



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 18, 2025 – 06:14 PM JST

PDB ID : 9JCU / pdb\_00009jcu  
Title : Compound bound to ROCK2 kinase domain  
Authors : Yan, H.  
Deposited on : 2024-08-30  
Resolution : 3.02 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.

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	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.46

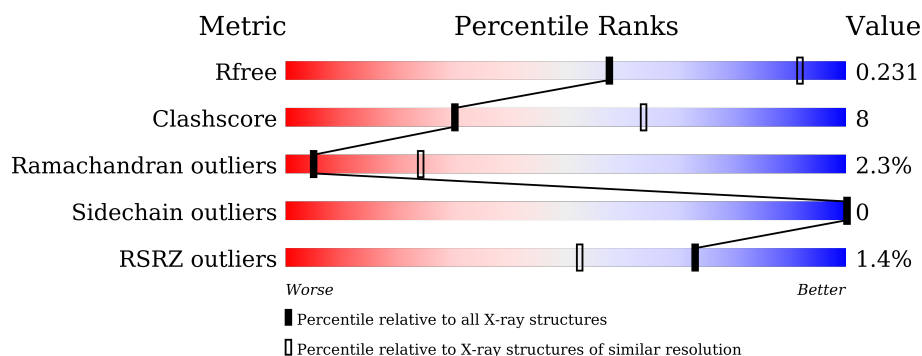
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.02 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))
$R_{free}$	164625	2927 (3.04-3.00)
Clashscore	180529	3300 (3.04-3.00)
Ramachandran outliers	177936	3188 (3.04-3.00)
Sidechain outliers	177891	3191 (3.04-3.00)
RSRZ outliers	164620	2939 (3.04-3.00)

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  $\geq 3$ , 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	391	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">%</span> </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>80%</span> <span>16%</span> <span>..</span> </div> </div>
1	B	391	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">2%</span> </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>79%</span> <span>18%</span> <span>..</span> </div> </div>
1	C	391	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">2%</span> </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>78%</span> <span>20%</span> <span>..</span> </div> </div>
1	D	391	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">%</span> </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>79%</span> <span>19%</span> <span>..</span> </div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12524 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 Rho-associated protein kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	0	0
			3133	2010	521	581	21			
1	B	389	Total	C	N	O	S	0	0	0
			3133	2010	521	581	21			
1	C	389	Total	C	N	O	S	0	0	0
			3132	2009	521	581	21			
1	D	387	Total	C	N	O	S	2	2	0
			3126	2007	519	579	21			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	157	CYS	TYR	conflict	UNP O75116
A	163	LYS	ARG	conflict	UNP O75116
A	270	TYR	PHE	conflict	UNP O75116
A	285	PHE	TYR	conflict	UNP O75116
A	349	LYS	ARG	conflict	UNP O75116
A	360	ASN	HIS	conflict	UNP O75116
B	157	CYS	TYR	conflict	UNP O75116
B	163	LYS	ARG	conflict	UNP O75116
B	270	TYR	PHE	conflict	UNP O75116
B	285	PHE	TYR	conflict	UNP O75116
B	349	LYS	ARG	conflict	UNP O75116
B	360	ASN	HIS	conflict	UNP O75116
C	157	CYS	TYR	conflict	UNP O75116
C	163	LYS	ARG	conflict	UNP O75116
C	270	TYR	PHE	conflict	UNP O75116
C	285	PHE	TYR	conflict	UNP O75116
C	349	LYS	ARG	conflict	UNP O75116
C	360	ASN	HIS	conflict	UNP O75116
D	157	CYS	TYR	conflict	UNP O75116
D	163	LYS	ARG	conflict	UNP O75116
D	270	TYR	PHE	conflict	UNP O75116

*Continued on next page...*

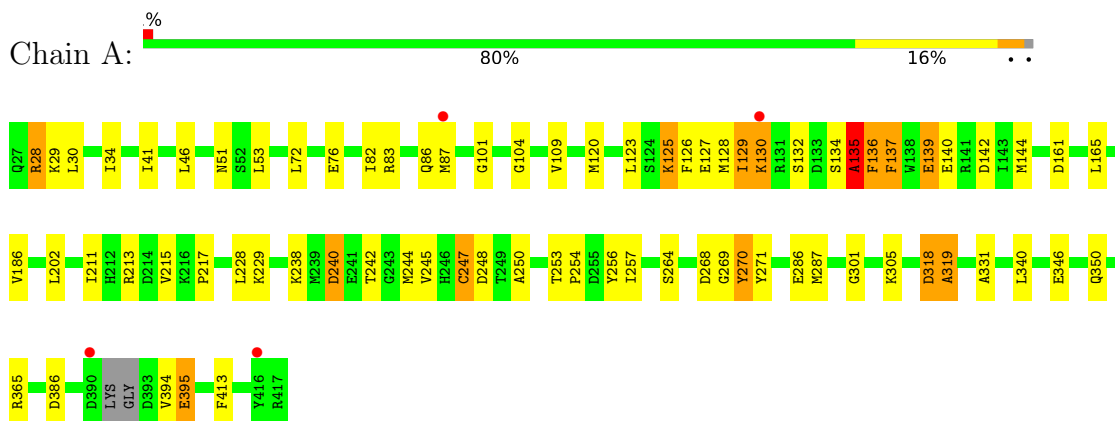
*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	285	PHE	TYR	conflict	UNP O75116
D	349	LYS	ARG	conflict	UNP O75116
D	360	ASN	HIS	conflict	UNP O75116

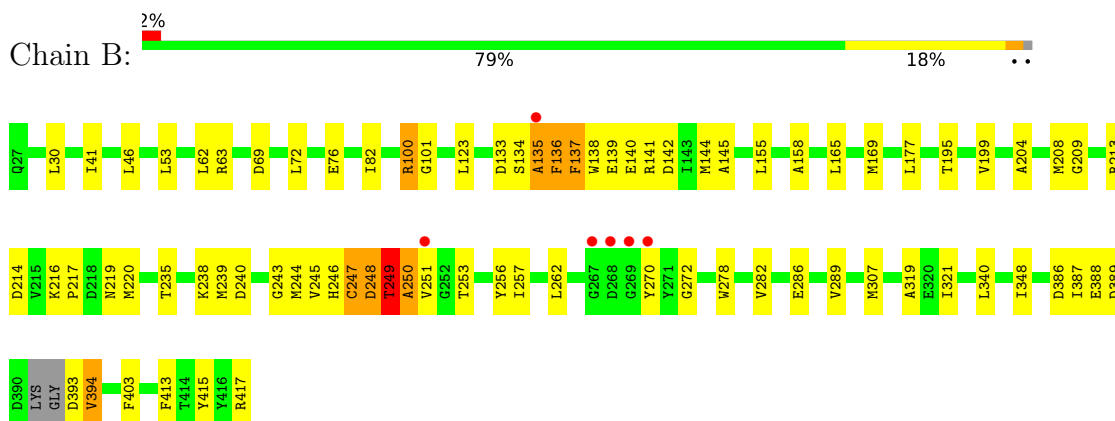
### 3 Residue-property plots [i](#)

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.

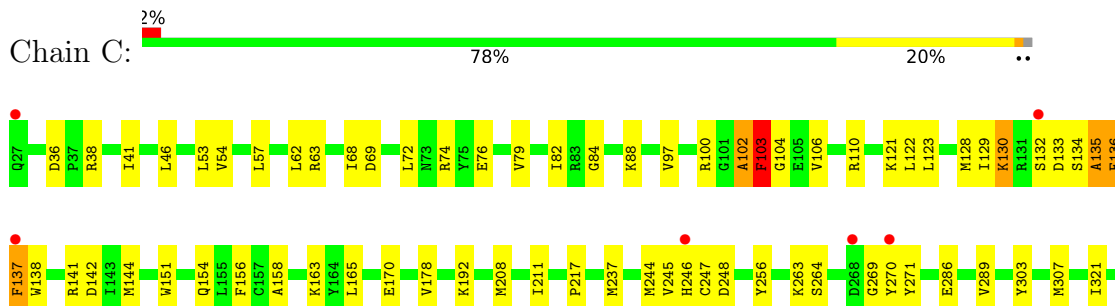
- Molecule 1: Rho-associated protein kinase 2

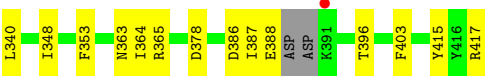


- Molecule 1: Rho-associated protein kinase 2

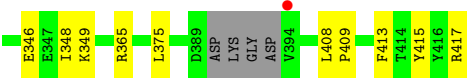
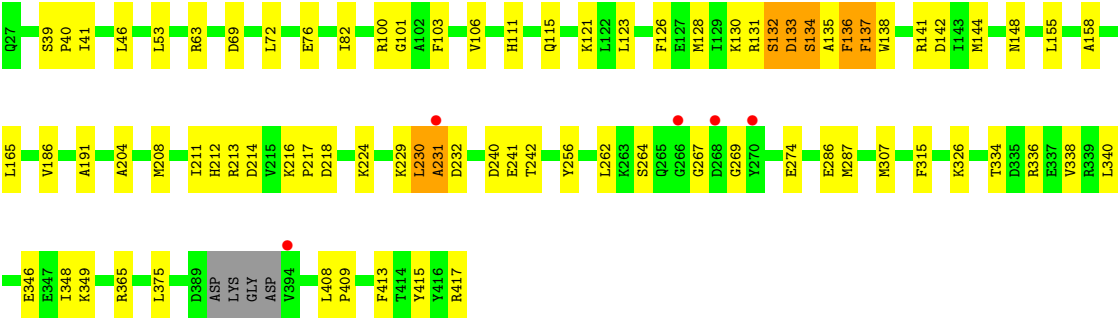
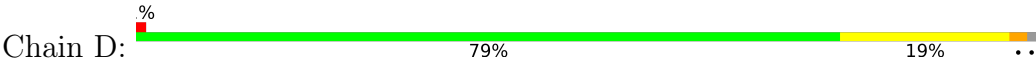


- Molecule 1: Rho-associated protein kinase 2





● Molecule 1: Rho-associated protein kinase 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	147.11Å 144.41Å 134.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.89 – 3.02 43.89 – 3.02	Depositor EDS
% Data completeness (in resolution range)	98.4 (43.89-3.02) 98.4 (43.89-3.02)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, $R_{free}$	0.184 , 0.220 0.203 , 0.231	Depositor DCC
$R_{free}$ test set	2766 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	72.9	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 59.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12524	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.60% 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

### 5.1 Standard geometry

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	0.18	0/3209	0.55	4/4336 (0.1%)
1	B	0.20	0/3209	0.54	5/4336 (0.1%)
1	C	0.18	0/3208	0.48	3/4334 (0.1%)
1	D	0.17	0/3208	0.49	6/4334 (0.1%)
All	All	0.18	0/12834	0.52	18/17340 (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
1	A	0	7
1	B	0	5
1	C	0	2
1	D	0	1
All	All	0	15

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	135	ALA	CA-C-N	7.90	135.93	121.70
1	B	135	ALA	C-N-CA	7.90	135.93	121.70
1	A	136	PHE	CA-C-N	7.90	135.92	121.70
1	A	136	PHE	C-N-CA	7.90	135.92	121.70
1	A	135	ALA	CA-C-N	7.84	135.82	121.70
1	A	135	ALA	C-N-CA	7.84	135.82	121.70
1	D	136	PHE	CA-C-N	7.79	135.72	121.70
1	D	136	PHE	C-N-CA	7.79	135.72	121.70
1	C	103	PHE	N-CA-C	6.37	128.84	111.00
1	B	249	THR	CA-C-N	6.28	133.00	121.70

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	249	THR	C-N-CA	6.28	133.00	121.70
1	C	102	ALA	CA-C-N	6.12	132.72	121.70
1	C	102	ALA	C-N-CA	6.12	132.72	121.70
1	B	249	THR	CB-CA-C	5.52	121.25	109.10
1	D	132	SER	CA-C-N	5.05	131.19	121.54
1	D	132	SER	C-N-CA	5.05	131.19	121.54
1	D	231	ALA	CA-C-N	5.03	130.76	121.70
1	D	231	ALA	C-N-CA	5.03	130.76	121.70

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	129	ILE	Peptide
1	A	130	LYS	Peptide
1	A	132	SER	Peptide
1	A	135	ALA	Peptide
1	A	247	CYS	Peptide
1	A	250	ALA	Peptide
1	A	394	VAL	Peptide
1	B	136	PHE	Peptide
1	B	139	GLU	Peptide
1	B	249	THR	Peptide
1	B	250	ALA	Peptide
1	B	251	VAL	Peptide
1	C	132	SER	Peptide
1	C	136	PHE	Peptide
1	D	230	LEU	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	3133	0	3057	50	0
1	B	3133	0	3057	52	0
1	C	3132	0	3058	57	0
1	D	3126	0	3061	59	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12524	0	12233	205	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 8.

All (205) 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:135:ALA:HB3	1:B:137:PHE:H	1.29	0.98
1:A:82:ILE:HD11	1:B:41:ILE:HD13	1.57	0.87
1:D:231:ALA:HB1	1:D:232:ASP:HA	1.56	0.87
1:C:363:ASN:O	1:C:365:ARG:N	2.12	0.82
1:A:256:TYR:OH	1:A:286:GLU:OE1	1.97	0.80
1:B:247:CYS:SG	1:B:248:ASP:N	2.56	0.79
1:B:249:THR:HB	1:B:250:ALA:HB2	1.68	0.76
1:D:264:SER:HB2	1:D:269:GLY:HA2	1.67	0.76
1:D:133:ASP:OD1	1:D:134:SER:N	2.14	0.75
1:B:244:MET:HG2	1:B:272:GLY:HA3	1.69	0.75
1:C:84:GLY:HA2	1:C:88:LYS:HD3	1.69	0.74
1:B:141:ARG:NH1	1:B:142:ASP:OD1	2.20	0.74
1:C:63:ARG:NH1	1:C:69:ASP:OD1	2.20	0.74
1:B:155:LEU:O	1:B:417:ARG:NH1	2.23	0.72
1:A:254:PRO:HA	1:A:257:ILE:HD13	1.71	0.72
1:C:256:TYR:OH	1:C:286:GLU:OE1	2.07	0.71
1:A:41:ILE:HD13	1:B:82:ILE:HD11	1.72	0.71
1:D:136:PHE:HA	1:D:137:PHE:HB3	1.73	0.71
1:C:248:ASP:OD1	1:C:269:GLY:N	2.25	0.70
1:B:144:MET:HA	1:B:208:MET:HE1	1.73	0.69
1:C:163:LYS:HG2	1:C:396:THR:HG21	1.74	0.69
1:A:213:ARG:NH1	1:A:247:CYS:SG	2.62	0.68
1:A:125:LYS:O	1:A:127:GLU:N	2.27	0.68
1:D:63:ARG:NH1	1:D:69:ASP:OD1	2.25	0.68
1:B:135:ALA:HB3	1:B:137:PHE:N	2.07	0.66
1:C:102:ALA:HA	1:C:104:GLY:N	2.12	0.64
1:D:212:HIS:HD1	1:D:214:ASP:H	1.44	0.64
1:D:141:ARG:NH1	1:D:142:ASP:OD1	2.31	0.64
1:D:141:ARG:NH2	1:D:413:PHE:O	2.31	0.63
1:B:134:SER:HB2	1:B:135:ALA:HA	1.79	0.63
1:D:216:LYS:HE3	1:D:218:ASP:HB2	1.82	0.61
1:C:74:ARG:HH21	1:D:40:PRO:HB3	1.66	0.61
1:B:256:TYR:OH	1:B:286:GLU:OE1	2.17	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:256:TYR:OH	1:D:286:GLU:OE1	2.12	0.61
1:C:41:ILE:HD13	1:D:82:ILE:HD11	1.84	0.60
1:C:72:LEU:O	1:C:76:GLU:HB2	2.02	0.59
1:C:82:ILE:HD11	1:D:41:ILE:HD13	1.84	0.59
1:C:123:LEU:HB2	1:C:165:LEU:HB2	1.85	0.59
1:A:82:ILE:HD11	1:B:41:ILE:CD1	2.29	0.59
1:A:213:ARG:NH2	1:A:271:TYR:OH	2.34	0.58
1:A:72:LEU:O	1:A:76:GLU:HB2	2.03	0.58
1:C:263:LYS:HG2	1:C:307:MET:HE1	1.85	0.58
1:B:72:LEU:O	1:B:76:GLU:HB2	2.03	0.58
1:A:346:GLU:O	1:A:350:GLN:HG2	2.04	0.58
1:D:72:LEU:O	1:D:76:GLU:HB2	2.04	0.58
1:B:214:ASP:O	1:B:219:ASN:ND2	2.37	0.57
1:A:125:LYS:NZ	1:A:161:ASP:O	2.37	0.57
1:B:393:ASP:O	1:B:394:VAL:HG22	2.06	0.56
1:C:106:VAL:HG22	1:C:121:LYS:HD3	1.87	0.55
1:C:100:ARG:HH22	1:C:388:GLU:C	2.14	0.55
1:D:155:LEU:O	1:D:417:ARG:NH1	2.40	0.55
1:C:264:SER:HB2	1:C:269:GLY:HA2	1.87	0.55
1:D:346:GLU:OE1	1:D:349:LYS:NZ	2.31	0.55
1:C:128:MET:O	1:C:133:ASP:HB2	2.07	0.55
1:C:244:MET:HE1	1:C:270:TYR:CD2	2.42	0.55
1:A:240:ASP:HB3	1:A:242:THR:H	1.71	0.54
1:C:82:ILE:HD11	1:D:41:ILE:HG21	1.89	0.54
1:A:240:ASP:HB2	1:A:244:MET:H	1.71	0.54
1:C:104:GLY:HA3	1:C:122:LEU:O	2.06	0.54
1:C:110:ARG:NH2	1:C:378:ASP:OD2	2.41	0.53
1:C:57:LEU:HD13	1:C:68:ILE:HG23	1.90	0.53
1:B:289:VAL:HG22	1:B:321:ILE:HD11	1.90	0.53
1:A:30:LEU:O	1:A:34:ILE:HG12	2.09	0.53
1:A:186:VAL:HG11	1:A:287:MET:HG2	1.92	0.52
1:B:63:ARG:NH1	1:B:69:ASP:OD1	2.42	0.52
1:D:144:MET:HG2	1:D:208:MET:HE1	1.90	0.52
1:A:53:LEU:HD13	1:B:53:LEU:HD13	1.93	0.51
1:C:264:SER:HB2	1:C:269:GLY:CA	2.40	0.51
1:B:246:HIS:HB3	1:B:270:TYR:HA	1.91	0.51
1:B:262:LEU:HD23	1:B:307:MET:HE3	1.93	0.51
1:C:211:ILE:HD11	1:C:245:VAL:HG22	1.91	0.51
1:A:123:LEU:HB3	1:A:128:MET:HE3	1.92	0.51
1:B:253:THR:O	1:B:257:ILE:HG13	2.11	0.51
1:D:128:MET:HE3	1:D:137:PHE:CZ	2.46	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:VAL:HG12	1:C:387:ILE:HD12	1.92	0.50
1:D:106:VAL:HG22	1:D:121:LYS:HD3	1.94	0.50
1:D:191:ALA:HA	1:D:287:MET:HE3	1.94	0.50
1:A:51:ASN:HD21	1:A:83:ARG:HG2	1.76	0.50
1:A:264:SER:HB3	1:A:269:GLY:N	2.27	0.50
1:A:139:GLU:OE2	1:A:238:LYS:NZ	2.31	0.50
1:A:211:ILE:HD11	1:A:245:VAL:HG22	1.94	0.50
1:B:100:ARG:HH22	1:B:388:GLU:C	2.20	0.50
1:B:141:ARG:NH2	1:B:413:PHE:O	2.44	0.50
1:D:123:LEU:HD13	1:D:128:MET:HE2	1.92	0.50
1:C:102:ALA:HA	1:C:103:PHE:C	2.37	0.50
1:B:248:ASP:HA	1:B:249:THR:HB	1.93	0.49
1:A:101:GLY:HA3	1:A:104:GLY:O	2.13	0.49
1:C:129:ILE:O	1:C:130:LYS:HB2	2.12	0.49
1:D:165:LEU:HG	1:D:413:PHE:CE2	2.47	0.49
1:A:229:LYS:HG3	1:A:365:ARG:NH2	2.28	0.48
1:C:46:LEU:HB3	1:D:46:LEU:HB3	1.95	0.48
1:B:177:LEU:HD12	1:B:220:MET:HB2	1.95	0.48
1:B:62:LEU:HD21	1:B:403:PHE:N	2.28	0.48
1:C:53:LEU:HD13	1:D:53:LEU:HD13	1.95	0.48
1:C:246:HIS:HA	1:C:269:GLY:O	2.14	0.47
1:C:244:MET:HE1	1:C:270:TYR:CG	2.50	0.47
1:C:74:ARG:NH2	1:D:40:PRO:HB3	2.28	0.47
1:B:340:LEU:HG	1:B:348:ILE:HG12	1.97	0.47
1:C:289:VAL:HG22	1:C:321:ILE:HD11	1.96	0.47
1:C:211:ILE:HD11	1:C:245:VAL:CG2	2.44	0.47
1:D:217:PRO:HD3	1:D:256:TYR:CZ	2.50	0.47
1:D:229:LYS:HE2	1:D:365:ARG:NH2	2.30	0.47
1:B:145:ALA:O	1:B:417:ARG:NH2	2.48	0.46
1:C:156:PHE:HE2	1:C:170:GLU:HB3	1.80	0.46
1:A:217:PRO:HD3	1:A:256:TYR:CZ	2.49	0.46
1:C:151:TRP:CZ2	1:C:365:ARG:HG3	2.51	0.46
1:C:62:LEU:HD21	1:C:403:PHE:N	2.30	0.46
1:D:131:ARG:HD2	1:D:131:ARG:N	2.31	0.46
1:B:165:LEU:HG	1:B:413:PHE:CE2	2.50	0.46
1:A:46:LEU:HB3	1:B:46:LEU:HB3	1.98	0.46
1:B:240:ASP:HB3	1:B:243:GLY:H	1.80	0.46
1:D:138:TRP:HB2	1:D:141:ARG:HG2	1.97	0.46
1:A:213:ARG:NH2	1:A:247:CYS:SG	2.89	0.45
1:D:204:ALA:O	1:D:208:MET:HG3	2.16	0.45
1:B:158:ALA:HB3	1:B:415:TYR:HB3	1.98	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:ALA:HB3	1:C:415:TYR:HB3	1.98	0.45
1:C:303:TYR:O	1:C:307:MET:HG2	2.17	0.45
1:D:334:THR:HG21	1:D:338:VAL:HG23	1.99	0.45
1:C:245:VAL:O	1:C:245:VAL:HG23	2.16	0.45
1:A:238:LYS:HB3	1:A:238:LYS:HE2	1.73	0.45
1:B:239:MET:HA	1:B:245:VAL:HG22	1.97	0.45
1:D:128:MET:HE3	1:D:137:PHE:CE1	2.51	0.45
1:C:141:ARG:NH1	1:C:142:ASP:OD1	2.49	0.45
1:A:109:VAL:HG11	1:A:120:MET:HE2	1.98	0.44
1:B:217:PRO:HD3	1:B:256:TYR:CZ	2.53	0.44
1:B:238:LYS:HE2	1:B:238:LYS:HB3	1.84	0.44
1:A:28:ARG:HG3	1:A:29:LYS:HG3	1.99	0.44
1:A:211:ILE:HD11	1:A:245:VAL:CG2	2.47	0.44
1:B:195:THR:O	1:B:199:VAL:HG23	2.18	0.44
1:D:267:GLY:C	1:D:269:GLY:N	2.73	0.44
1:C:135:ALA:HA	1:C:136:PHE:HA	1.76	0.44
1:B:133:ASP:HA	1:B:134:SER:HA	1.56	0.44
1:A:245:VAL:O	1:A:270:TYR:HA	2.17	0.44
1:D:136:PHE:HA	1:D:137:PHE:CB	2.45	0.44
1:D:224:LYS:HD2	1:D:375:LEU:HD12	1.99	0.44
1:D:375:LEU:HD23	1:D:375:LEU:HA	1.78	0.44
1:A:228:LEU:O	1:A:365:ARG:NH1	2.48	0.44
1:B:100:ARG:HA	1:B:101:GLY:HA3	1.63	0.44
1:C:136:PHE:C	1:C:137:PHE:O	2.60	0.44
1:C:154:GLN:HE21	1:C:417:ARG:NH2	2.15	0.44
1:D:262:LEU:HB2	1:D:307:MET:HE3	1.99	0.44
1:D:241:GLU:H	1:D:241:GLU:CD	2.25	0.43
1:D:408:LEU:N	1:D:409:PRO:HD2	2.33	0.43
1:A:395:GLU:H	1:A:395:GLU:HG3	1.64	0.43
1:A:202:LEU:HD21	1:A:215:VAL:HG21	2.00	0.43
1:A:386:ASP:N	1:A:386:ASP:OD1	2.52	0.43
1:D:111:HIS:O	1:D:115:GLN:N	2.49	0.43
1:C:36:ASP:OD1	1:C:38:ARG:N	2.44	0.43
1:D:141:ARG:HG3	1:D:142:ASP:N	2.34	0.43
1:A:129:ILE:O	1:A:129:ILE:HG22	2.17	0.43
1:A:139:GLU:HA	1:A:142:ASP:HB2	2.01	0.43
1:D:346:GLU:HA	1:D:349:LYS:HE3	2.01	0.43
1:A:34:ILE:HD13	1:A:41:ILE:HD12	2.00	0.42
1:B:386:ASP:C	1:B:387:ILE:HG12	2.44	0.42
1:A:140:GLU:O	1:A:144:MET:HG3	2.18	0.42
1:C:136:PHE:O	1:C:136:PHE:CG	2.71	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:PHE:CZ	1:D:130:LYS:HE2	2.55	0.42
1:B:123:LEU:HB2	1:B:165:LEU:HB2	2.01	0.42
1:A:331:ALA:HB1	1:A:340:LEU:HB2	2.01	0.42
1:B:141:ARG:HD2	1:B:155:LEU:HD22	2.02	0.42
1:B:216:LYS:HE2	1:B:219:ASN:OD1	2.20	0.42
1:D:274:GLU:HG3	1:D:336:ARG:HB2	2.02	0.42
1:A:318:ASP:CG	1:A:319:ALA:H	2.28	0.42
1:B:204:ALA:O	1:B:208:MET:HG3	2.19	0.42
1:D:39:SER:HA	1:D:40:PRO:HD3	1.93	0.42
1:D:137:PHE:HD2	1:D:138:TRP:CE3	2.38	0.42
1:D:158:ALA:HB3	1:D:415:TYR:HB3	2.02	0.41
1:B:169:MET:HE3	1:B:169:MET:HB2	1.80	0.41
1:C:237:MET:HE1	1:C:247:CYS:HB2	2.00	0.41
1:D:240:ASP:HB3	1:D:242:THR:H	1.85	0.41
1:A:135:ALA:HB1	1:A:136:PHE:HB3	2.02	0.41
1:B:209:GLY:HA2	1:B:239:MET:HE2	2.01	0.41
1:B:248:ASP:HA	1:B:249:THR:CB	2.50	0.41
1:D:211:ILE:HG13	1:D:213:ARG:HG3	2.03	0.41
1:A:130:LYS:HB3	1:A:130:LYS:HE3	1.62	0.41
1:B:213:ARG:NH1	1:B:235:THR:O	2.49	0.41
1:C:217:PRO:HD3	1:C:256:TYR:CZ	2.56	0.41
1:D:101:GLY:O	1:D:103:PHE:N	2.48	0.41
1:A:86:GLN:HG2	1:B:30:LEU:HD11	2.01	0.41
1:B:278:TRP:O	1:B:282:VAL:HG23	2.21	0.41
1:C:100:ARG:NH2	1:C:387:ILE:HG22	2.36	0.41
1:C:144:MET:HG2	1:C:208:MET:HE1	2.03	0.41
1:C:340:LEU:HG	1:C:348:ILE:HG12	2.01	0.41
1:A:86:GLN:O	1:A:87:MET:HG2	2.21	0.41
1:A:165:LEU:HG	1:A:413:PHE:CE2	2.56	0.41
1:C:192:LYS:HE3	1:C:353:PHE:O	2.20	0.41
1:D:123:LEU:HB2	1:D:165:LEU:HB2	2.03	0.41
1:A:253:THR:HA	1:A:254:PRO:HD3	1.85	0.41
1:C:138:TRP:HB2	1:C:141:ARG:HD3	2.02	0.41
1:D:136:PHE:O	1:D:136:PHE:CG	2.73	0.41
1:D:230:LEU:HD23	1:D:230:LEU:HA	1.88	0.41
1:D:218:ASP:OD1	1:D:218:ASP:N	2.53	0.40
1:C:54:VAL:HG21	1:C:79:VAL:HG21	2.02	0.40
1:C:178:VAL:HG23	1:C:217:PRO:HB2	2.03	0.40
1:D:186:VAL:HG21	1:D:287:MET:HG3	2.03	0.40
1:A:136:PHE:N	1:A:137:PHE:HB2	2.37	0.40
1:B:134:SER:HB2	1:B:135:ALA:CA	2.49	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:GLY:O	1:A:305:LYS:HB2	2.22	0.40
1:B:246:HIS:O	1:B:247:CYS:HB3	2.21	0.40
1:D:315:PHE:CE1	1:D:326:LYS:HG3	2.57	0.40
1:A:134:SER:O	1:A:135:ALA:HB3	2.22	0.40
1:C:244:MET:HE3	1:C:271:TYR:C	2.46	0.40
1:C:386:ASP:C	1:C:387:ILE:HG13	2.45	0.40
1:D:340:LEU:HG	1:D:348:ILE:HG12	2.03	0.40

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	385/391 (98%)	341 (89%)	32 (8%)	12 (3%)	3	17
1	B	385/391 (98%)	341 (89%)	34 (9%)	10 (3%)	4	21
1	C	385/391 (98%)	350 (91%)	29 (8%)	6 (2%)	8	32
1	D	385/391 (98%)	356 (92%)	22 (6%)	7 (2%)	7	30
All	All	1540/1564 (98%)	1388 (90%)	117 (8%)	35 (2%)	5	24

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	PHE
1	A	139	GLU
1	A	240	ASP
1	A	248	ASP
1	A	395	GLU
1	B	140	GLU
1	B	247	CYS
1	B	248	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	389	ASP
1	C	103	PHE
1	C	130	LYS
1	C	134	SER
1	C	135	ALA
1	C	137	PHE
1	C	364	ILE
1	D	134	SER
1	D	135	ALA
1	A	28	ARG
1	A	319	ALA
1	B	136	PHE
1	B	138	TRP
1	B	394	VAL
1	D	100	ARG
1	D	133	ASP
1	D	137	PHE
1	D	148	ASN
1	A	125	LYS
1	B	100	ARG
1	B	137	PHE
1	B	319	ALA
1	A	270	TYR
1	A	268	ASP
1	A	318	ASP
1	D	132	SER
1	A	126	PHE

### 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	340/344 (99%)	340 (100%)	0	100	100
1	B	340/344 (99%)	340 (100%)	0	100	100
1	C	340/344 (99%)	340 (100%)	0	100	100

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	340/344 (99%)	340 (100%)	0	100	100
All	All	1360/1376 (99%)	1360 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	GLN
1	B	70	ASN
1	B	360	ASN
1	B	383	ASN
1	C	154	GLN
1	C	350	GLN
1	D	70	ASN

### 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](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	389/391 (99%)	-0.41	4 (1%)	79 61	46, 75, 117, 174	0
1	B	389/391 (99%)	-0.30	6 (1%)	71 51	51, 84, 137, 163	0
1	C	389/391 (99%)	-0.49	7 (1%)	67 45	41, 66, 108, 140	0
1	D	387/391 (98%)	-0.56	5 (1%)	74 54	44, 69, 111, 146	2 (0%)
All	All	1554/1564 (99%)	-0.44	22 (1%)	73 52	41, 73, 122, 174	2 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	268	ASP	5.3
1	B	267	GLY	3.8
1	B	251	VAL	3.7
1	A	390	ASP	3.7
1	D	270	TYR	3.3
1	C	270	TYR	3.3
1	B	270	TYR	3.2
1	C	137	PHE	3.1
1	C	27	GLN	3.0
1	A	130	LYS	2.9
1	D	268	ASP	2.8
1	A	87	MET	2.8
1	A	416	TYR	2.7
1	D	231	ALA	2.5
1	C	391	LYS	2.5
1	D	266	GLY	2.4
1	C	268	ASP	2.3
1	C	132	SER	2.3
1	C	246	HIS	2.3
1	B	269	GLY	2.2
1	B	135	ALA	2.1
1	D	394	VAL	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.