	2.16	0.53
1:B:202:GLN:C	1:B:204:ALA:N	2.64	0.53
1:B:62:LEU:O	1:B:62:LEU:CD1	2.56	0.52
2:C:269:PHE:HB3	2:C:273:LEU:HD22	1.91	0.52
2:D:303:LYS:CD	2:D:313:LEU:HD11	2.34	0.52
2:D:192:VAL:O	2:D:198:LYS:NZ	2.37	0.52
1:A:165:HIS:CE1	1:B:185:PRO:HB3	2.45	0.52
1:A:202:GLN:O	1:A:205:SER:N	2.43	0.51
1:B:202:GLN:O	1:B:205:SER:N	2.43	0.51
1:A:91:ASN:N	2:C:47:ARG:NH1	2.44	0.51
1:A:119:MET:HE2	1:A:137:CYS:HB2	1.91	0.51
2:C:137:MET:HE2	2:C:137:MET:HA	1.92	0.51
2:C:191:ARG:HH11	2:C:191:ARG:CB	2.24	0.51
2:D:193:ALA:HB3	2:D:198:LYS:HG2	1.93	0.50
2:C:191:ARG:HG3	2:C:191:ARG:NH1	2.23	0.50
2:D:224:SER:OG	2:D:230:GLU:HG2	2.11	0.49
1:A:112:VAL:HG21	1:B:143:VAL:HG12	1.95	0.49
2:C:27:GLU:OE1	2:C:76:LYS:HE3	2.13	0.49
2:C:269:PHE:O	2:C:273:LEU:HB2	2.12	0.49
1:A:185:PRO:HB3	1:B:165:HIS:CE1	2.46	0.49
2:C:265:LEU:HD22	2:C:269:PHE:CD1	2.47	0.49
2:D:103:ASP:O	2:D:107:ARG:HA	2.12	0.49
1:A:119:MET:HE3	1:A:137:CYS:HB2	1.94	0.49
1:A:209:SER:CB	1:A:210:PRO:HD2	2.38	0.48
2:C:191:ARG:HH11	2:C:191:ARG:HB3	1.78	0.48
2:D:134:ARG:HG2	2:D:323:TYR:CZ	2.48	0.48
1:B:202:GLN:C	1:B:204:ALA:H	2.22	0.48
2:C:178:LEU:HD22	2:C:192:VAL:HG12	1.95	0.48
2:C:122:LYS:HG2	2:C:122:LYS:O	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:33:TRP:CZ2	2:D:102:LYS:HE2	2.49	0.48
1:A:87:TYR:O	1:A:90:THR:OG1	2.32	0.47
1:A:193:HIS:CD2	1:A:195:MET:N	2.76	0.47
1:B:62:LEU:HD12	1:B:62:LEU:C	2.40	0.47
2:D:247:LYS:HG2	2:D:276:HIS:CE1	2.49	0.47
2:C:334:MET:HA	2:C:334:MET:HE2	1.97	0.46
1:B:40:ASN:HA	1:B:46:TYR:CD1	2.50	0.46
2:D:129:THR:H	2:D:132:ASP:HB2	1.80	0.46
2:C:202:LEU:HD11	2:C:213:LEU:HD11	1.96	0.46
2:D:227:PHE:HA	2:D:289:ASN:HD22	1.81	0.46
1:A:165:HIS:HB3	1:B:192:ILE:CD1	2.44	0.46
2:C:50:TYR:CD2	2:C:73:VAL:HG11	2.51	0.46
1:A:112:VAL:CG2	1:B:143:VAL:HG12	2.45	0.45
1:A:202:GLN:O	1:A:203:ALA:C	2.59	0.45
2:C:53:VAL:HG22	2:C:68:LYS:HG3	1.98	0.45
2:D:137:MET:HE2	2:D:222:LEU:HD13	1.97	0.45
2:C:283:ARG:O	2:C:283:ARG:HG2	2.16	0.45
1:A:124:LEU:HD11	1:B:112:VAL:HG11	1.98	0.45
2:C:159:PRO:HD3	2:C:221:MET:HG2	1.98	0.45
1:B:63:GLU:C	1:B:65:ASN:H	2.24	0.45
2:D:80:ARG:HD3	2:D:179:ALA:O	2.16	0.45
2:C:36:GLN:N	2:C:101:VAL:HG21	2.32	0.45
2:C:121:PHE:HB3	2:C:126:GLN:HG2	1.99	0.45
2:D:5:VAL:HA	2:D:6:PRO:HD3	1.84	0.45
1:A:200:GLN:NE2	1:B:169:MET:HE2	2.31	0.44
2:C:134:ARG:HG2	2:C:323:TYR:CZ	2.53	0.44
2:D:56:ALA:HB3	2:D:65:VAL:HG23	1.99	0.44
2:D:122:LYS:O	2:D:126:GLN:HG3	2.17	0.44
2:C:134:ARG:HD3	2:C:323:TYR:O	2.17	0.44
2:C:121:PHE:HE1	2:C:128:LEU:HD23	1.82	0.43
1:B:106:PHE:HB2	1:B:119:MET:O	2.17	0.43
1:B:194:PRO:C	1:B:196:ALA:H	2.26	0.43
1:B:170:VAL:HG22	2:D:44:LYS:HE3	2.01	0.43
1:A:43:VAL:HG12	1:A:78:MET:HE3	2.00	0.43
1:A:209:SER:O	1:A:210:PRO:C	2.62	0.42
1:B:193:HIS:CD2	1:B:194:PRO:CD	2.99	0.42
2:C:236:HIS:ND1	2:C:240:ASP:CB	2.82	0.42
2:D:322:PRO:HA	2:D:325:TYR:CD1	2.53	0.42
2:D:139:GLU:HB2	2:D:171:LEU:HD13	2.01	0.42
1:B:202:GLN:O	1:B:203:ALA:C	2.62	0.42
1:A:193:HIS:HD2	1:A:195:MET:N	2.15	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:GLY:HA2	1:B:165:HIS:CD2	2.55	0.42
2:C:5:VAL:HB	2:C:261:TYR:HA	2.01	0.42
2:D:269:PHE:HB3	2:D:273:LEU:HD22	2.02	0.42
1:A:185:PRO:CB	1:B:165:HIS:CE1	3.03	0.41
1:B:193:HIS:CD2	1:B:195:MET:HB2	2.55	0.41
2:C:68:LYS:HD3	2:C:113:PHE:CE2	2.55	0.41
2:D:304:LEU:O	2:D:312:ARG:HG2	2.21	0.41
2:C:155:ARG:HD2	2:C:192:VAL:HG21	2.02	0.41
2:C:36:GLN:NE2	2:C:104:PRO:HD2	2.36	0.41
2:D:302:ASP:O	2:D:306:ARG:NH1	2.54	0.41
1:A:119:MET:CE	1:A:144:TYR:CD1	3.01	0.41
2:C:126:GLN:CG	2:C:127:THR:N	2.82	0.41
1:A:215:ARG:HH11	1:A:215:ARG:HG3	1.85	0.41
1:B:60:GLU:CG	1:B:61:GLU:H	2.26	0.41
2:C:121:PHE:C	2:C:123:GLN:N	2.79	0.41
2:D:121:PHE:O	2:D:125:ARG:HG3	2.21	0.41
1:B:94:ILE:O	1:B:98:LEU:HB2	2.21	0.40
1:A:165:HIS:O	1:A:169:MET:HG2	2.22	0.40
1:A:196:ALA:CB	2:D:42:VAL:O	2.69	0.40
1:B:117:GLN:HA	1:B:118:PRO:HD2	1.94	0.40
1:B:205:SER:O	1:B:206:ASN:C	2.64	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	196/215 (91%)	185 (94%)	10 (5%)	1 (0%)	24	60
1	B	199/215 (93%)	190 (96%)	8 (4%)	1 (0%)	24	60
2	C	332/335 (99%)	305 (92%)	26 (8%)	1 (0%)	36	70
2	D	326/335 (97%)	306 (94%)	20 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1053/1100 (96%)	986 (94%)	64 (6%)	3 (0%)	36 70

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	ALA
1	B	203	ALA
2	C	75	LYS

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	176/191 (92%)	169 (96%)	7 (4%)	28 62
1	B	177/191 (93%)	169 (96%)	8 (4%)	24 59
2	C	306/307 (100%)	282 (92%)	24 (8%)	11 39
2	D	302/307 (98%)	283 (94%)	19 (6%)	16 48
All	All	961/996 (96%)	903 (94%)	58 (6%)	17 50

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	THR
1	A	65	ASN
1	A	71	LEU
1	A	111	ARG
1	A	120	LEU
1	A	184	VAL
1	A	215	ARG
1	B	59	ASP
1	B	63	GLU
1	B	69	SER
1	B	114	CYS
1	B	161	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	166	MET
1	B	169	MET
1	B	178	ARG
2	C	8	ARG
2	C	27	GLU
2	C	60	THR
2	C	71	LYS
2	C	75	LYS
2	C	89	ARG
2	C	120	ASP
2	C	122	LYS
2	C	123	GLN
2	C	124	LEU
2	C	125	ARG
2	C	126	GLN
2	C	137	MET
2	C	170	LYS
2	C	172	ARG
2	C	186	GLN
2	C	191	ARG
2	C	228	ARG
2	C	275	ARG
2	C	283	ARG
2	C	288	GLU
2	C	290	GLN
2	C	329	LYS
2	C	331	GLN
2	D	15	VAL
2	D	18	HIS
2	D	21	ARG
2	D	22	GLU
2	D	32	GLU
2	D	44	LYS
2	D	71	LYS
2	D	74	LYS
2	D	75	LYS
2	D	83	LYS
2	D	105	VAL
2	D	116	VAL
2	D	128	LEU
2	D	170	LYS
2	D	172	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	208	MET
2	D	230	GLU
2	D	268	ARG
2	D	275	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	91	ASN
1	A	96	GLN
1	A	153	HIS
1	A	165	HIS
1	A	193	HIS
1	A	206	ASN
1	B	68	GLN
1	B	91	ASN
1	B	151	HIS
1	B	165	HIS
1	B	171	HIS
1	B	193	HIS
2	C	18	HIS
2	C	36	GLN
2	C	117	ASN
2	C	270	ASN
2	C	276	HIS
2	C	291	HIS
2	C	331	GLN
2	D	29	HIS
2	D	35	ASN
2	D	36	GLN
2	D	186	GLN
2	D	276	HIS
2	D	290	GLN
2	D	291	HIS

5.3.3 RNA ⓘ

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 2 ligands modelled in this entry, 2 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 [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, 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	200/215 (93%)	-0.16	2 (1%) 79 59	72, 102, 155, 190	0
1	B	201/215 (93%)	-0.44	0 100 100	71, 89, 123, 174	0
2	C	334/335 (99%)	-0.44	5 (1%) 72 49	59, 83, 123, 180	0
2	D	328/335 (97%)	-0.46	1 (0%) 90 79	58, 85, 116, 158	0
All	All	1063/1100 (96%)	-0.39	8 (0%) 82 64	58, 88, 133, 190	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	116	VAL	5.0
2	C	128	LEU	4.5
1	A	214	ILE	3.0
2	C	123	GLN	2.9
2	C	119	THR	2.4
2	C	49	LYS	2.4
1	A	56	LEU	2.2
2	C	124	LEU	2.1

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	A	301	1/1	1.00	0.02	75,75,75,75	0
3	ZN	B	301	1/1	1.00	0.02	73,73,73,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.