



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 1, 2026 – 02:20 AM UTC

PDB ID : 6AJ4 / pdb_00006aj4
Title : Crystal structure of the DHR-2 domain of DOCK7 in complex with Cdc42
Authors : Kukimoto-Niino, M.; Shirouzu, M.
Deposited on : 2018-08-27
Resolution : 3.26 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

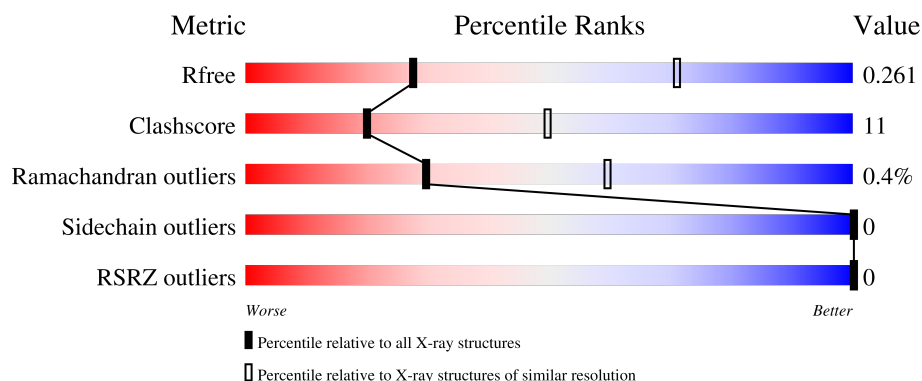
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.26 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	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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	290	 65% 30% 5%
1	C	290	 74% 20% 5%
1	E	290	 73% 22% 5%
1	G	290	 66% 28% 5%
2	B	195	 62% 29% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	195	 71%21%9%
2	F	195	 67%24%•9%
2	H	195	 68%23%•9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14684 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 Deducator of cytokinesis protein 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2283	1460	391	422	10			
1	C	275	Total	C	N	O	S	0	0	0
			2283	1460	391	422	10			
1	E	275	Total	C	N	O	S	0	0	0
			2283	1460	391	422	10			
1	G	275	Total	C	N	O	S	0	0	0
			2283	1460	391	422	10			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1794	GLY	-	expression tag	UNP Q96N67
A	1795	SER	-	expression tag	UNP Q96N67
A	1796	SER	-	expression tag	UNP Q96N67
A	1797	GLY	-	expression tag	UNP Q96N67
A	1798	SER	-	expression tag	UNP Q96N67
A	1799	SER	-	expression tag	UNP Q96N67
A	1800	GLY	-	expression tag	UNP Q96N67
C	1794	GLY	-	expression tag	UNP Q96N67
C	1795	SER	-	expression tag	UNP Q96N67
C	1796	SER	-	expression tag	UNP Q96N67
C	1797	GLY	-	expression tag	UNP Q96N67
C	1798	SER	-	expression tag	UNP Q96N67
C	1799	SER	-	expression tag	UNP Q96N67
C	1800	GLY	-	expression tag	UNP Q96N67
E	1794	GLY	-	expression tag	UNP Q96N67
E	1795	SER	-	expression tag	UNP Q96N67
E	1796	SER	-	expression tag	UNP Q96N67
E	1797	GLY	-	expression tag	UNP Q96N67
E	1798	SER	-	expression tag	UNP Q96N67
E	1799	SER	-	expression tag	UNP Q96N67
E	1800	GLY	-	expression tag	UNP Q96N67

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	1794	GLY	-	expression tag	UNP Q96N67
G	1795	SER	-	expression tag	UNP Q96N67
G	1796	SER	-	expression tag	UNP Q96N67
G	1797	GLY	-	expression tag	UNP Q96N67
G	1798	SER	-	expression tag	UNP Q96N67
G	1799	SER	-	expression tag	UNP Q96N67
G	1800	GLY	-	expression tag	UNP Q96N67

- Molecule 2 is a protein called Cell division control protein 42 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	178	Total	C	N	O	S	0	0	0
			1388	893	221	267	7			
2	D	178	Total	C	N	O	S	0	0	0
			1388	893	221	267	7			
2	F	178	Total	C	N	O	S	0	0	0
			1388	893	221	267	7			
2	H	178	Total	C	N	O	S	0	0	0
			1388	893	221	267	7			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	GLY	-	expression tag	UNP P60953
B	-5	SER	-	expression tag	UNP P60953
B	-4	SER	-	expression tag	UNP P60953
B	-3	GLY	-	expression tag	UNP P60953
B	-2	SER	-	expression tag	UNP P60953
B	-1	SER	-	expression tag	UNP P60953
B	0	GLY	-	expression tag	UNP P60953
B	188	SER	CYS	engineered mutation	UNP P60953
D	-6	GLY	-	expression tag	UNP P60953
D	-5	SER	-	expression tag	UNP P60953
D	-4	SER	-	expression tag	UNP P60953
D	-3	GLY	-	expression tag	UNP P60953
D	-2	SER	-	expression tag	UNP P60953
D	-1	SER	-	expression tag	UNP P60953
D	0	GLY	-	expression tag	UNP P60953
D	188	SER	CYS	engineered mutation	UNP P60953
F	-6	GLY	-	expression tag	UNP P60953
F	-5	SER	-	expression tag	UNP P60953
F	-4	SER	-	expression tag	UNP P60953

Continued on next page...

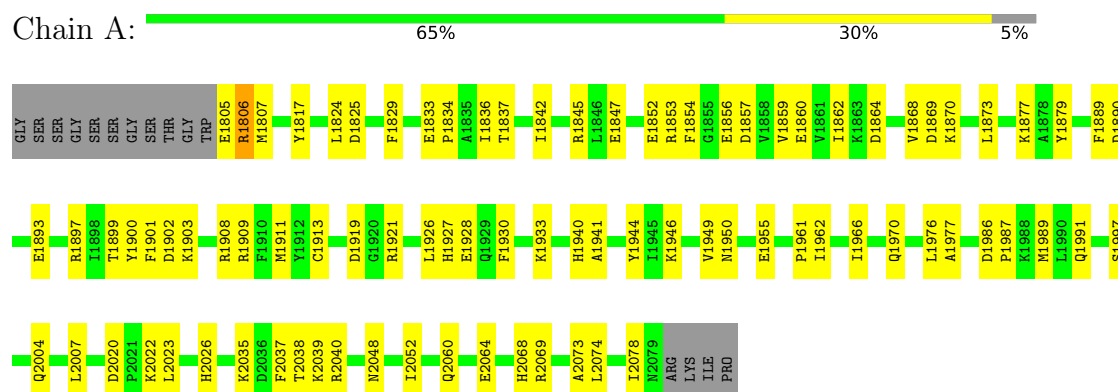
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	-3	GLY	-	expression tag	UNP P60953
F	-2	SER	-	expression tag	UNP P60953
F	-1	SER	-	expression tag	UNP P60953
F	0	GLY	-	expression tag	UNP P60953
F	188	SER	CYS	engineered mutation	UNP P60953
H	-6	GLY	-	expression tag	UNP P60953
H	-5	SER	-	expression tag	UNP P60953
H	-4	SER	-	expression tag	UNP P60953
H	-3	GLY	-	expression tag	UNP P60953
H	-2	SER	-	expression tag	UNP P60953
H	-1	SER	-	expression tag	UNP P60953
H	0	GLY	-	expression tag	UNP P60953
H	188	SER	CYS	engineered mutation	UNP P60953

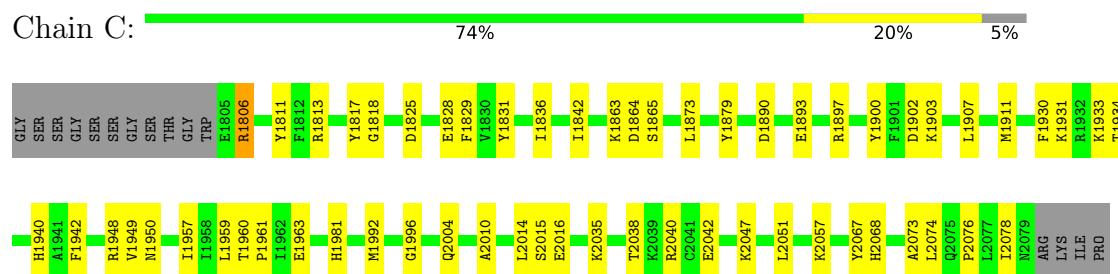
3 Residue-property plots

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.

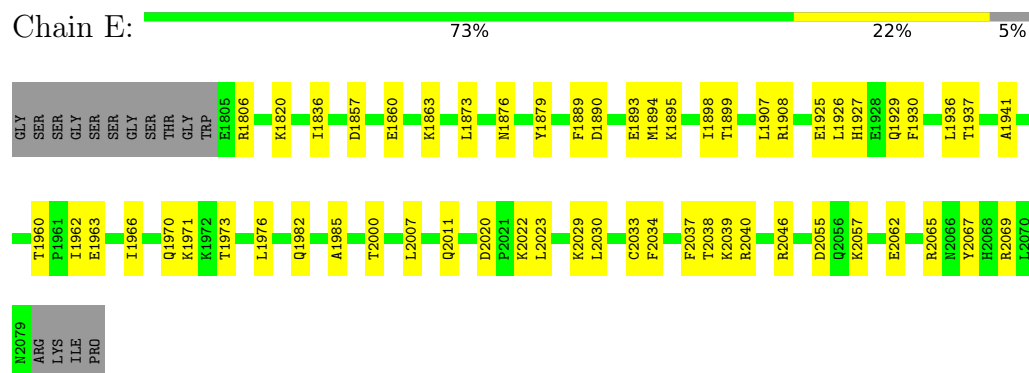
• Molecule 1: Dedicator of cytokinesis protein 7



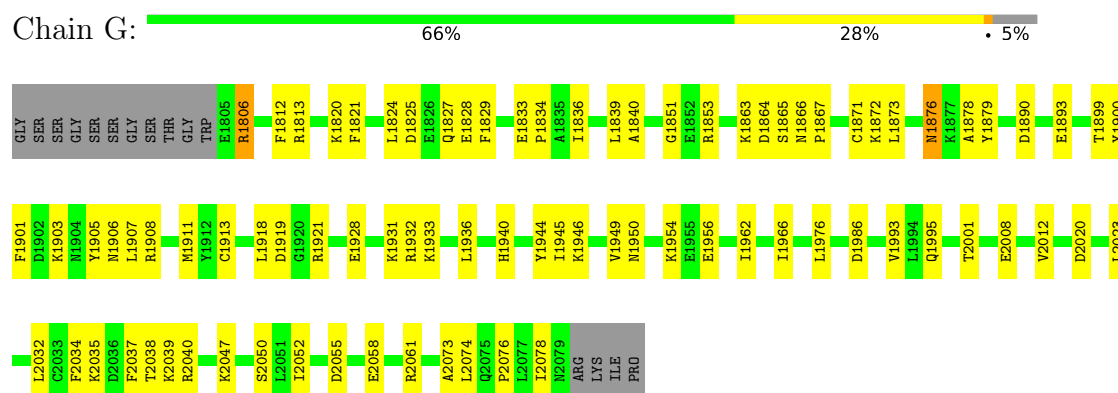
• Molecule 1: Dedicator of cytokinesis protein 7



• Molecule 1: Dedicator of cytokinesis protein 7



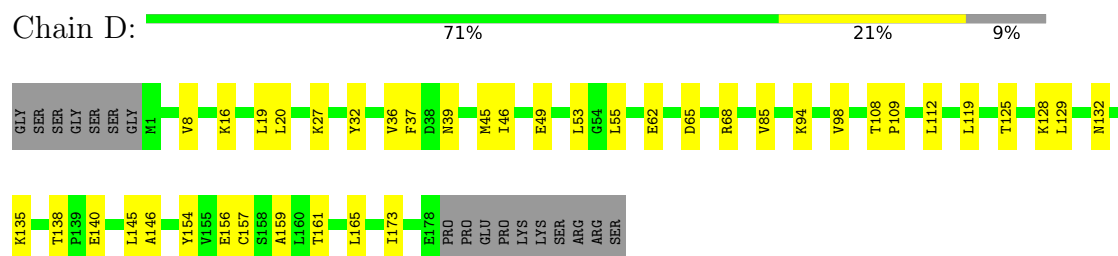
- Molecule 1: Deducator of cytokinesis protein 7



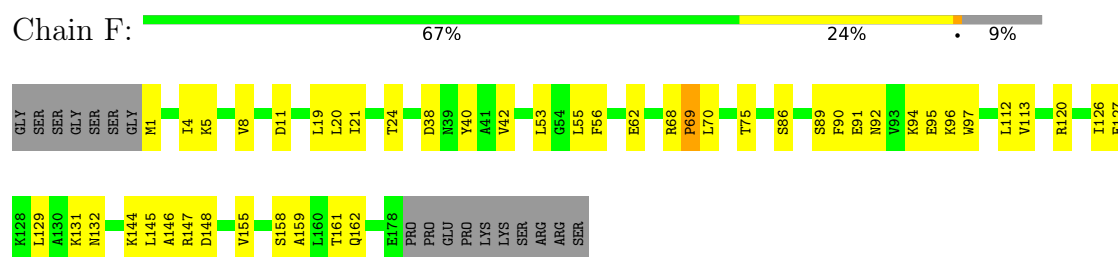
- Molecule 2: Cell division control protein 42 homolog



- Molecule 2: Cell division control protein 42 homolog

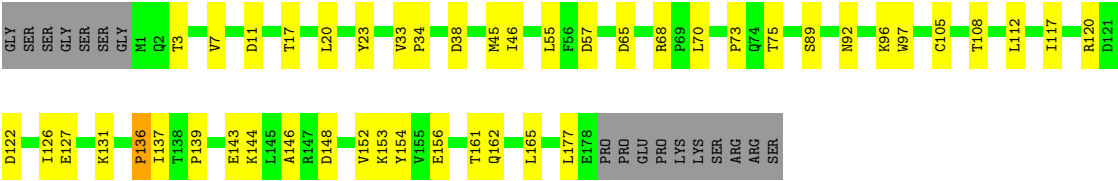


- Molecule 2: Cell division control protein 42 homolog



- Molecule 2: Cell division control protein 42 homolog





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	196.46Å 105.56Å 118.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.80 – 3.26 46.80 – 3.26	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.80-3.26) 99.4 (46.80-3.26)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 3.25Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.184 , 0.259 0.187 , 0.261	Depositor DCC
R_{free} test set	1993 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	88.6	Xtriage
Anisotropy	0.433	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 88.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14684	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 2.98% 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	0.49	0/2337	0.70	0/3150
1	C	0.51	0/2337	0.71	0/3150
1	E	0.46	0/2337	0.71	0/3150
1	G	0.51	0/2337	0.75	2/3150 (0.1%)
2	B	0.48	0/1418	1.10	3/1930 (0.2%)
2	D	0.50	1/1418 (0.1%)	0.69	0/1930
2	F	0.38	0/1418	0.63	0/1930
2	H	0.42	0/1418	0.65	0/1930
All	All	0.47	1/15020 (0.0%)	0.75	5/20320 (0.0%)

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	1
1	C	0	1
1	G	0	1
2	B	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	98	VAL	CA-CB	-7.10	1.50	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	134	GLN	CG-CD-NE2	-26.61	76.48	116.40
2	B	134	GLN	OE1-CD-NE2	-18.91	103.69	122.60
2	B	134	GLN	CG-CD-OE1	16.87	154.54	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	1905	TYR	CA-C-N	-5.73	112.76	121.53
1	G	1905	TYR	C-N-CA	-5.73	112.76	121.53

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1806	ARG	Peptide
2	B	134	GLN	Sidechain
1	C	1806	ARG	Peptide
1	G	1806	ARG	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	2283	0	2257	65	0
1	C	2283	0	2257	46	0
1	E	2283	0	2257	48	0
1	G	2283	0	2257	58	0
2	B	1388	0	1405	45	0
2	D	1388	0	1405	29	0
2	F	1388	0	1405	33	0
2	H	1388	0	1405	29	0
All	All	14684	0	14648	333	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 11.

The worst 5 of 333 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)
2:D:112:LEU:HD22	2:D:146:ALA:HB2	1.44	0.98
2:B:6:CYS:SG	2:B:79:LEU:HD13	2.04	0.98
2:B:144:LYS:HD3	2:B:148:ASP:CG	1.99	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:144:LYS:HD3	2:B:148:ASP:OD2	1.76	0.86
1:G:1863:LYS:HE2	2:H:161:THR:HA	1.58	0.85

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	273/290 (94%)	245 (90%)	28 (10%)	0	100	100
1	C	273/290 (94%)	256 (94%)	16 (6%)	1 (0%)	30	59
1	E	273/290 (94%)	249 (91%)	23 (8%)	1 (0%)	30	59
1	G	273/290 (94%)	248 (91%)	23 (8%)	2 (1%)	18	48
2	B	176/195 (90%)	162 (92%)	13 (7%)	1 (1%)	21	51
2	D	176/195 (90%)	158 (90%)	18 (10%)	0	100	100
2	F	176/195 (90%)	162 (92%)	13 (7%)	1 (1%)	21	51
2	H	176/195 (90%)	154 (88%)	21 (12%)	1 (1%)	21	51
All	All	1796/1940 (93%)	1634 (91%)	155 (9%)	7 (0%)	30	59

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1981	HIS
1	E	1926	LEU
2	H	136	PRO
2	B	121	ASP
1	G	1876	ASN

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	250/261 (96%)	250 (100%)	0	100	100
1	C	250/261 (96%)	250 (100%)	0	100	100
1	E	250/261 (96%)	250 (100%)	0	100	100
1	G	250/261 (96%)	250 (100%)	0	100	100
2	B	158/172 (92%)	158 (100%)	0	100	100
2	D	158/172 (92%)	158 (100%)	0	100	100
2	F	158/172 (92%)	158 (100%)	0	100	100
2	H	158/172 (92%)	158 (100%)	0	100	100
All	All	1632/1732 (94%)	1632 (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. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	2011	GLN
1	E	2075	GLN
1	G	2028	ASN
2	F	167	ASN
1	G	1940	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	275/290 (94%)	-0.55	0 100 100	46, 80, 133, 250	0
1	C	275/290 (94%)	-0.63	0 100 100	41, 74, 122, 192	0
1	E	275/290 (94%)	-0.52	0 100 100	55, 98, 161, 215	0
1	G	275/290 (94%)	-0.54	0 100 100	43, 78, 136, 199	0
2	B	178/195 (91%)	-0.61	0 100 100	53, 79, 150, 257	0
2	D	178/195 (91%)	-0.60	0 100 100	50, 78, 162, 233	0
2	F	178/195 (91%)	-0.58	0 100 100	71, 94, 177, 228	0
2	H	178/195 (91%)	-0.56	0 100 100	57, 91, 175, 246	0
All	All	1812/1940 (93%)	-0.57	0 100 100	41, 84, 147, 257	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.