



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 12:41 AM UTC

PDB ID : 4D28 / pdb_00004d28
Title : Crystal structure of the kinase domain of CIPK24/SOS2
Authors : Gonzalez-Rubio, J.M.; Chaves-Sanjuan, A.; Sanchez-Barrena, M.J.; Albert, A.
Deposited on : 2014-05-08
Resolution : 3.30 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

<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

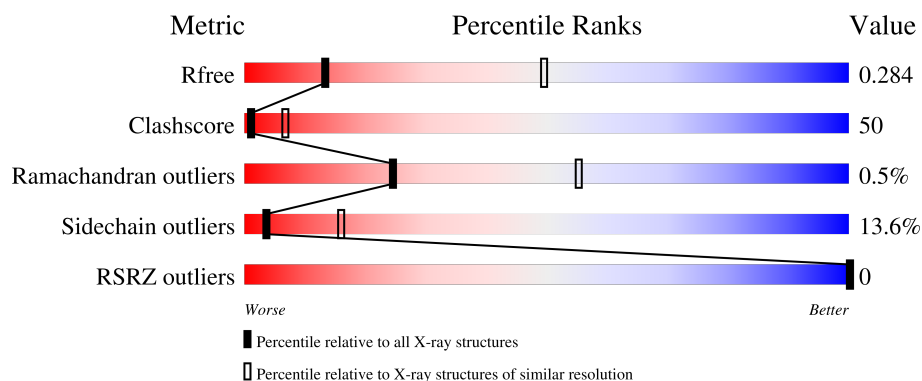
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	446	
1	B	446	
1	C	446	
1	D	446	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8821 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 CBL-INTERACTING SERINE/THREONINE-PROTEIN KINASE 24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2192	1404	382	399	7			
1	B	277	Total	C	N	O	S	0	0	0
			2217	1419	388	403	7			
1	C	279	Total	C	N	O	S	0	0	0
			2234	1430	390	407	7			
1	D	271	Total	C	N	O	S	0	0	0
			2178	1397	379	395	7			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	81	LYS	PRO	engineered mutation	UNP Q9LDI3
A	107	LYS	GLU	engineered mutation	UNP Q9LDI3
A	109	ASP	SER	engineered mutation	UNP Q9LDI3
A	127	SER	CYS	engineered mutation	UNP Q9LDI3
A	167	ASN	ARG	conflict	UNP Q9LDI3
A	168	ASP	THR	engineered mutation	UNP Q9LDI3
A	228	ASP	SER	engineered mutation	UNP Q9LDI3
A	266	LYS	LEU	engineered mutation	UNP Q9LDI3
B	81	LYS	PRO	engineered mutation	UNP Q9LDI3
B	107	LYS	GLU	engineered mutation	UNP Q9LDI3
B	109	ASP	SER	engineered mutation	UNP Q9LDI3
B	127	SER	CYS	engineered mutation	UNP Q9LDI3
B	167	ASN	ARG	conflict	UNP Q9LDI3
B	168	ASP	THR	engineered mutation	UNP Q9LDI3
B	228	ASP	SER	engineered mutation	UNP Q9LDI3
B	266	LYS	LEU	engineered mutation	UNP Q9LDI3
C	81	LYS	PRO	engineered mutation	UNP Q9LDI3
C	107	LYS	GLU	engineered mutation	UNP Q9LDI3
C	109	ASP	SER	engineered mutation	UNP Q9LDI3
C	127	SER	CYS	engineered mutation	UNP Q9LDI3

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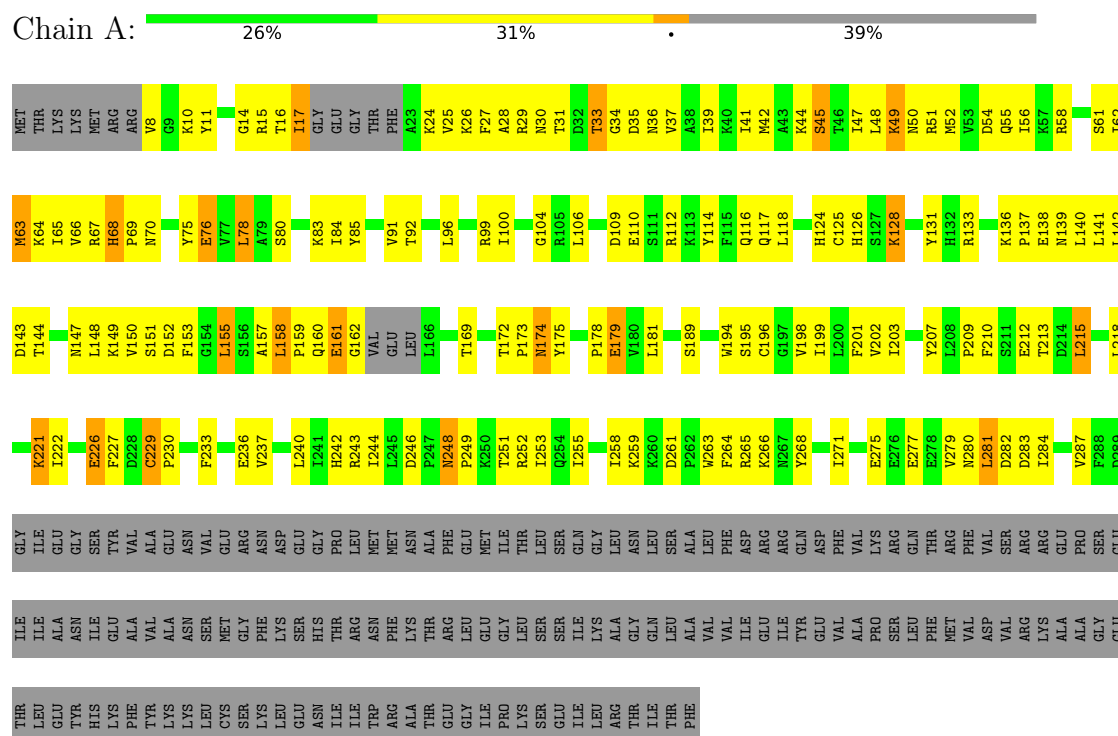
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Chain	Residue	Modelled	Actual	Comment	Reference
C	167	ASN	ARG	conflict	UNP Q9LDI3
C	168	ASP	THR	engineered mutation	UNP Q9LDI3
C	228	ASP	SER	engineered mutation	UNP Q9LDI3
C	266	LYS	LEU	engineered mutation	UNP Q9LDI3
D	81	LYS	PRO	engineered mutation	UNP Q9LDI3
D	107	LYS	GLU	engineered mutation	UNP Q9LDI3
D	109	ASP	SER	engineered mutation	UNP Q9LDI3
D	127	SER	CYS	engineered mutation	UNP Q9LDI3
D	167	ASN	ARG	conflict	UNP Q9LDI3
D	168	ASP	THR	engineered mutation	UNP Q9LDI3
D	228	ASP	SER	engineered mutation	UNP Q9LDI3
D	266	LYS	LEU	engineered mutation	UNP Q9LDI3

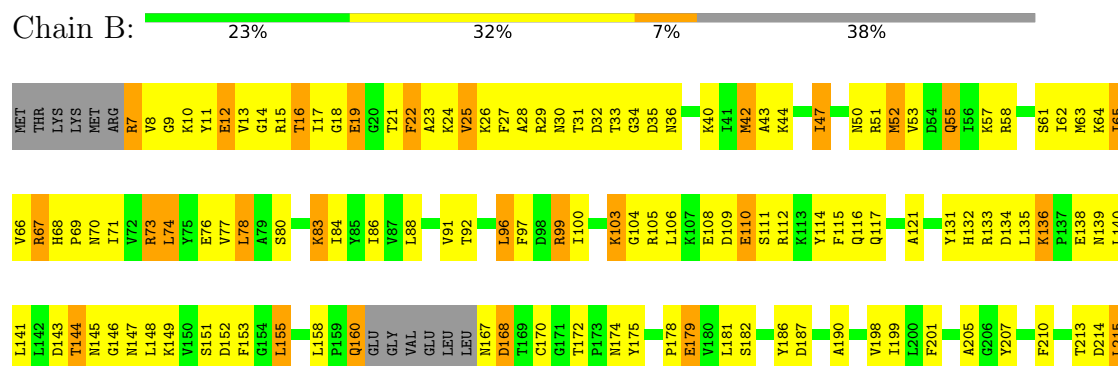
3 Residue-property plots

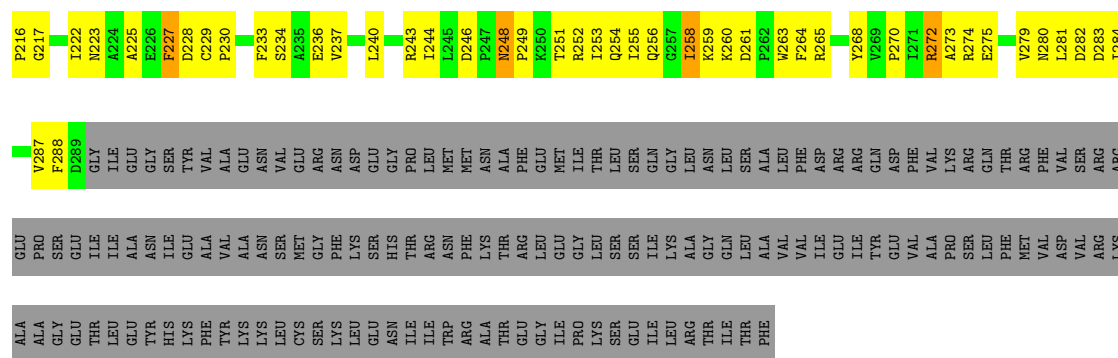
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: CBL-INTERACTING SERINE/THREONINE-PROTEIN KINASE 24

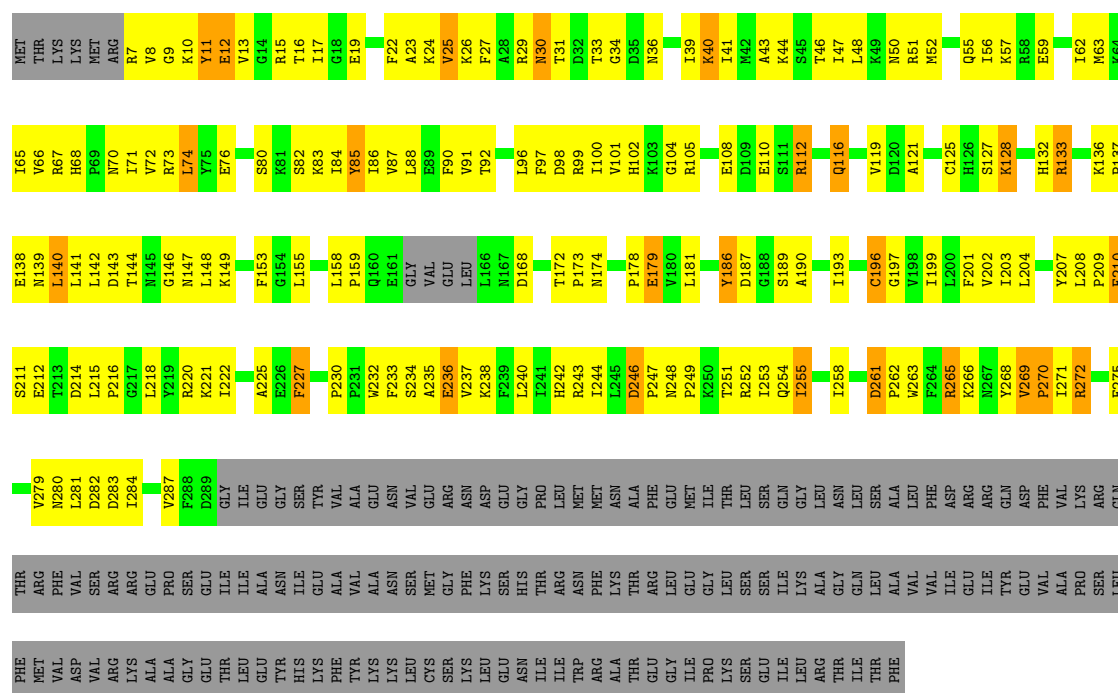
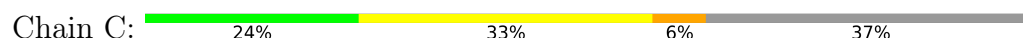


• Molecule 1: CBL-INTERACTING SERINE/THREONINE-PROTEIN KINASE 24

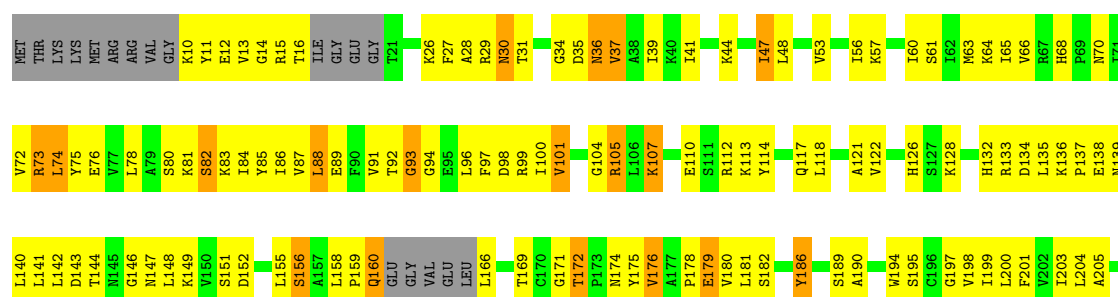
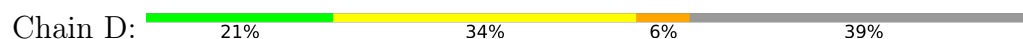




● Molecule 1: CBL-INTERACTING SERINE/THREONINE-PROTEIN KINASE 24



● Molecule 1: CBL-INTERACTING SERINE/THREONINE-PROTEIN KINASE 24



LEU	GLN	E276	F210
PHE	THR		S211
MET	ARG	V279	E212
VAL	PHE	N280	T213
ASP	VAL	L281	D214
VAL	SER	D282	L215
ARG	ARG	D283	T216
LYS	ARG	L284	G217
ALA	GLU		L218
ALA	PRO	V287	L219
GLY	SER	F288	R220
GLU	GLU	D289	K221
THR	ILE		I222
LEU	ILE	ILE	N223
GLU	ALA	GLU	
TYR	ASN	GLY	E226
HIS	ILE	SER	F227
LYS	GLU	TYR	
PHE	ALA	VAL	P230
TYR	VAL	ALA	T231
LYS	ALA	GLU	W232
LYS	ASN	ASN	F233
LEU	SER	VAL	
CYS	MET	GLU	E236
SER	GLY	ARG	V237
LYS	PHE	ASN	K238
LEU	LYS	ASP	F239
GLU	SER	GLU	L240
ASN	HIS	GLY	I241
ILE	THR	PRO	H242
ILE	ARG	LEU	R243
TRP	ASN	MET	L244
ARG	PHE	MET	L245
ALA	LYS	ASN	D246
THR	THR	ALA	P247
GLU	ARG	PHE	N248
GLY	LEU	GLU	P249
ILE	GLU	MET	K250
PRO	GLY	ILE	T251
SER	LEU	THR	R252
SER	SER	LEU	L253
GLU	SER	SER	Q254
ILE	ILE	GLN	T255
LEU	LYS	GLY	Q256
ARG	ALA	LEU	G257
THR	GLY	ASN	L258
ILE	GLN	LEU	K259
THR	LEU	SER	K260
PHE	ALA	ALA	D261
	VAL	VAL	P262
	VAL	PHE	W263
	ILE	ASP	F264
	GLU	ARG	R265
	ILE	ARG	K266
	TYR	GLN	N267
	GLU	ASP	V268
	VAL	PHE	V269
	ALA	VAL	P270
	PRO	LYS	
	SER	ARG	F275

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	69.11Å 71.35Å 77.83Å 104.85° 100.32° 118.96°	Depositor
Resolution (Å)	70.23 – 3.30 70.23 – 3.30	Depositor EDS
% Data completeness (in resolution range)	90.8 (70.23-3.30) 90.8 (70.23-3.30)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.271 , 0.283 0.275 , 0.284	Depositor DCC
R_{free} test set	810 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	72.5	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 88.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.045 for k,h,-h-k-l 0.043 for -k,-h,-l 0.069 for -h,-k,h+k+l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8821	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.13% 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

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	0.40	0/2236	0.96	7/3020 (0.2%)
1	B	0.41	0/2263	0.94	2/3057 (0.1%)
1	C	0.40	0/2280	0.92	5/3080 (0.2%)
1	D	0.39	0/2223	0.89	2/3003 (0.1%)
All	All	0.40	0/9002	0.93	16/12160 (0.1%)

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	248	ASN	CA-C-N	-11.47	107.65	120.04
1	B	248	ASN	C-N-CA	-11.47	107.65	120.04
1	A	248	ASN	CA-C-N	-7.70	111.72	120.04
1	A	248	ASN	C-N-CA	-7.70	111.72	120.04
1	A	261	ASP	CA-C-N	7.59	129.32	119.84

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	2192	0	2222	174	0
1	B	2217	0	2244	211	0
1	C	2234	0	2261	250	0
1	D	2178	0	2206	252	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8821	0	8933	880	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 50.

The worst 5 of 880 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:C:174:ASN:OD1	1:C:212:GLU:OE2	1.60	1.15
1:B:99:ARG:NH2	1:B:110:GLU:CD	2.04	1.14
1:D:86:ILE:HG22	1:D:88:LEU:HD11	1.17	1.14
1:B:92:THR:OG1	1:B:144:THR:HG23	1.49	1.12
1:B:7:ARG:HD2	1:B:12:GLU:OE2	1.48	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	268/446 (60%)	254 (95%)	14 (5%)	0	100	100
1	B	273/446 (61%)	249 (91%)	23 (8%)	1 (0%)	30	60
1	C	275/446 (62%)	263 (96%)	11 (4%)	1 (0%)	30	60
1	D	265/446 (59%)	247 (93%)	15 (6%)	3 (1%)	11	39
All	All	1081/1784 (61%)	1013 (94%)	63 (6%)	5 (0%)	24	55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	93	GLY

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Mol	Chain	Res	Type
1	B	23	ALA
1	D	176	VAL
1	D	267	ASN
1	C	270	PRO

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	239/388 (62%)	214 (90%)	25 (10%)	6	25
1	B	241/388 (62%)	197 (82%)	44 (18%)	2	7
1	C	243/388 (63%)	215 (88%)	28 (12%)	5	21
1	D	238/388 (61%)	204 (86%)	34 (14%)	3	14
All	All	961/1552 (62%)	830 (86%)	131 (14%)	3	16

5 of 131 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	174	ASN
1	D	186	TYR
1	D	275	GLU
1	B	110	GLU
1	B	108	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	102	HIS
1	D	36	ASN
1	D	242	HIS
1	C	223	ASN
1	D	102	HIS

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 [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	274/446 (61%)	-1.55	0 100 100	40, 61, 100, 124	0
1	B	277/446 (62%)	-1.53	0 100 100	39, 64, 125, 146	0
1	C	279/446 (62%)	-1.54	0 100 100	44, 65, 121, 136	0
1	D	271/446 (60%)	-1.44	0 100 100	47, 67, 109, 132	0
All	All	1101/1784 (61%)	-1.52	0 100 100	39, 64, 116, 146	0

There are no RSRZ outliers to report.

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.