



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 04:59 pm BST

PDB ID : 6AJ4  
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 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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

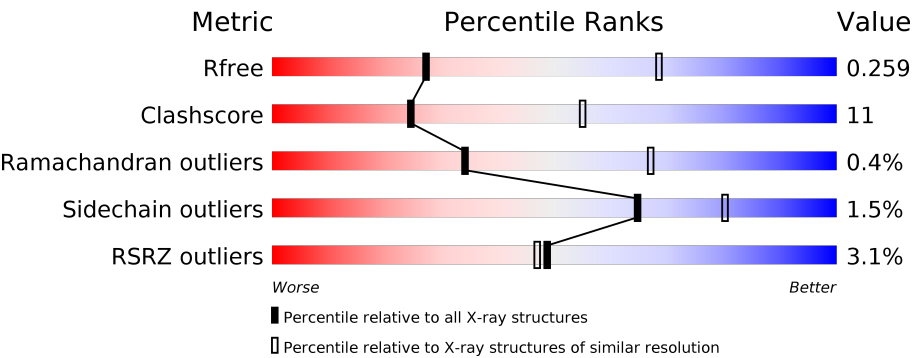
# 1 Overall quality at a glance i

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))
$R_{free}$	130704	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (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 on 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	290	<div><div></div><div>64%30%• 5%</div></div>
1	C	290	<div><div>%</div><div>74%20%• 5%</div></div>
1	E	290	<div><div>5%</div><div>72%22%5%</div></div>
1	G	290	<div><div>%</div><div>66%27%• 5%</div></div>
2	B	195	<div><div>5%</div><div>62%29%• 9%</div></div>
2	D	195	<div><div>5%</div><div>71%21%9%</div></div>

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Mol	Chain	Length	Quality of chain
2	F	195	<div><div>4%</div><div><div></div><div>67%</div><div>23%</div><div>9%</div></div></div>
2	H	195	<div><div>5%</div><div><div></div><div>66%</div><div>25%</div><div>9%</div></div></div>

## 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 Dedicator 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

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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

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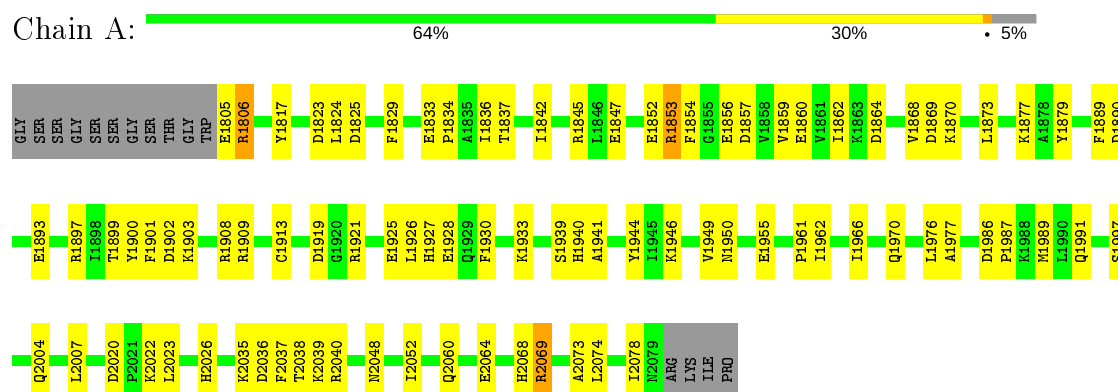
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Chain	Residue	Modelled	Actual	Comment	Reference
F	-3	GLY	-	expression tag	UNP P60953
F	-2	SER	-	expression tag	UNP P60953
F	-1	SER	-	expression tag	UNP P60953
F	0	GLY	-	expression tag	UNP P60953
F	188	SER	CYS	engineered mutation	UNP P60953
H	-6	GLY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

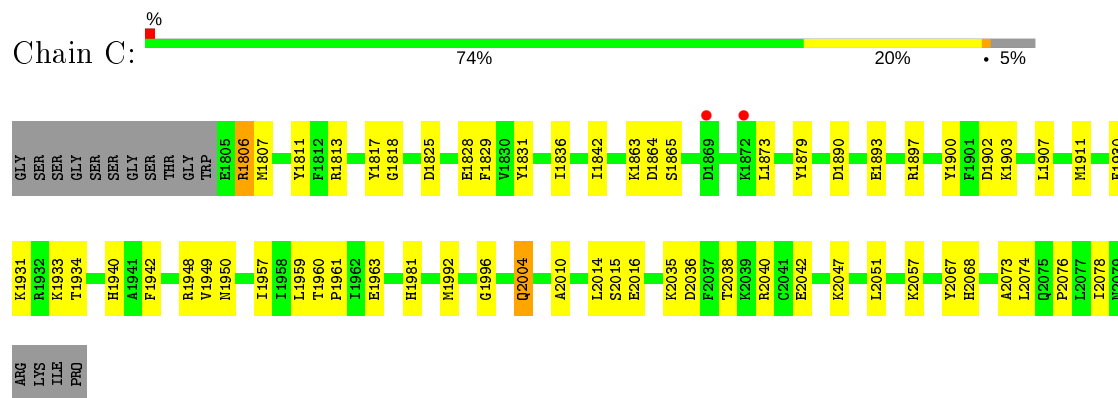
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

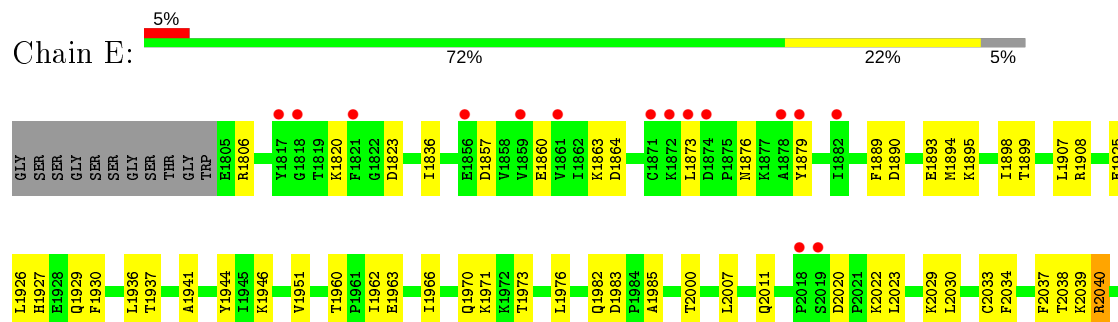
- Molecule 1: Dedicator of cytokinesis protein 7

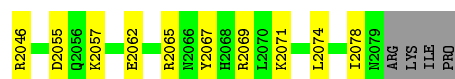


- Molecule 1: Dedicator of cytokinesis protein 7

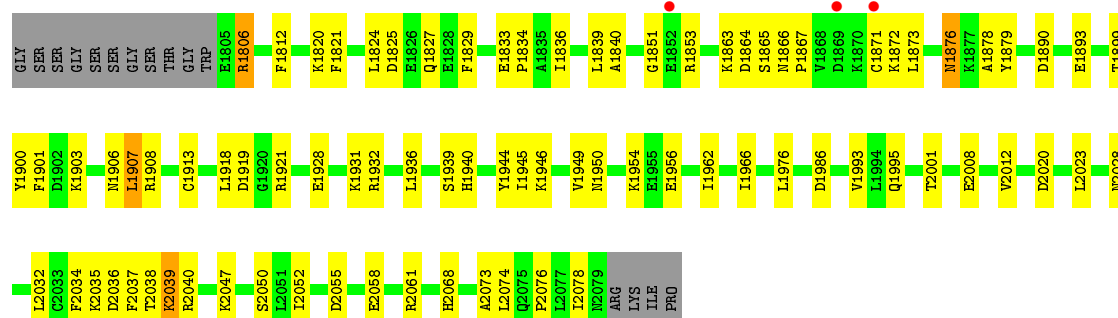


- Molecule 1: Dedicator of cytokinesis protein 7

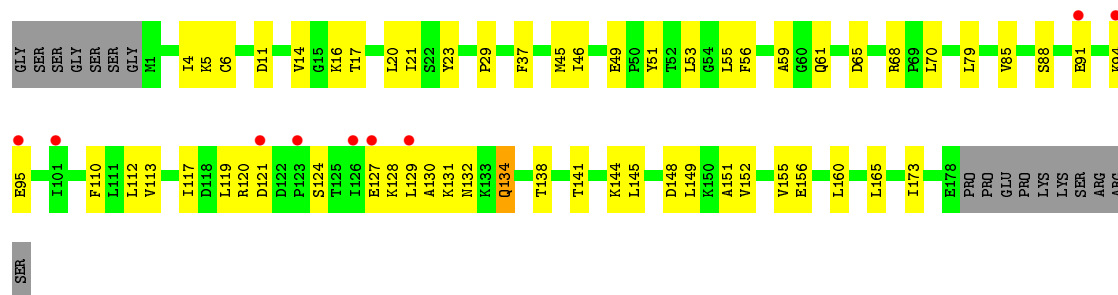




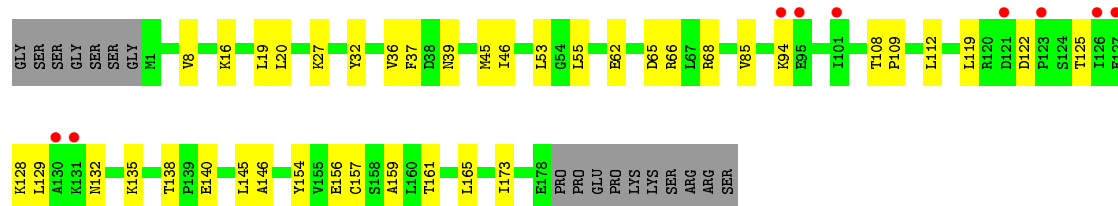
• Molecule 1: Dedicator of cytokinesis protein 7



• 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, $\alpha$ , $\beta$ , $\gamma$	196.46 Å   105.56 Å   118.14 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	46.80 – 3.26 46.49 – 3.26	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.80-3.26) 99.4 (46.49-3.26)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.57 (at 3.25 Å)	Xtriage
Refinement program	PHENIX (1.13 _2998: ???)	Depositor
R, $R_{free}$	0.184   ,   0.259 0.184   ,   0.259	Depositor DCC
$R_{free}$ test set	1993 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	88.6	Xtriage
Anisotropy	0.433	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 67.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14684	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<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	0.51	0/2337	0.69	0/3150
1	C	0.55	0/2337	0.69	0/3150
1	E	0.52	0/2337	0.69	1/3150 (0.0%)
1	G	0.56	0/2337	0.74	1/3150 (0.0%)
2	B	0.50	0/1418	0.91	4/1930 (0.2%)
2	D	0.51	0/1418	0.69	0/1930
2	F	0.44	0/1418	0.65	0/1930
2	H	0.47	0/1418	0.66	0/1930
All	All	0.52	0/15020	0.72	6/20320 (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

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	134	GLN	CG-CD-NE2	-16.76	76.48	116.70
2	B	134	GLN	CG-CD-OE1	16.47	154.54	121.60
2	B	134	GLN	OE1-CD-NE2	-7.92	103.69	121.90
1	E	2040	ARG	NE-CZ-NH1	-6.40	117.10	120.30
1	G	1907	LEU	CB-CG-CD2	5.90	121.03	111.00
2	B	129	LEU	CA-CB-CG	5.45	127.84	115.30

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 ⓘ

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	64	0
1	C	2283	0	2257	44	0
1	E	2283	0	2257	48	0
1	G	2283	0	2257	56	0
2	B	1388	0	1405	40	0
2	D	1388	0	1405	28	0
2	F	1388	0	1405	31	0
2	H	1388	0	1405	28	0
All	All	14684	0	14648	320	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.

All (320) 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:OD2	1.76	0.86
1:G:1863:LYS:HE2	2:H:161:THR:HA	1.58	0.85
1:A:1852:GLU:HA	1:E:2046:ARG:HH22	1.44	0.82
2:B:144:LYS:HD3	2:B:148:ASP:CG	1.99	0.82
2:B:144:LYS:HD3	2:B:148:ASP:OD1	1.82	0.78
2:H:65:ASP:OD1	2:H:68:ARG:NH2	2.16	0.78
2:H:120:ARG:O	2:H:126:ILE:HD11	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1921:ARG:NH1	1:G:1928:GLU:OE1	2.19	0.74
1:G:2058:GLU:HG3	1:G:2061:ARG:HD2	1.70	0.74
1:G:2058:GLU:OE2	1:G:2061:ARG:NH1	2.21	0.73
1:G:1873:LEU:HD22	1:G:1879:TYR:CE2	2.25	0.72
2:F:94:LYS:HG2	2:F:145:LEU:HD21	1.73	0.71
1:A:2068:HIS:CE1	1:G:1946:LYS:HA	2.27	0.69
2:D:112:LEU:HD22	2:D:146:ALA:CB	2.22	0.69
1:A:1806:ARG:HH11	1:A:1836:ILE:HA	1.58	0.68
1:C:2068:HIS:CE1	1:E:1946:LYS:HA	2.27	0.68
2:B:85:VAL:HG11	2:B:119:LEU:HB2	1.75	0.68
2:D:125:THR:HG23	2:D:128:LYS:HD3	1.76	0.68
1:C:1873:LEU:HD22	1:C:1879:TYR:CE2	2.31	0.66
2:F:11:ASP:OD2	2:F:92:ASN:ND2	2.28	0.66
1:A:2060:GLN:NE2	1:A:2064:GLU:OE2	2.27	0.66
2:B:5:LYS:HG3	2:B:56:PHE:CE1	2.31	0.66
1:G:1986:ASP:OD2	2:H:3:THR:OG1	2.12	0.66
1:E:2062:GLU:OE1	1:E:2065:ARG:NH2	2.29	0.65
1:G:1899:THR:OG1	1:G:1900:TYR:N	2.29	0.65
1:C:2035:LYS:O	1:C:2038:THR:HG22	1.97	0.65
2:H:139:PRO:O	2:H:143:GLU:N	2.27	0.65
2:B:144:LYS:CD	2:B:148:ASP:OD1	2.45	0.64
1:G:1890:ASP:HB2	1:G:1893:GLU:H	1.63	0.64
1:G:2020:ASP:HB3	1:G:2023:LEU:HB2	1.79	0.64
1:C:1931:LYS:HE2	1:C:1959:LEU:HD22	1.79	0.64
2:B:144:LYS:HE2	2:B:148:ASP:OD1	1.97	0.64
1:A:1806:ARG:NH1	1:A:1836:ILE:HA	2.14	0.63
1:A:1860:GLU:HG3	1:A:1877:LYS:HD3	1.81	0.63
1:C:1897:ARG:O	1:C:1903:LYS:HD3	1.99	0.62
1:E:1889:PHE:HZ	1:E:1907:LEU:HD22	1.64	0.61
1:G:1820:LYS:NZ	1:G:1876:ASN:O	2.33	0.61
2:D:154:TYR:OH	2:D:156:GLU:OE2	2.09	0.60
1:E:1929:GLN:NE2	1:E:1930:PHE:O	2.34	0.60
2:B:144:LYS:CE	2:B:148:ASP:OD1	2.49	0.60
1:C:1811:TYR:OH	1:C:1907:LEU:HD12	2.01	0.60
1:G:1806:ARG:HH11	1:G:1836:ILE:HA	1.66	0.60
1:G:2058:GLU:HA	1:G:2061:ARG:HB3	1.83	0.59
2:B:112:LEU:HD21	2:B:145:LEU:HD12	1.84	0.59
1:A:1899:THR:OG1	1:A:1900:TYR:N	2.35	0.59
2:H:112:LEU:HB3	2:H:154:TYR:HD1	1.68	0.59
1:E:1890:ASP:HB2	1:E:1893:GLU:HG3	1.84	0.58
1:G:2055:ASP:N	1:G:2055:ASP:OD1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:117:ILE:HG21	2:B:156:GLU:HB2	1.85	0.58
2:D:65:ASP:OD1	2:D:68:ARG:NH2	2.29	0.57
1:G:1913:CYS:SG	1:G:1931:LYS:HE3	2.44	0.57
1:A:1869:ASP:OD1	1:A:1870:LYS:N	2.38	0.57
1:E:1806:ARG:HD2	1:E:1836:ILE:HD13	1.86	0.56
2:B:131:LYS:O	2:B:132:ASN:ND2	2.39	0.56
1:C:1829:PHE:HA	1:C:1950:ASN:HA	1.87	0.56
2:F:62:GLU:OE1	2:F:62:GLU:N	2.39	0.56
2:B:17:THR:O	2:B:21:ILE:HG22	2.06	0.55
1:E:1820:LYS:NZ	1:E:1876:ASN:O	2.35	0.55
1:C:1829:PHE:CD2	1:C:1948:ARG:HD2	2.41	0.55
2:B:124:SER:O	2:B:128:LYS:HB2	2.06	0.55
1:C:1873:LEU:HD22	1:C:1879:TYR:CD2	2.41	0.55
2:F:8:VAL:HG21	2:F:20:LEU:HD11	1.88	0.55
1:A:1852:GLU:HA	1:E:2046:ARG:NH2	2.16	0.55
1:C:2068:HIS:NE2	1:E:1946:LYS:HG2	2.21	0.55
1:A:1944:TYR:HE1	1:A:1946:LYS:HB2	1.70	0.55
2:H:127:GLU:HG3	2:H:131:LYS:HE2	1.88	0.54
2:D:20:LEU:HD22	2:D:55:LEU:HD13	1.90	0.54
2:B:120:ARG:NH2	2:B:156:GLU:OE2	2.41	0.54
2:F:68:ARG:HB3	2:F:69:PRO:HD3	1.89	0.54
1:A:1913:CYS:SG	1:A:1933:LYS:HG2	2.48	0.54
2:D:125:THR:HA	2:D:128:LYS:HB3	1.90	0.53
1:C:2068:HIS:HE1	1:E:1946:LYS:HA	1.73	0.53
1:G:2035:LYS:O	1:G:2038:THR:HG22	2.08	0.53
2:H:112:LEU:HD22	2:H:146:ALA:HB2	1.89	0.53
1:A:1862:ILE:O	1:A:1864:ASP:N	2.42	0.53
1:G:1866:ASN:HB2	1:G:1867:PRO:HD2	1.90	0.53
2:F:144:LYS:HG2	2:F:148:ASP:OD1	2.08	0.52
1:E:1806:ARG:HH11	1:E:1836:ILE:HD13	1.74	0.52
2:B:29:PRO:HG2	2:B:160:LEU:HA	1.90	0.52
2:B:45:MET:O	2:B:46:ILE:HG13	2.09	0.52
2:F:144:LYS:O	2:F:147:ARG:N	2.42	0.52
1:A:1829:PHE:HA	1:A:1950:ASN:HA	1.90	0.52
1:E:2039:LYS:HZ2	1:E:2040:ARG:NH2	2.08	0.51
2:F:129:LEU:HA	2:F:132:ASN:OD1	2.10	0.51
1:A:1909:ARG:NH1	1:A:1955:GLU:OE1	2.43	0.51
2:D:8:VAL:HG12	2:D:16:LYS:HD2	1.93	0.51
1:G:1906:ASN:H	1:G:1907:LEU:HD23	1.75	0.51
2:D:27:LYS:HG3	2:D:32:TYR:HA	1.92	0.51
1:G:1825:ASP:O	1:G:1827:GLN:NE2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:127:GLU:HG3	2:B:131:LYS:HE2	1.93	0.51
2:B:138:THR:OG1	2:B:141:THR:HG23	2.11	0.51
1:A:1987:PRO:O	1:A:1991:GLN:HG3	2.10	0.51
1:C:1829:PHE:CD2	1:C:1950:ASN:HB3	2.46	0.51
1:A:1944:TYR:CE1	1:A:1946:LYS:HB2	2.46	0.51
2:D:129:LEU:HA	2:D:132:ASN:OD1	2.11	0.51
2:F:112:LEU:HD21	2:F:145:LEU:HD12	1.93	0.51
2:D:53:LEU:HD22	2:D:173:ILE:HD11	1.94	0.50
2:F:20:LEU:HD22	2:F:55:LEU:HD13	1.92	0.50
1:G:1919:ASP:OD2	1:G:1921:ARG:NH2	2.37	0.50
2:B:145:LEU:O	2:B:149:LEU:HG	2.11	0.50
2:B:59:ALA:HB1	2:B:61:GLN:OE1	2.11	0.50
1:G:1995:GLN:O	1:G:1995:GLN:NE2	2.44	0.50
1:G:2008:GLU:O	1:G:2012:VAL:HG23	2.12	0.50
1:C:1900:TYR:O	1:C:1903:LYS:NZ	2.33	0.50
1:E:2020:ASP:OD1	1:E:2022:LYS:HB2	2.11	0.50
1:A:1857:ASP:N	1:A:1857:ASP:OD1	2.43	0.50
2:D:140:GLU:N	2:D:140:GLU:OE1	2.40	0.50
2:H:117:ILE:HG21	2:H:156:GLU:HB2	1.94	0.50
2:D:45:MET:O	2:D:46:ILE:HG13	2.12	0.50
2:H:17:THR:HG23	2:H:57:ASP:OD2	2.12	0.50
1:A:1997:SER:HA	2:B:37:PHE:HD1	1.76	0.49
1:C:2015:SER:O	1:C:2016:GLU:HG3	2.12	0.49
1:E:1960:THR:O	1:E:1963:GLU:N	2.44	0.49
1:E:2020:ASP:HB3	1:E:2023:LEU:HD13	1.94	0.49
1:E:2000:THR:HG22	2:F:38:ASP:HB2	1.93	0.49
2:B:130:ALA:C	2:B:132:ASN:H	2.16	0.49
2:B:11:ASP:O	2:B:14:VAL:HG22	2.11	0.49
1:A:1997:SER:HA	2:B:37:PHE:CD1	2.48	0.49
1:C:1806:ARG:HH21	1:C:1836:ILE:HA	1.77	0.49
1:A:1900:TYR:CE2	1:A:1902:ASP:HB3	2.48	0.49
2:D:85:VAL:HG11	2:D:119:LEU:HB2	1.95	0.49
1:E:1857:ASP:OD1	1:E:1857:ASP:N	2.36	0.49
1:G:1840:ALA:HB2	2:H:162:GLN:OE1	2.13	0.49
1:G:1871:CYS:SG	1:G:1872:LYS:N	2.86	0.49
1:C:2042:GLU:OE1	1:C:2067:TYR:OH	2.27	0.49
1:C:2074:LEU:O	1:C:2078:ILE:HG12	2.13	0.49
1:G:1976:LEU:HD23	1:G:1993:VAL:HG12	1.94	0.49
2:B:23:TYR:HB2	2:B:165:LEU:HD21	1.95	0.49
2:H:20:LEU:HD22	2:H:55:LEU:HD13	1.95	0.49
1:G:1833:GLU:HB3	1:G:1834:PRO:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2010:ALA:O	1:C:2014:LEU:HB2	2.14	0.48
1:A:1873:LEU:HD22	1:A:1879:TYR:CE2	2.49	0.48
1:C:1960:THR:HG23	1:C:1963:GLU:OE1	2.14	0.48
2:D:85:VAL:HG21	2:D:119:LEU:HD12	1.96	0.48
1:A:1962:ILE:HD13	1:A:2026:HIS:HB3	1.95	0.48
1:C:1864:ASP:OD1	1:C:1865:SER:N	2.41	0.48
2:D:19:LEU:HB3	2:D:159:ALA:HB2	1.94	0.48
2:F:86:SER:OG	2:F:89:SER:HB3	2.14	0.48
1:C:1818:GLY:N	1:C:1825:ASP:OD1	2.47	0.48
1:G:1940:HIS:H	1:G:1949:VAL:HG21	1.78	0.48
2:F:127:GLU:HG3	2:F:131:LYS:HE2	1.95	0.48
1:G:1944:TYR:CG	1:G:1945:ILE:N	2.82	0.47
1:C:1996:GLY:O	2:D:37:PHE:HB3	2.14	0.47
1:A:1930:PHE:CE2	1:A:1961:PRO:HD3	2.49	0.47
1:C:1890:ASP:OD2	1:C:1893:GLU:HG3	2.14	0.47
1:G:2032:LEU:O	1:G:2032:LEU:HD23	2.15	0.47
1:A:1966:ILE:O	1:A:1970:GLN:HG3	2.15	0.47
2:B:49:GLU:HB2	2:B:51:TYR:CE1	2.49	0.47
1:C:1863:LYS:HE2	2:D:161:THR:HA	1.97	0.47
1:G:1962:ILE:O	1:G:1966:ILE:HG13	2.13	0.47
1:G:1907:LEU:N	1:G:1907:LEU:HD23	2.30	0.47
1:C:2040:ARG:HA	1:C:2040:ARG:HD3	1.68	0.47
1:A:1836:ILE:HG21	2:B:45:MET:HG3	1.96	0.47
2:D:16:LYS:O	2:D:20:LEU:HG	2.15	0.47
1:G:2073:ALA:O	1:G:2076:PRO:HD2	2.15	0.47
1:A:1853:ARG:HB3	1:A:1854:PHE:CD1	2.50	0.46
1:A:1873:LEU:HD22	1:A:1879:TYR:CD2	2.50	0.46
1:A:1908:ARG:HB3	1:A:1941:ALA:HB2	1.97	0.46
2:B:65:ASP:OD1	2:B:68:ARG:NH2	2.48	0.46
2:B:91:GLU:O	2:B:95:GLU:HG2	2.15	0.46
1:E:1936:LEU:HD22	1:E:1951:VAL:HG11	1.97	0.46
1:E:1982:GLN:HG3	1:E:1985:ALA:HA	1.97	0.46
1:E:2067:TYR:CE2	1:E:2071:LYS:HE3	2.49	0.46
2:F:19:LEU:HB3	2:F:159:ALA:HB2	1.96	0.46
1:C:1933:LYS:HE3	1:C:1957:ILE:HD12	1.97	0.46
2:B:113:VAL:HA	2:B:155:VAL:O	2.16	0.46
1:E:2034:PHE:O	1:E:2038:THR:HG22	2.16	0.46
1:G:1873:LEU:HD22	1:G:1879:TYR:CD2	2.50	0.46
1:C:1911:MET:HA	1:C:1934:THR:O	2.16	0.46
1:E:1863:LYS:HE2	2:F:161:THR:HG22	1.96	0.46
1:A:2048:ASN:O	1:A:2052:ILE:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1806:ARG:HE	1:C:1836:ILE:H	1.64	0.46
1:C:1940:HIS:H	1:C:1949:VAL:HG21	1.81	0.46
1:C:1907:LEU:HB2	1:C:1942:PHE:HB2	1.97	0.46
1:C:2004:GLN:HG2	2:D:36:VAL:HB	1.97	0.46
2:D:94:LYS:HG2	2:D:145:LEU:HD21	1.98	0.46
1:E:1889:PHE:CZ	1:E:1907:LEU:HD22	2.49	0.46
1:E:1971:LYS:HB2	1:E:1971:LYS:HE2	1.79	0.46
2:H:122:ASP:O	2:H:126:ILE:HG13	2.16	0.46
1:A:2074:LEU:O	1:A:2078:ILE:HG12	2.16	0.46
1:E:2033:CYS:O	1:E:2037:PHE:N	2.41	0.45
1:G:2039:LYS:HE3	1:G:2039:LYS:HB3	1.72	0.45
1:A:2004:GLN:H	1:A:2004:GLN:HG2	1.38	0.45
2:D:62:GLU:N	2:D:62:GLU:OE1	2.49	0.45
1:G:1829:PHE:HA	1:G:1950:ASN:HA	1.99	0.45
1:E:1966:ILE:HD13	1:E:2029:LYS:HD3	1.99	0.45
1:G:2040:ARG:HD3	1:G:2040:ARG:HA	1.53	0.45
2:B:53:LEU:HD13	2:B:173:ILE:HG12	1.97	0.45
1:C:1930:PHE:CE2	1:C:1961:PRO:HD3	2.52	0.45
1:E:1873:LEU:HD22	1:E:1879:TYR:CD2	2.51	0.45
2:F:5:LYS:HB3	2:F:75:THR:HA	1.99	0.45
1:G:1851:GLY:C	1:G:1853:ARG:H	2.18	0.45
1:A:1997:SER:HB3	1:A:2037:PHE:HZ	1.81	0.45
1:A:1890:ASP:HB2	1:A:1893:GLU:H	1.82	0.45
2:H:96:LYS:HD2	2:H:97:TRP:CE2	2.51	0.45
1:C:1813:ARG:NH1	1:C:1828:GLU:OE2	2.50	0.45
1:G:1812:PHE:HE2	1:G:1839:LEU:HA	1.80	0.45
2:H:45:MET:O	2:H:46:ILE:HG13	2.17	0.45
1:A:1986:ASP:HB3	1:A:1989:MET:HB3	1.99	0.45
1:A:2007:LEU:HD11	1:A:2073:ALA:CB	2.47	0.44
1:C:2073:ALA:O	1:C:2076:PRO:HD2	2.17	0.44
1:G:2039:LYS:NZ	1:G:2040:ARG:NE	2.65	0.44
2:H:70:LEU:O	2:H:73:PRO:HD2	2.17	0.44
1:E:1908:ARG:HG2	1:E:1937:THR:HG23	2.00	0.44
2:F:4:ILE:HB	2:F:53:LEU:HD12	2.00	0.44
1:A:2069:ARG:HE	1:A:2069:ARG:HB3	1.71	0.44
1:C:1942:PHE:CZ	1:C:1949:VAL:HG12	2.52	0.44
1:E:1860:GLU:O	1:E:1879:TYR:HA	2.17	0.44
2:H:11:ASP:OD2	2:H:92:ASN:ND2	2.43	0.44
2:H:152:VAL:HG12	2:H:153:LYS:HG2	1.98	0.44
1:A:1919:ASP:HB3	1:A:1921:ARG:HE	1.83	0.44
2:D:138:THR:HB	2:D:140:GLU:OE1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1894:MET:O	1:E:1898:ILE:HG13	2.18	0.44
1:G:1932:ARG:HD2	1:G:1956:GLU:HG2	1.99	0.44
2:F:90:PHE:CZ	2:F:145:LEU:HG	2.53	0.43
1:G:2039:LYS:NZ	1:G:2040:ARG:HE	2.16	0.43
2:H:144:LYS:HE2	2:H:148:ASP:OD2	2.18	0.43
1:A:1806:ARG:HD2	1:A:1836:ILE:H	1.83	0.43
2:D:85:VAL:O	2:D:129:LEU:HD11	2.18	0.43
1:G:2034:PHE:HA	1:G:2037:PHE:HB3	2.00	0.43
1:A:1834:PRO:O	1:A:1837:THR:OG1	2.36	0.43
1:E:1890:ASP:HB2	1:E:1893:GLU:H	1.82	0.43
1:E:2074:LEU:HD23	1:E:2074:LEU:HA	1.85	0.43
1:G:2047:LYS:O	1:G:2050:SER:N	2.43	0.43
1:E:1895:LYS:O	1:E:1899:THR:HG23	2.17	0.43
1:C:2057:LYS:HB3	1:C:2057:LYS:HE2	1.87	0.43
2:F:112:LEU:HD22	2:F:146:ALA:HB2	2.01	0.43
2:H:105:CYS:HB3	2:H:108:THR:HB	2.01	0.43
2:B:4:ILE:HD12	2:B:173:ILE:HG23	2.00	0.43
1:E:2055:ASP:OD1	1:E:2055:ASP:N	2.52	0.43
1:G:1906:ASN:O	1:G:1908:ARG:N	2.51	0.43
2:F:158:SER:O	2:F:162:GLN:N	2.52	0.43
1:G:1806:ARG:NH1	1:G:1836:ILE:HA	2.33	0.43
1:G:1864:ASP:OD1	1:G:1865:SER:N	2.46	0.43
1:A:1897:ARG:O	1:A:1903:LYS:HD3	2.19	0.43
1:E:2040:ARG:HA	1:E:2040:ARG:HD3	1.39	0.43
1:E:2069:ARG:HE	1:E:2069:ARG:HB3	1.67	0.43
1:A:2074:LEU:HA	1:A:2074:LEU:HD23	1.59	0.43
1:C:2047:LYS:HE2	1:C:2051:LEU:HD11	1.99	0.43
1:A:1842:ILE:HG21	1:A:1842:ILE:HD13	1.83	0.43
1:A:1873:LEU:HA	1:A:1873:LEU:HD23	1.77	0.43
1:A:2060:GLN:O	1:A:2064:GLU:HG3	2.19	0.43
1:E:1966:ILE:O	1:E:1970:GLN:HG3	2.18	0.42
2:F:113:VAL:HG13	2:F:155:VAL:HG23	2.01	0.42
1:E:2039:LYS:HB3	1:E:2039:LYS:HE2	1.54	0.42
1:A:1856:GLU:OE1	1:A:1856:GLU:N	2.47	0.42
2:B:70:LEU:HD23	2:B:70:LEU:HA	1.64	0.42
1:G:1901:PHE:O	1:G:1903:LYS:HG3	2.19	0.42
2:H:33:VAL:HG13	2:H:34:PRO:HD2	2.01	0.42
1:A:1900:TYR:HE2	1:A:1902:ASP:HB3	1.84	0.42
2:B:94:LYS:HG2	2:B:145:LEU:HD21	2.02	0.42
1:E:1941:ALA:O	1:E:1944:TYR:HB2	2.19	0.42
1:C:1992:MET:HG2	2:D:39:ASN:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1821:PHE:CE2	1:G:1878:ALA:HB1	2.54	0.42
1:A:2035:LYS:O	1:A:2038:THR:HG22	2.20	0.42
2:F:68:ARG:O	2:F:70:LEU:N	2.53	0.42
1:C:1831:TYR:OH	1:C:1948:ARG:NH1	2.52	0.42
1:C:1828:GLU:O	1:C:1950:ASN:HB2	2.20	0.42
1:G:1976:LEU:CD2	1:G:1993:VAL:HG12	2.49	0.42
1:A:1940:HIS:HB2	1:A:1949:VAL:HG21	2.01	0.42
2:F:5:LYS:HG3	2:F:56:PHE:CE1	2.55	0.42
1:A:1889:PHE:CE1	1:A:1897:ARG:NH1	2.88	0.42
2:F:96:LYS:HE3	2:F:97:TRP:CH2	2.55	0.42
2:H:23:TYR:HB2	2:H:165:LEU:HD21	2.01	0.42
1:A:1926:LEU:HD23	1:A:1926:LEU:HA	1.76	0.41
1:A:2039:LYS:HB3	1:A:2040:ARG:HH12	1.85	0.41
1:A:1824:LEU:O	1:A:1825:ASP:C	2.58	0.41
1:E:2007:LEU:HD22	1:E:2011:GLN:NE2	2.35	0.41
1:C:1842:ILE:HG21	1:C:1842:ILE:HD13	1.82	0.41
1:A:1805:GLU:O	1:A:1805:GLU:HG3	2.21	0.41
2:B:110:PHE:CE2	2:B:151:ALA:HB2	2.55	0.41
2:D:108:THR:HA	2:D:109:PRO:HD2	1.91	0.41
1:E:2039:LYS:NZ	1:E:2040:ARG:NH2	2.68	0.41
2:F:158:SER:HG	2:F:161:THR:H	1.64	0.41
2:F:24:THR:HG22	2:F:42:VAL:HB	2.02	0.41
1:A:1817:TYR:CZ	1:A:1868:VAL:HG21	2.56	0.41
1:A:1927:HIS:CE1	1:A:1928:GLU:HG3	2.55	0.41
2:B:20:LEU:HD22	2:B:55:LEU:HD13	2.01	0.41
1:E:1962:ILE:HG13	1:E:2030:LEU:HD22	2.02	0.41
2:F:91:GLU:O	2:F:95:GLU:HG2	2.21	0.41
1:C:1900:TYR:CE2	1:C:1902:ASP:HB3	2.55	0.41
1:E:2038:THR:HG23	1:E:2039:LYS:N	2.36	0.41
2:H:11:ASP:OD2	2:H:89:SER:HA	2.21	0.41
1:A:1962:ILE:O	1:A:1966:ILE:HG13	2.21	0.41
1:G:1824:LEU:HA	1:G:1824:LEU:HD23	1.75	0.41
1:G:2037:PHE:O	1:G:2040:ARG:HB2	2.20	0.41
1:G:2001:THR:N	2:H:38:ASP:OD2	2.52	0.41
2:H:7:VAL:HG23	2:H:75:THR:HG23	2.02	0.41
1:A:2020:ASP:OD1	1:A:2022:LYS:HB2	2.21	0.41
2:D:135:LYS:HB3	2:D:135:LYS:HE2	1.75	0.41
1:E:1925:GLU:O	1:E:1927:HIS:N	2.54	0.41
2:F:127:GLU:O	2:F:131:LYS:HE2	2.21	0.41
2:F:53:LEU:HA	2:F:53:LEU:HD12	1.90	0.41
1:G:2034:PHE:O	1:G:2038:THR:HB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2020:ASP:HB3	1:A:2023:LEU:HD22	2.03	0.41
1:A:2040:ARG:HD3	1:A:2040:ARG:HA	1.90	0.41
1:C:1817:TYR:HB2	1:C:1879:TYR:HB2	2.03	0.41
1:E:1973:THR:O	1:E:1976:LEU:HB2	2.21	0.41
1:E:2057:LYS:HE2	1:E:2057:LYS:HB3	1.80	0.41
1:A:1925:GLU:OE1	1:A:1925:GLU:HA	2.21	0.40
2:F:21:ILE:HG13	2:F:40:TYR:CE2	2.56	0.40
2:H:136:PRO:O	2:H:137:ILE:HD13	2.22	0.40
1:A:1833:GLU:OE1	1:A:1845:ARG:NH1	2.52	0.40
2:B:20:LEU:HA	2:B:20:LEU:HD23	1.80	0.40
1:C:1960:THR:H	1:C:1960:THR:HG23	1.66	0.40
2:D:157:CYS:HB2	2:D:165:LEU:HD12	2.02	0.40
2:H:153:LYS:HB3	2:H:153:LYS:HE2	1.85	0.40
2:H:177:LEU:HA	2:H:177:LEU:HD23	1.71	0.40
1:A:1847:GLU:HA	1:A:1859:VAL:HG11	2.03	0.40
2:B:110:PHE:O	2:B:152:VAL:HG23	2.21	0.40
1:E:2074:LEU:O	1:E:2078:ILE:HG12	2.22	0.40
2:F:120:ARG:O	2:F:126:ILE:HD11	2.22	0.40
1:G:1918:LEU:HG	1:G:1918:LEU:H	1.64	0.40
1:G:2074:LEU:O	1:G:2078:ILE:HG12	2.22	0.40
1:A:1901:PHE:O	1:A:1903:LYS:HG3	2.21	0.40
1:A:1976:LEU:O	1:A:1977:ALA:C	2.59	0.40
2:B:16:LYS:HE2	2:B:16:LYS:HB3	1.82	0.40
1:G:1936:LEU:CD2	1:G:1954:LYS:HE2	2.51	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	273/290 (94%)	245 (90%)	28 (10%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	273/290 (94%)	256 (94%)	16 (6%)	1 (0%)	34	67
1	E	273/290 (94%)	249 (91%)	23 (8%)	1 (0%)	34	67
1	G	273/290 (94%)	248 (91%)	23 (8%)	2 (1%)	22	56
2	B	176/195 (90%)	162 (92%)	13 (7%)	1 (1%)	25	59
2	D	176/195 (90%)	158 (90%)	18 (10%)	0	100	100
2	F	176/195 (90%)	162 (92%)	13 (7%)	1 (1%)	25	59
2	H	176/195 (90%)	154 (88%)	21 (12%)	1 (1%)	25	59
All	All	1796/1940 (93%)	1634 (91%)	155 (9%)	7 (0%)	34	67

All (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
1	G	2052	ILE
2	F	69	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	250/261 (96%)	245 (98%)	5 (2%)	55	76
1	C	250/261 (96%)	247 (99%)	3 (1%)	71	83
1	E	250/261 (96%)	247 (99%)	3 (1%)	71	83
1	G	250/261 (96%)	245 (98%)	5 (2%)	55	76
2	B	158/172 (92%)	157 (99%)	1 (1%)	86	91
2	D	158/172 (92%)	156 (99%)	2 (1%)	69	82
2	F	158/172 (92%)	156 (99%)	2 (1%)	69	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	H	158/172 (92%)	155 (98%)	3 (2%)	57 76
All	All	1632/1732 (94%)	1608 (98%)	24 (2%)	65 80

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1823	ASP
1	A	1853	ARG
1	A	1939	SER
1	A	2036	ASP
1	A	2069	ARG
2	B	88	SER
1	C	1807	MET
1	C	2004	GLN
1	C	2036	ASP
2	D	66	ARG
2	D	122	ASP
1	E	1823	ASP
1	E	1864	ASP
1	E	1983	ASP
2	F	158	SER
2	F	178	GLU
1	G	1939	SER
1	G	2028	ASN
1	G	2036	ASP
1	G	2039	LYS
1	G	2068	HIS
2	H	88	SER
2	H	124	SER
2	H	132	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1927	HIS
1	A	2068	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 carbohydrates 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 ⓘ

### 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	275/290 (94%)	-0.14	0 100 100	46, 80, 133, 250	0
1	C	275/290 (94%)	-0.14	2 (0%) 87 88	41, 74, 122, 192	0
1	E	275/290 (94%)	0.26	15 (5%) 25 23	55, 98, 161, 215	0
1	G	275/290 (94%)	-0.07	3 (1%) 80 80	43, 78, 136, 199	0
2	B	178/195 (91%)	0.22	9 (5%) 28 26	53, 79, 150, 257	0
2	D	178/195 (91%)	0.12	9 (5%) 28 26	50, 78, 162, 233	0
2	F	178/195 (91%)	0.17	8 (4%) 33 31	71, 94, 177, 228	0
2	H	178/195 (91%)	0.28	10 (5%) 24 22	57, 91, 175, 246	0
All	All	1812/1940 (93%)	0.06	56 (3%) 49 47	41, 84, 147, 257	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	123	PRO	9.9
2	D	123	PRO	7.9
2	H	127	GLU	7.6
2	H	121	ASP	7.3
2	D	127	GLU	6.8
2	B	123	PRO	5.8
2	F	121	ASP	5.0
2	F	123	PRO	4.8
2	D	126	ILE	4.6
2	B	127	GLU	4.4
2	H	126	ILE	4.0
2	B	91	GLU	4.0
2	H	131	LYS	3.9
1	E	1874	ASP	3.9
2	B	95	GLU	3.6
2	F	126	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
2	H	130	ALA	3.5
2	B	121	ASP	3.3
2	F	127	GLU	3.3
1	E	1871	CYS	3.2
1	E	1879	TYR	3.1
2	B	129	LEU	3.0
1	E	1818	GLY	3.0
2	B	94	LYS	3.0
1	E	1873	LEU	3.0
1	E	1859	VAL	2.9
1	E	2018	PRO	2.9
2	F	104	HIS	2.8
2	H	129	LEU	2.8
1	C	1872	LYS	2.7
1	E	1821	PHE	2.7
2	F	130	ALA	2.7
1	E	1817	TYR	2.6
2	D	121	ASP	2.6
1	E	1878	ALA	2.6
1	G	1869	ASP	2.5
2	B	126	ILE	2.5
1	E	1856	GLU	2.5
2	H	135	LYS	2.5
2	F	134	GLN	2.4
1	E	1882	ILE	2.4
2	D	130	ALA	2.3
2	H	112	LEU	2.3
2	D	131	LYS	2.3
1	G	1852	GLU	2.3
1	E	1861	VAL	2.2
2	D	101	ILE	2.2
2	D	94	LYS	2.2
2	H	120	ARG	2.2
1	C	1869	ASP	2.1
2	F	131	LYS	2.1
2	D	95	GLU	2.1
1	E	2019	SER	2.1
1	G	1871	CYS	2.1
1	E	1872	LYS	2.0
2	B	101	ILE	2.0

## 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.