



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:10 pm GMT

PDB ID : 2C35  
Title : Subunits Rpb4 and Rpb7 of human RNA polymerase II  
Authors : Meka, H.; Werner, F.; Cordell, S.C.; Onesti, S.; Brick, P.  
Deposited on : 2005-10-04  
Resolution : 2.70 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

<http://wwpdb.org/validation/2016/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)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

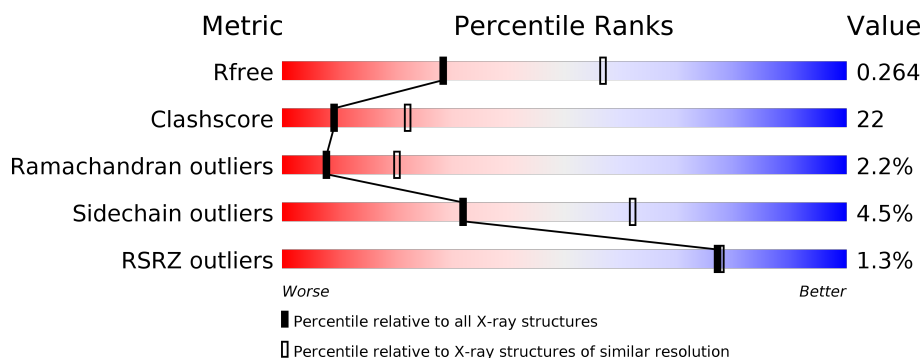
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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. 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	152	<div> <div>%</div> <div> <div></div> <div>49%</div> <div>34%</div> <div>•</div> <div>15%</div> </div> </div>
1	C	152	<div> <div>%</div> <div> <div></div> <div>49%</div> <div>34%</div> <div>•</div> <div>15%</div> </div> </div>
1	E	152	<div> <div>%</div> <div> <div></div> <div>49%</div> <div>30%</div> <div>•</div> <div>17%</div> </div> </div>
1	G	152	<div> <div>3%</div> <div> <div></div> <div>51%</div> <div>27%</div> <div>5%</div> <div>17%</div> </div> </div>
2	B	172	<div> <div>%</div> <div> <div></div> <div>62%</div> <div>35%</div> <div>••</div> </div> </div>
2	D	172	<div> <div>%</div> <div> <div></div> <div>60%</div> <div>37%</div> <div>••</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	172	<div><div>%</div><div><div></div></div><div>56%41%..</div></div>
2	H	172	<div><div>%</div><div><div></div></div><div>57%40%..</div></div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9290 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 DNA-DIRECTED RNA POLYMERASE II 16 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	129	Total	C	N	O	S	0	0	1
			998	629	170	195	4			
1	C	129	Total	C	N	O	S	0	0	1
			998	629	170	195	4			
1	E	126	Total	C	N	O	S	0	0	0
			981	617	167	193	4			
1	G	126	Total	C	N	O	S	0	0	0
			981	617	167	193	4			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II 19 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	171	Total	C	N	O	S	0	0	0
			1305	852	205	240	8			
2	D	171	Total	C	N	O	S	0	0	0
			1305	852	205	240	8			
2	F	171	Total	C	N	O	S	0	0	0
			1334	866	213	247	8			
2	H	171	Total	C	N	O	S	0	0	0
			1334	866	213	247	8			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	O	0	0
			3	3		
3	B	10	Total	O	0	0
			10	10		
3	C	3	Total	O	0	0
			3	3		

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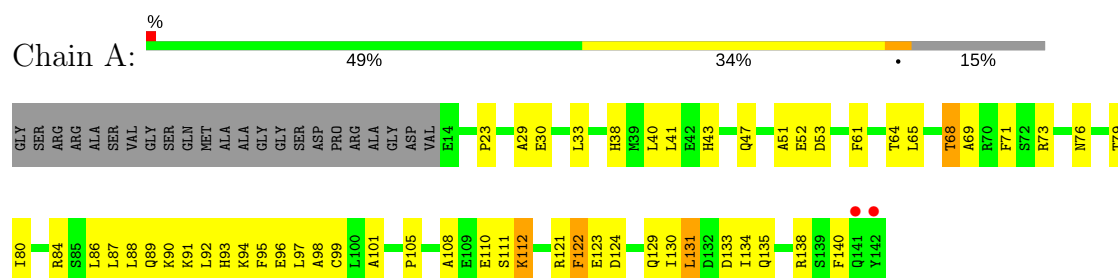
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	10	Total 10	O 10	0	0
3	E	4	Total 4	O 4	0	0
3	F	10	Total 10	O 10	0	0
3	G	4	Total 4	O 4	0	0
3	H	10	Total 10	O 10	0	0

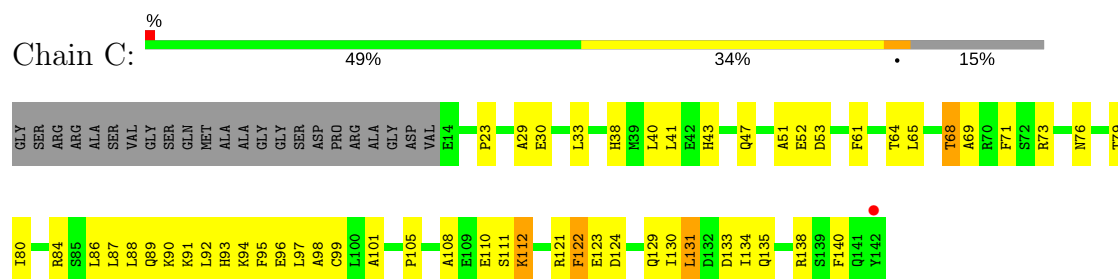
### 3 Residue-property plots [i](#)

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.

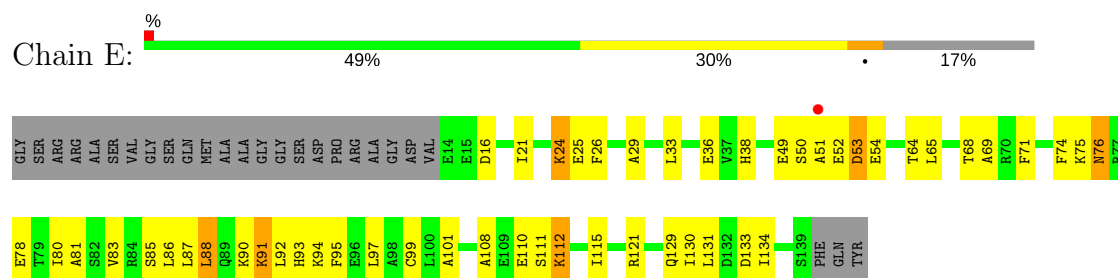
- Molecule 1: DNA-DIRECTED RNA POLYMERASE II 16 KDA POLYPEPTIDE



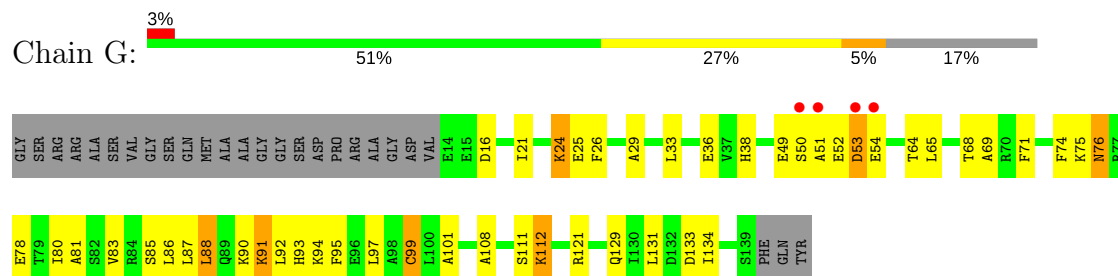
- Molecule 1: DNA-DIRECTED RNA POLYMERASE II 16 KDA POLYPEPTIDE



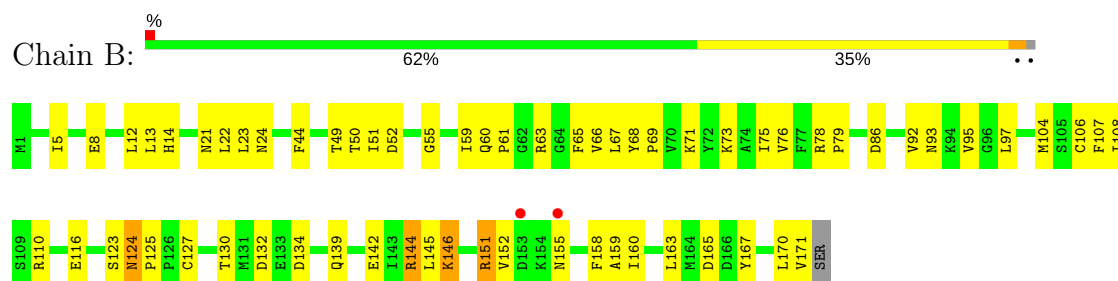
- Molecule 1: DNA-DIRECTED RNA POLYMERASE II 16 KDA POLYPEPTIDE



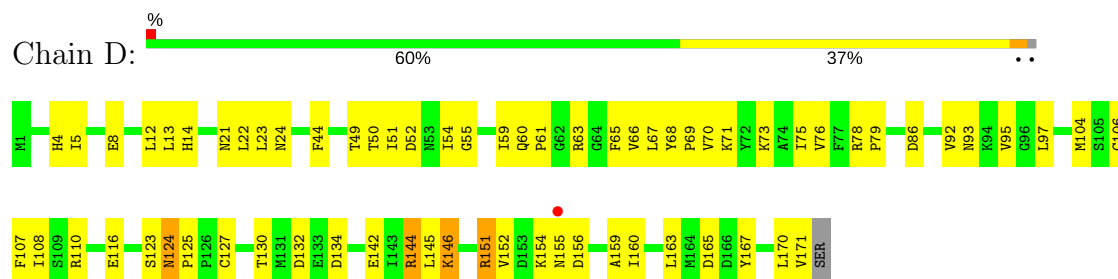
- Molecule 1: DNA-DIRECTED RNA POLYMERASE II 16 KDA POLYPEPTIDE



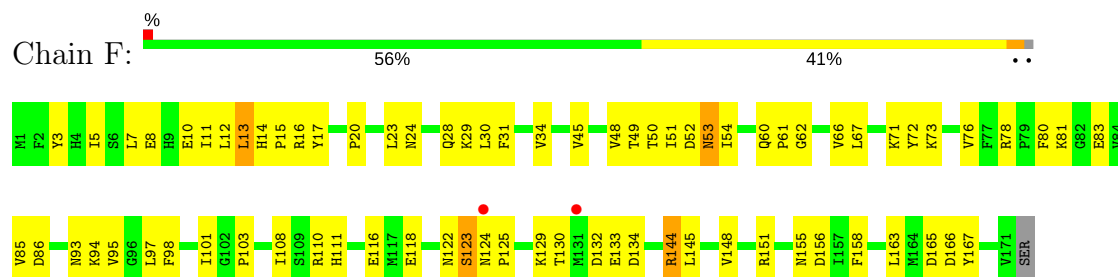
• Molecule 2: DNA-DIRECTED RNA POLYMERASE II 19 KDA POLYPEPTIDE



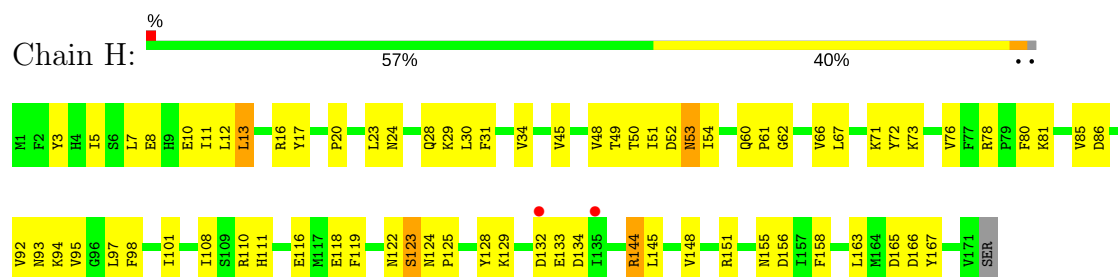
• Molecule 2: DNA-DIRECTED RNA POLYMERASE II 19 KDA POLYPEPTIDE



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• Molecule 2: DNA-DIRECTED RNA POLYMERASE II 19 KDA POLYPEPTIDE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.69Å 83.19Å 99.31Å 85.53° 81.80° 81.77°	Depositor
Resolution (Å)	43.26 – 2.70 43.26 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.2 (43.26-2.70) 93.4 (43.26-2.70)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.24 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.230 , 0.266 0.230 , 0.264	Depositor DCC
$R_{free}$ test set	1860 reflections (5.23%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.6	Xtriage
Anisotropy	0.564	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 50.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9290	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% 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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.41	0/1012	0.59	0/1366
1	C	0.41	0/1012	0.58	0/1366
1	E	0.40	0/994	0.57	0/1341
1	G	0.40	0/994	0.57	0/1341
2	B	0.43	0/1336	0.73	0/1820
2	D	0.44	0/1336	0.72	0/1820
2	F	0.44	0/1365	0.73	0/1854
2	H	0.44	0/1365	0.73	0/1854
All	All	0.42	0/9414	0.67	0/12762

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	998	0	953	47	0
1	C	998	0	953	46	0
1	E	981	0	942	42	0
1	G	981	0	942	41	0
2	B	1305	0	1267	67	0
2	D	1305	0	1267	63	0
2	F	1334	0	1326	71	0
2	H	1334	0	1326	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	3	0	0	0	0
3	B	10	0	0	0	0
3	C	3	0	0	0	0
3	D	10	0	0	0	0
3	E	4	0	0	0	0
3	F	10	0	0	0	0
3	G	4	0	0	0	0
3	H	10	0	0	0	0
All	All	9290	0	8976	402	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 22.

All (402) 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:93:ASN:HD22	2:D:95:VAL:H	1.09	0.98
2:F:93:ASN:HD22	2:F:95:VAL:H	1.04	0.98
2:B:93:ASN:HD22	2:B:95:VAL:H	1.11	0.96
2:D:160:ILE:HD12	2:H:111:HIS:HE2	1.32	0.92
2:H:93:ASN:HD22	2:H:95:VAL:H	1.02	0.92
2:D:93:ASN:ND2	2:D:95:VAL:H	1.67	0.91
2:B:93:ASN:ND2	2:B:95:VAL:H	1.70	0.88
2:B:86:ASP:OD1	2:B:144:ARG:HG2	1.75	0.87
1:E:87:LEU:HD21	1:E:134:ILE:HD11	1.56	0.86
1:G:87:LEU:HD21	1:G:134:ILE:HD11	1.60	0.84
2:D:160:ILE:HD12	2:H:111:HIS:NE2	1.93	0.84
2:D:86:ASP:OD1	2:D:144:ARG:HG2	1.78	0.82
2:D:146:LYS:HE3	2:D:165:ASP:OD2	1.82	0.80
2:D:151:ARG:HH11	2:D:151:ARG:HG2	1.46	0.78
1:E:93:HIS:HD2	1:E:95:PHE:H	1.32	0.77
2:B:151:ARG:HG2	2:B:151:ARG:HH11	1.48	0.77
2:F:124:ASN:CB	2:F:125:PRO:HD3	2.15	0.77
1:A:23:PRO:HG3	2:B:78:ARG:HH12	1.49	0.76
2:B:146:LYS:HE3	2:B:165:ASP:OD2	1.84	0.76
1:C:23:PRO:HG3	2:D:78:ARG:HH12	1.50	0.76
2:H:124:ASN:CB	2:H:125:PRO:HD3	2.15	0.75
1:G:93:HIS:HD2	1:G:95:PHE:H	1.34	0.75
2:D:8:GLU:OE2	2:D:71:LYS:HG2	1.85	0.75
1:C:86:LEU:HD11	1:C:133:ASP:HB3	1.67	0.75
1:A:86:LEU:HD11	1:A:133:ASP:HB3	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:HIS:HD2	1:A:94:LYS:N	1.86	0.74
1:E:93:HIS:CD2	1:E:95:PHE:H	2.05	0.74
1:C:38:HIS:HB2	1:C:68:THR:HG23	1.69	0.74
1:G:93:HIS:CD2	1:G:95:PHE:H	2.06	0.74
2:D:93:ASN:HD22	2:D:95:VAL:N	1.85	0.73
1:C:93:HIS:HD2	1:C:94:LYS:N	1.86	0.73
1:A:93:HIS:CD2	1:A:95:PHE:H	2.07	0.73
1:G:65:LEU:O	1:G:68:THR:HG22	1.88	0.73
1:C:93:HIS:CD2	1:C:95:PHE:H	2.07	0.72
2:D:124:ASN:CB	2:D:125:PRO:HD3	2.20	0.71
2:B:8:GLU:OE2	2:B:71:LYS:HG2	1.90	0.71
1:A:38:HIS:HB2	1:A:68:THR:HG23	1.73	0.71
1:E:65:LEU:O	1:E:68:THR:HG22	1.90	0.70
2:B:124:ASN:CB	2:B:125:PRO:HD3	2.22	0.70
2:B:132:ASP:OD2	2:B:134:ASP:HB2	1.92	0.70
1:C:108:ALA:O	1:C:112:LYS:HD3	1.92	0.70
2:H:10:GLU:HB3	2:H:67:LEU:HD21	1.73	0.70
2:F:30:LEU:O	2:F:34:VAL:HG22	1.91	0.69
1:A:76:ASN:HB3	1:A:79:THR:OG1	1.92	0.69
2:H:30:LEU:O	2:H:34:VAL:HG22	1.93	0.68
2:B:93:ASN:HD22	2:B:95:VAL:N	1.87	0.68
2:F:10:GLU:HB3	2:F:67:LEU:HD21	1.75	0.68
2:D:132:ASP:OD2	2:D:134:ASP:HB2	1.92	0.68
1:C:76:ASN:HB3	1:C:79:THR:OG1	1.94	0.68
1:A:108:ALA:O	1:A:112:LYS:HD3	1.93	0.67
2:H:93:ASN:HD22	2:H:95:VAL:N	1.84	0.67
2:H:45:VAL:HA	2:H:76:VAL:HG12	1.77	0.67
2:D:95:VAL:HG11	2:H:98:PHE:CE2	2.29	0.67
2:B:95:VAL:HG11	2:F:98:PHE:CE2	2.30	0.66
1:E:24:LYS:CG	1:E:25:GLU:H	2.08	0.66
2:H:86:ASP:OD1	2:H:144:ARG:HG2	1.94	0.66
2:H:11:ILE:HD12	2:H:29:LYS:HG3	1.78	0.66
2:F:86:ASP:OD1	2:F:144:ARG:HG2	1.94	0.65
1:C:33:LEU:HD22	1:C:101:ALA:HB3	1.77	0.65
2:D:93:ASN:ND2	2:D:95:VAL:N	2.44	0.65
2:H:118:GLU:HG2	2:H:129:LYS:O	1.96	0.65
1:A:33:LEU:HD22	1:A:101:ALA:HB3	1.78	0.65
2:F:132:ASP:OD2	2:F:134:ASP:HB2	1.97	0.65
2:F:45:VAL:HA	2:F:76:VAL:HG12	1.79	0.65
2:H:93:ASN:ND2	2:H:95:VAL:H	1.86	0.65
2:F:93:ASN:HD22	2:F:95:VAL:N	1.86	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:HIS:CD2	1:C:94:LYS:N	2.66	0.64
2:F:118:GLU:HG2	2:F:129:LYS:O	1.97	0.64
1:G:86:LEU:HD11	1:G:133:ASP:HB3	1.80	0.64
1:A:93:HIS:CD2	1:A:94:LYS:N	2.66	0.64
2:D:93:ASN:ND2	2:D:95:VAL:HB	2.12	0.63
2:B:158:PHE:CD2	2:F:94:LYS:HD2	2.32	0.63
1:G:24:LYS:CG	1:G:25:GLU:H	2.11	0.63
1:C:76:ASN:O	1:C:80:ILE:HG13	1.98	0.63
1:A:76:ASN:O	1:A:80:ILE:HG13	1.98	0.63
2:B:170:LEU:HD12	2:B:171:VAL:H	1.64	0.63
2:B:93:ASN:ND2	2:B:95:VAL:HB	2.12	0.63
2:F:11:ILE:HD12	2:F:29:LYS:HG3	1.81	0.63
1:E:36:GLU:HG2	1:E:80:ILE:HG21	1.81	0.62
1:E:86:LEU:HD11	1:E:133:ASP:HB3	1.82	0.62
1:A:41:LEU:HD22	1:A:61:PHE:CE1	2.35	0.62
2:H:132:ASP:OD2	2:H:134:ASP:HB2	2.00	0.61
2:D:170:LEU:HD12	2:D:171:VAL:H	1.65	0.61
2:F:8:GLU:OE1	2:F:71:LYS:HD3	2.01	0.61
2:H:53:ASN:HD22	2:H:54:ILE:H	1.49	0.61
2:F:23:LEU:N	2:F:23:LEU:HD22	2.16	0.60
2:F:85:VAL:HG21	2:F:101:ILE:HD13	1.83	0.60
2:F:93:ASN:ND2	2:F:95:VAL:H	1.88	0.60
1:C:84:ARG:O	1:C:88:LEU:HB2	2.01	0.60
2:H:8:GLU:OE1	2:H:71:LYS:HD3	2.02	0.60
1:A:30:GLU:HG3	1:A:94:LYS:NZ	2.17	0.60
1:A:29:ALA:CB	2:B:5:ILE:HG22	2.32	0.60
2:B:93:ASN:ND2	2:B:95:VAL:N	2.46	0.59
1:C:41:LEU:HD22	1:C:61:PHE:CE1	2.37	0.59
2:H:23:LEU:N	2:H:23:LEU:HD22	2.17	0.59
2:H:85:VAL:HG21	2:H:101:ILE:HD13	1.85	0.59
1:G:38:HIS:HB2	1:G:68:THR:HG23	1.85	0.59
1:E:29:ALA:HB1	2:F:5:ILE:HG22	1.84	0.59
2:B:132:ASP:C	2:B:134:ASP:H	2.06	0.59
1:E:52:GLU:O	1:E:53:ASP:CB	2.51	0.59
1:G:36:GLU:HG2	1:G:80:ILE:HG21	1.84	0.59
2:B:158:PHE:HB3	2:F:94:LYS:NZ	2.18	0.59
1:C:29:ALA:CB	2:D:5:ILE:HG22	2.32	0.58
1:G:108:ALA:O	1:G:111:SER:HB3	2.03	0.58
1:G:29:ALA:HB1	2:H:5:ILE:HG22	1.85	0.58
1:C:30:GLU:HG3	1:C:94:LYS:NZ	2.18	0.58
2:H:16:ARG:HB2	2:H:17:TYR:CE1	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:108:ALA:O	1:E:111:SER:HB3	2.04	0.58
2:F:53:ASN:HD22	2:F:54:ILE:H	1.49	0.57
2:F:16:ARG:HB2	2:F:17:TYR:CE1	2.39	0.57
2:F:108:ILE:HD13	2:F:163:LEU:HD13	1.87	0.57
1:G:52:GLU:O	1:G:53:ASP:CB	2.52	0.57
1:A:135:GLN:OE1	1:A:138:ARG:NH1	2.38	0.57
2:D:132:ASP:C	2:D:134:ASP:H	2.07	0.57
2:H:145:LEU:C	2:H:145:LEU:HD12	2.25	0.57
2:F:145:LEU:HD12	2:F:145:LEU:C	2.25	0.57
2:H:53:ASN:ND2	2:H:54:ILE:H	2.02	0.56
2:B:67:LEU:C	2:B:67:LEU:HD23	2.25	0.56
2:D:79:PRO:HG3	2:D:104:MET:SD	2.45	0.56
2:B:158:PHE:HB3	2:F:94:LYS:HZ2	1.69	0.56
1:A:84:ARG:O	1:A:88:LEU:HB2	2.05	0.56
2:B:95:VAL:HG12	2:B:107:PHE:HZ	1.70	0.56
1:G:29:ALA:HB1	2:H:5:ILE:CG2	2.36	0.56
2:D:95:VAL:HG12	2:D:107:PHE:HZ	1.70	0.56
2:F:24:ASN:O	2:F:28:GLN:HG2	2.05	0.56
2:F:11:ILE:HG23	2:F:29:LYS:HG2	1.87	0.56
2:H:108:ILE:HD13	2:H:163:LEU:HD13	1.88	0.56
2:D:67:LEU:C	2:D:67:LEU:HD23	2.25	0.55
1:E:38:HIS:HB2	1:E:68:THR:HG23	1.86	0.55
2:H:24:ASN:O	2:H:28:GLN:HG2	2.06	0.55
1:G:38:HIS:CE1	1:G:69:ALA:HB2	2.42	0.55
1:E:29:ALA:HB1	2:F:5:ILE:CG2	2.36	0.55
2:F:53:ASN:ND2	2:F:54:ILE:H	2.03	0.55
2:H:11:ILE:HG23	2:H:29:LYS:HG2	1.87	0.55
1:A:90:LYS:O	1:A:92:LEU:N	2.40	0.55
2:D:116:GLU:O	2:D:130:THR:HA	2.06	0.55
2:F:108:ILE:HD13	2:F:163:LEU:CD1	2.37	0.55
2:B:79:PRO:HG3	2:B:104:MET:SD	2.48	0.54
1:C:97:LEU:C	1:C:97:LEU:HD23	2.27	0.54
1:A:97:LEU:C	1:A:97:LEU:HD23	2.28	0.54
2:D:52:ASP:OD1	2:D:73:LYS:HE2	2.07	0.54
1:G:75:LYS:O	1:G:76:ASN:HB2	2.08	0.54
2:B:116:GLU:O	2:B:130:THR:HA	2.08	0.54
2:F:155:ASN:O	2:F:156:ASP:HB2	2.07	0.54
1:E:75:LYS:O	1:E:76:ASN:HB2	2.08	0.54
2:H:155:ASN:O	2:H:156:ASP:HB2	2.07	0.54
2:B:93:ASN:HD22	2:B:95:VAL:HB	1.72	0.54
1:E:97:LEU:HD23	1:E:97:LEU:C	2.29	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:THR:O	1:C:68:THR:HB	2.08	0.54
2:F:52:ASP:OD1	2:F:73:LYS:HE2	2.07	0.54
2:D:124:ASN:CB	2:D:125:PRO:CD	2.86	0.53
1:A:30:GLU:HG3	1:A:94:LYS:HZ3	1.73	0.53
1:E:38:HIS:CE1	1:E:69:ALA:HB2	2.43	0.53
2:H:31:PHE:CE1	2:H:48:VAL:HB	2.44	0.53
2:F:31:PHE:CE1	2:F:48:VAL:HB	2.44	0.53
2:H:50:THR:HG22	2:H:51:ILE:N	2.23	0.53
1:C:87:LEU:HD21	1:C:134:ILE:HD11	1.90	0.53
2:F:3:TYR:HH	2:F:80:PHE:HE1	1.57	0.53
2:H:3:TYR:HH	2:H:80:PHE:HE1	1.55	0.53
2:D:108:ILE:HD13	2:D:163:LEU:HD13	1.90	0.53
2:F:123:SER:O	2:F:124:ASN:C	2.47	0.53
2:B:151:ARG:NH1	2:B:151:ARG:HG2	2.21	0.53
1:C:90:LYS:O	1:C:92:LEU:N	2.41	0.53
2:F:50:THR:HG22	2:F:51:ILE:N	2.24	0.53
1:A:64:THR:O	1:A:68:THR:HB	2.09	0.52
2:B:124:ASN:CB	2:B:125:PRO:CD	2.87	0.52
2:B:52:ASP:OD1	2:B:73:LYS:HE2	2.08	0.52
2:D:151:ARG:HG2	2:D:151:ARG:NH1	2.19	0.52
2:H:123:SER:O	2:H:124:ASN:C	2.48	0.52
2:D:93:ASN:HD22	2:D:95:VAL:HB	1.75	0.52
1:G:50:SER:O	1:G:51:ALA:HB3	2.10	0.52
1:A:65:LEU:O	1:A:68:THR:HG22	2.10	0.52
1:G:97:LEU:HD23	1:G:97:LEU:C	2.30	0.52
1:E:108:ALA:O	1:E:112:LYS:HD3	2.09	0.52
1:G:93:HIS:CD2	1:G:94:LYS:N	2.78	0.52
2:H:108:ILE:HD13	2:H:163:LEU:CD1	2.39	0.52
2:F:166:ASP:O	2:F:167:TYR:HB2	2.10	0.51
2:H:11:ILE:CG2	2:H:13:LEU:HD13	2.40	0.51
1:A:87:LEU:HD21	1:A:134:ILE:HD11	1.92	0.51
2:B:108:ILE:HD13	2:B:163:LEU:HD13	1.92	0.51
2:B:151:ARG:HH11	2:B:151:ARG:CG	2.22	0.51
2:F:11:ILE:CG2	2:F:13:LEU:HD13	2.39	0.51
2:H:52:ASP:OD1	2:H:73:LYS:HE2	2.10	0.51
2:F:23:LEU:HD22	2:F:23:LEU:H	1.75	0.51
1:C:65:LEU:O	1:C:68:THR:HG22	2.11	0.51
2:F:10:GLU:CB	2:F:67:LEU:HD21	2.41	0.51
1:E:93:HIS:CD2	1:E:94:LYS:N	2.79	0.51
2:D:110:ARG:HE	2:H:151:ARG:NH1	2.09	0.51
1:E:50:SER:O	1:E:51:ALA:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:53:ASN:ND2	2:H:54:ILE:N	2.59	0.50
2:H:10:GLU:CB	2:H:67:LEU:HD21	2.39	0.50
2:D:23:LEU:HD22	2:D:23:LEU:H	1.76	0.50
2:H:23:LEU:H	2:H:23:LEU:HD22	1.76	0.50
1:A:121:ARG:HB3	1:A:122:PHE:CD1	2.47	0.50
2:B:23:LEU:HD22	2:B:23:LEU:H	1.77	0.50
2:F:124:ASN:CB	2:F:125:PRO:CD	2.89	0.50
2:B:132:ASP:C	2:B:134:ASP:N	2.65	0.49
1:C:108:ALA:O	1:C:111:SER:HB3	2.12	0.49
1:C:135:GLN:OE1	1:C:138:ARG:NH1	2.45	0.49
2:D:132:ASP:C	2:D:134:ASP:N	2.66	0.49
1:A:97:LEU:HD23	1:A:98:ALA:N	2.27	0.49
1:G:93:HIS:HD2	1:G:94:LYS:N	2.10	0.49
2:F:81:LYS:NZ	2:F:148:VAL:HG13	2.28	0.49
2:D:12:LEU:O	2:D:13:LEU:HD12	2.13	0.49
1:E:90:LYS:O	1:E:92:LEU:N	2.45	0.49
1:A:108:ALA:O	1:A:111:SER:HB3	2.13	0.48
1:G:95:PHE:O	1:G:99:CYS:HB2	2.12	0.48
1:A:135:GLN:O	1:A:138:ARG:HB2	2.13	0.48
1:A:68:THR:CG2	1:A:69:ALA:N	2.75	0.48
2:F:53:ASN:ND2	2:F:54:ILE:N	2.61	0.48
2:B:170:LEU:HD12	2:B:171:VAL:N	2.28	0.48
2:H:10:GLU:CD	2:H:67:LEU:HD21	2.34	0.48
1:C:121:ARG:HB3	1:C:122:PHE:CD1	2.49	0.48
2:D:21:ASN:ND2	2:D:24:ASN:CB	2.77	0.48
2:H:166:ASP:O	2:H:167:TYR:HB2	2.14	0.48
2:H:49:THR:HG22	2:H:50:THR:N	2.28	0.48
1:A:110:GLU:HG3	2:B:167:TYR:CD2	2.49	0.48
1:E:93:HIS:HD2	1:E:94:LYS:N	2.12	0.48
2:F:10:GLU:CD	2:F:67:LEU:HD21	2.33	0.48
1:C:38:HIS:CB	1:C:68:THR:HG23	2.41	0.47
1:G:64:THR:O	1:G:68:THR:HB	2.13	0.47
1:C:68:THR:CG2	1:C:69:ALA:N	2.78	0.47
1:G:108:ALA:O	1:G:112:LYS:HD3	2.13	0.47
1:A:105:PRO:O	1:A:131:LEU:HG	2.14	0.47
1:C:97:LEU:HD23	1:C:98:ALA:N	2.29	0.47
2:D:170:LEU:HD12	2:D:171:VAL:N	2.29	0.47
1:G:90:LYS:O	1:G:92:LEU:N	2.47	0.47
2:H:116:GLU:H	2:H:116:GLU:CD	2.18	0.47
2:D:14:HIS:CE1	2:D:65:PHE:HB3	2.50	0.47
1:A:121:ARG:HB3	1:A:122:PHE:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:24:LYS:CG	1:E:25:GLU:N	2.75	0.47
2:B:12:LEU:O	2:B:13:LEU:HD12	2.15	0.47
1:C:86:LEU:O	1:C:89:GLN:HG2	2.15	0.47
1:C:110:GLU:HG3	2:D:167:TYR:CD2	2.49	0.47
2:F:116:GLU:H	2:F:116:GLU:CD	2.18	0.47
2:F:60:GLN:HB3	2:F:61:PRO:HD2	1.97	0.47
1:C:111:SER:HB2	1:C:131:LEU:HD21	1.97	0.46
2:D:106:CYS:HA	2:D:159:ALA:O	2.16	0.46
1:G:24:LYS:CG	1:G:25:GLU:N	2.78	0.46
2:H:81:LYS:NZ	2:H:148:VAL:HG13	2.30	0.46
2:B:59:ILE:N	2:B:59:ILE:HD12	2.31	0.46
2:B:60:GLN:O	2:B:61:PRO:C	2.53	0.46
1:E:64:THR:O	1:E:68:THR:HB	2.15	0.46
1:C:121:ARG:HB3	1:C:122:PHE:CE1	2.51	0.46
2:D:50:THR:HG22	2:D:51:ILE:N	2.30	0.46
2:H:124:ASN:CB	2:H:125:PRO:CD	2.89	0.46
1:C:73:ARG:HB3	1:C:138:ARG:HD2	1.98	0.46
2:D:60:GLN:O	2:D:61:PRO:C	2.54	0.46
1:G:38:HIS:HA	1:G:68:THR:HG21	1.96	0.46
1:A:71:PHE:CZ	2:B:142:GLU:HG2	2.51	0.46
1:E:111:SER:HB2	1:E:131:LEU:HD21	1.97	0.46
1:C:29:ALA:HB2	2:D:5:ILE:HG22	1.98	0.46
2:D:93:ASN:ND2	2:D:95:VAL:CB	2.77	0.46
1:A:86:LEU:O	1:A:89:GLN:HG2	2.16	0.46
1:A:40:LEU:HD13	2:B:75:ILE:HD11	1.98	0.46
2:B:22:LEU:HD21	2:B:68:TYR:CZ	2.50	0.46
1:C:105:PRO:O	1:C:131:LEU:HG	2.16	0.46
1:E:87:LEU:CD2	1:E:134:ILE:HD11	2.39	0.45
2:H:10:GLU:HB3	2:H:67:LEU:CD2	2.45	0.45
1:A:111:SER:HB2	1:A:131:LEU:HD21	1.98	0.45
1:E:38:HIS:HA	1:E:68:THR:HG21	1.98	0.45
2:F:94:LYS:O	2:F:110:ARG:HD2	2.17	0.45
2:B:21:ASN:ND2	2:B:24:ASN:CB	2.79	0.45
1:E:71:PHE:CE2	2:F:86:ASP:HB3	2.50	0.45
1:G:54:GLU:HG3	2:H:28:GLN:OE1	2.16	0.45
1:A:135:GLN:HA	1:A:138:ARG:HG3	1.99	0.45
2:B:151:ARG:NH1	2:B:151:ARG:CG	2.80	0.45
2:B:93:ASN:ND2	2:B:95:VAL:CB	2.78	0.45
2:H:132:ASP:O	2:H:133:GLU:CB	2.64	0.45
2:B:50:THR:HG22	2:B:51:ILE:N	2.32	0.45
1:C:135:GLN:O	1:C:138:ARG:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:63:ARG:N	2:D:63:ARG:HD2	2.32	0.45
2:D:22:LEU:HD21	2:D:68:TYR:CZ	2.52	0.45
1:C:130:ILE:O	1:C:134:ILE:HG13	2.17	0.45
1:C:38:HIS:HA	1:C:68:THR:HG21	1.99	0.45
2:F:49:THR:HG22	2:F:50:THR:N	2.32	0.45
2:B:146:LYS:CE	2:B:165:ASP:OD2	2.61	0.45
2:D:49:THR:HG22	2:D:50:THR:OG1	2.17	0.45
2:H:11:ILE:HD13	2:H:11:ILE:HA	1.81	0.45
1:A:29:ALA:HB2	2:B:5:ILE:HG22	1.99	0.44
1:G:33:LEU:HD22	1:G:101:ALA:HB3	1.99	0.44
1:E:78:GLU:O	1:E:81:ALA:HB3	2.17	0.44
2:H:71:LYS:HB2	2:H:71:LYS:HE2	1.84	0.44
2:B:110:ARG:HE	2:F:151:ARG:NH1	2.15	0.44
1:C:30:GLU:HG3	1:C:94:LYS:HZ3	1.83	0.44
2:F:53:ASN:HD22	2:F:54:ILE:N	2.15	0.44
1:A:38:HIS:HA	1:A:68:THR:HG21	1.99	0.44
2:B:44:PHE:O	2:B:76:VAL:HA	2.17	0.44
2:B:49:THR:HG22	2:B:50:THR:OG1	2.18	0.44
2:H:53:ASN:HD22	2:H:54:ILE:N	2.14	0.44
1:A:130:ILE:O	1:A:134:ILE:HG13	2.17	0.44
1:C:135:GLN:HA	1:C:138:ARG:HG3	2.00	0.44
1:E:95:PHE:O	1:E:99:CYS:HB2	2.17	0.44
2:F:23:LEU:H	2:F:23:LEU:CD2	2.31	0.44
2:D:146:LYS:CE	2:D:165:ASP:OD2	2.60	0.44
1:C:71:PHE:CZ	2:D:142:GLU:HG2	2.52	0.44
1:G:38:HIS:CB	1:G:68:THR:HG23	2.46	0.44
2:D:110:ARG:HD3	2:H:158:PHE:CD1	2.53	0.44
2:H:60:GLN:HB3	2:H:61:PRO:HD2	2.00	0.44
1:A:52:GLU:O	1:A:53:ASP:CB	2.66	0.43
1:E:33:LEU:HD22	1:E:101:ALA:HB3	2.00	0.43
1:E:54:GLU:HG3	2:F:28:GLN:OE1	2.18	0.43
1:G:71:PHE:CE2	2:H:86:ASP:HB3	2.52	0.43
2:B:14:HIS:CE1	2:B:65:PHE:HB3	2.53	0.43
1:A:73:ARG:HB3	1:A:138:ARG:HD2	2.00	0.43
2:D:44:PHE:O	2:D:76:VAL:HA	2.17	0.43
2:B:123:SER:O	2:B:124:ASN:O	2.35	0.43
1:C:29:ALA:HB1	2:D:5:ILE:HG22	1.99	0.43
2:D:59:ILE:N	2:D:59:ILE:HD12	2.33	0.43
2:B:107:PHE:CD2	2:F:95:VAL:HG11	2.53	0.43
1:E:38:HIS:CB	1:E:68:THR:HG23	2.48	0.43
2:B:106:CYS:HA	2:B:159:ALA:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:152:VAL:HG13	2:D:152:VAL:O	2.19	0.43
2:H:122:ASN:O	2:H:123:SER:C	2.56	0.43
2:B:139:GLN:HE21	2:B:139:GLN:HB2	1.64	0.43
1:A:43:HIS:O	1:A:47:GLN:HG3	2.19	0.43
2:B:160:ILE:HD12	2:F:111:HIS:NE2	2.33	0.43
2:F:14:HIS:HA	2:F:15:PRO:HD3	1.91	0.43
2:B:92:VAL:HG11	2:B:127:CYS:HA	2.00	0.43
1:C:52:GLU:O	1:C:53:ASP:CB	2.65	0.43
1:G:91:LYS:O	1:G:121:ARG:NH1	2.47	0.43
2:H:81:LYS:HD3	2:H:148:VAL:O	2.19	0.43
1:A:123:GLU:O	1:A:124:ASP:C	2.57	0.43
1:E:85:SER:HA	1:E:88:LEU:HB2	2.01	0.43
1:E:91:LYS:O	1:E:121:ARG:NH1	2.48	0.43
2:H:132:ASP:O	2:H:133:GLU:HB3	2.19	0.43
2:H:23:LEU:N	2:H:23:LEU:CD2	2.82	0.43
1:A:93:HIS:CD2	1:A:93:HIS:C	2.93	0.42
1:A:38:HIS:CB	1:A:68:THR:HG23	2.43	0.42
2:B:63:ARG:HD2	2:B:63:ARG:N	2.34	0.42
2:D:123:SER:O	2:D:124:ASN:O	2.36	0.42
2:D:92:VAL:HG11	2:D:127:CYS:HA	2.01	0.42
2:B:110:ARG:HD3	2:F:158:PHE:CD1	2.55	0.42
1:E:26:PHE:CZ	2:F:78:ARG:HG2	2.54	0.42
2:F:132:ASP:O	2:F:133:GLU:CB	2.67	0.42
2:H:23:LEU:H	2:H:23:LEU:CD2	2.32	0.42
1:A:93:HIS:HB3	1:A:96:GLU:HG3	2.00	0.42
2:D:145:LEU:HD12	2:D:145:LEU:C	2.39	0.42
2:F:7:LEU:HB2	2:F:72:TYR:CZ	2.54	0.42
1:C:93:HIS:HD2	1:C:95:PHE:H	1.64	0.42
1:G:74:PHE:CD2	1:G:83:VAL:HG21	2.55	0.42
2:B:55:GLY:HA3	2:B:69:PRO:HG2	2.01	0.42
2:F:11:ILE:HG23	2:F:29:LYS:CG	2.50	0.42
2:F:71:LYS:HB2	2:F:71:LYS:HE2	1.86	0.42
1:G:16:ASP:H	1:G:21:ILE:HB	1.84	0.42
1:G:29:ALA:CB	2:H:5:ILE:CG2	2.98	0.42
2:H:7:LEU:HB2	2:H:72:TYR:CZ	2.55	0.42
1:G:87:LEU:CD2	1:G:134:ILE:HD11	2.42	0.42
2:H:94:LYS:O	2:H:110:ARG:HD2	2.18	0.42
2:B:145:LEU:C	2:B:145:LEU:HD12	2.40	0.42
2:F:81:LYS:HD3	2:F:148:VAL:O	2.20	0.42
1:G:85:SER:HA	1:G:88:LEU:HB2	2.01	0.42
1:C:43:HIS:O	1:C:47:GLN:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:23:LEU:N	2:F:23:LEU:CD2	2.82	0.42
1:A:29:ALA:HB1	2:B:5:ILE:HG22	1.99	0.41
2:B:116:GLU:CD	2:B:116:GLU:H	2.23	0.41
2:F:122:ASN:O	2:F:123:SER:C	2.57	0.41
2:D:151:ARG:NH1	2:H:111:HIS:ND1	2.68	0.41
1:A:96:GLU:OE2	1:A:121:ARG:NH2	2.51	0.41
2:B:93:ASN:HD22	2:B:95:VAL:CB	2.33	0.41
1:C:93:HIS:CD2	1:C:93:HIS:C	2.93	0.41
1:E:29:ALA:CB	2:F:5:ILE:CG2	2.98	0.41
1:G:111:SER:HB2	1:G:131:LEU:HD21	2.01	0.41
2:D:54:ILE:HD13	2:D:70:VAL:HG13	2.02	0.41
2:F:132:ASP:O	2:F:133:GLU:HB3	2.21	0.41
1:G:75:LYS:O	1:G:76:ASN:CB	2.68	0.41
2:D:14:HIS:HA	2:D:65:PHE:HA	2.03	0.41
1:G:78:GLU:O	1:G:81:ALA:HB3	2.20	0.41
1:G:87:LEU:HD21	1:G:134:ILE:CD1	2.42	0.41
2:H:144:ARG:CG	2:H:144:ARG:HH11	2.33	0.41
2:D:151:ARG:CG	2:D:151:ARG:NH1	2.78	0.41
2:D:4:HIS:HE1	2:D:49:THR:CB	2.34	0.41
1:C:40:LEU:HD13	2:D:75:ILE:HD11	2.03	0.41
1:E:90:LYS:HE2	1:E:130:ILE:HD11	2.03	0.41
1:E:75:LYS:O	1:E:76:ASN:CB	2.68	0.41
2:H:49:THR:HG22	2:H:50:THR:OG1	2.21	0.41
2:F:144:ARG:HH11	2:F:144:ARG:CG	2.33	0.41
1:G:26:PHE:CZ	2:H:78:ARG:HG2	2.55	0.41
2:H:92:VAL:HG13	2:H:128:TYR:CD1	2.56	0.41
1:G:68:THR:CG2	1:G:69:ALA:N	2.83	0.41
2:H:92:VAL:HG12	2:H:119:PHE:HE1	1.86	0.41
2:D:107:PHE:CD2	2:H:95:VAL:HG11	2.56	0.41
1:E:115:ILE:O	1:E:115:ILE:HG22	2.21	0.41
2:D:55:GLY:HA3	2:D:69:PRO:HG2	2.02	0.41
1:E:110:GLU:HG3	2:F:167:TYR:CD2	2.56	0.40
1:C:123:GLU:O	1:C:124:ASP:C	2.59	0.40
2:F:11:ILE:HA	2:F:11:ILE:HD13	1.79	0.40
2:F:83:GLU:HG2	2:F:85:VAL:HG13	2.02	0.40
1:E:68:THR:CG2	1:E:69:ALA:N	2.84	0.40
1:E:74:PHE:CD2	1:E:83:VAL:HG21	2.57	0.40
2:F:10:GLU:CG	2:F:67:LEU:HD21	2.51	0.40
2:F:130:THR:OG1	2:F:132:ASP:HB3	2.22	0.40
1:G:88:LEU:HD12	1:G:88:LEU:HA	1.90	0.40
2:B:14:HIS:HA	2:B:65:PHE:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:GLU:OE2	1:C:121:ARG:NH2	2.52	0.40
2:D:93:ASN:HD22	2:D:95:VAL:CB	2.35	0.40
1:E:16:ASP:H	1:E:21:ILE:HB	1.84	0.40
1:A:40:LEU:CD1	2:B:75:ILE:HD11	2.52	0.40
2:B:130:THR:C	2:B:132:ASP:N	2.75	0.40
2:B:152:VAL:HG13	2:B:152:VAL:O	2.21	0.40
2:B:8:GLU:CD	2:B:71:LYS:HG2	2.41	0.40
2:D:154:LYS:O	2:D:156:ASP:N	2.54	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	127/152 (84%)	110 (87%)	14 (11%)	3 (2%)	7	17
1	C	127/152 (84%)	111 (87%)	13 (10%)	3 (2%)	7	17
1	E	124/152 (82%)	110 (89%)	9 (7%)	5 (4%)	3	7
1	G	124/152 (82%)	111 (90%)	8 (6%)	5 (4%)	3	7
2	B	169/172 (98%)	159 (94%)	8 (5%)	2 (1%)	15	37
2	D	169/172 (98%)	161 (95%)	6 (4%)	2 (1%)	15	37
2	F	169/172 (98%)	148 (88%)	18 (11%)	3 (2%)	10	25
2	H	169/172 (98%)	146 (86%)	20 (12%)	3 (2%)	10	25
All	All	1178/1296 (91%)	1056 (90%)	96 (8%)	26 (2%)	8	20

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	LYS
1	A	140	PHE

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Mol	Chain	Res	Type
2	B	124	ASN
1	C	91	LYS
1	C	140	PHE
2	D	124	ASN
1	E	76	ASN
1	G	76	ASN
1	E	53	ASP
1	G	53	ASP
2	B	155	ASN
2	D	155	ASN
1	E	24	LYS
2	F	123	SER
1	G	24	LYS
2	H	123	SER
1	E	49	GLU
1	E	91	LYS
1	G	49	GLU
1	A	51	ALA
1	C	51	ALA
1	G	91	LYS
2	F	62	GLY
2	H	62	GLY
2	H	20	PRO
2	F	20	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	104/133 (78%)	98 (94%)	6 (6%)	23	50	
1	C	104/133 (78%)	98 (94%)	6 (6%)	23	50	
1	E	103/133 (77%)	100 (97%)	3 (3%)	48	77	
1	G	103/133 (77%)	99 (96%)	4 (4%)	37	68	
2	B	138/153 (90%)	133 (96%)	5 (4%)	40	70	

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	138/153 (90%)	133 (96%)	5 (4%)	40	70
2	F	148/153 (97%)	140 (95%)	8 (5%)	26	54
2	H	148/153 (97%)	141 (95%)	7 (5%)	30	60
All	All	986/1144 (86%)	942 (96%)	44 (4%)	32	62

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	THR
1	A	99	CYS
1	A	112	LYS
1	A	122	PHE
1	A	129	GLN
1	A	131	LEU
2	B	66	VAL
2	B	97	LEU
2	B	144	ARG
2	B	146	LYS
2	B	151	ARG
1	C	68	THR
1	C	99	CYS
1	C	112	LYS
1	C	122	PHE
1	C	129	GLN
1	C	131	LEU
2	D	66	VAL
2	D	97	LEU
2	D	144	ARG
2	D	146	LYS
2	D	151	ARG
1	E	88	LEU
1	E	112	LYS
1	E	129	GLN
2	F	12	LEU
2	F	13	LEU
2	F	53	ASN
2	F	66	VAL
2	F	97	LEU
2	F	103	PRO
2	F	144	ARG
2	F	165	ASP

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Mol	Chain	Res	Type
1	G	88	LEU
1	G	99	CYS
1	G	112	LYS
1	G	129	GLN
2	H	12	LEU
2	H	13	LEU
2	H	53	ASN
2	H	66	VAL
2	H	97	LEU
2	H	144	ARG
2	H	165	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	48	ASN
1	A	66	ASN
1	A	89	GLN
1	A	93	HIS
2	B	4	HIS
2	B	21	ASN
2	B	93	ASN
2	B	139	GLN
1	C	34	ASN
1	C	48	ASN
1	C	66	ASN
1	C	89	GLN
1	C	93	HIS
2	D	4	HIS
2	D	21	ASN
2	D	93	ASN
2	D	139	GLN
1	E	48	ASN
1	E	66	ASN
1	E	89	GLN
1	E	93	HIS
2	F	4	HIS
2	F	9	HIS
2	F	14	HIS
2	F	53	ASN
2	F	93	ASN

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Mol	Chain	Res	Type
1	G	48	ASN
1	G	66	ASN
1	G	89	GLN
1	G	93	HIS
2	H	4	HIS
2	H	9	HIS
2	H	14	HIS
2	H	53	ASN
2	H	91	GLN
2	H	93	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 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	129/152 (84%)	0.19	2 (1%) 72 73	30, 48, 73, 81	0
1	C	129/152 (84%)	0.15	1 (0%) 86 86	31, 48, 72, 81	0
1	E	126/152 (82%)	0.16	1 (0%) 86 86	32, 51, 82, 93	0
1	G	126/152 (82%)	0.30	4 (3%) 48 48	32, 50, 82, 92	0
2	B	171/172 (99%)	0.15	2 (1%) 79 80	27, 38, 64, 70	0
2	D	171/172 (99%)	0.13	1 (0%) 89 90	26, 38, 64, 70	0
2	F	171/172 (99%)	0.14	2 (1%) 79 80	30, 43, 64, 74	0
2	H	171/172 (99%)	0.21	2 (1%) 79 80	30, 43, 65, 74	0
All	All	1194/1296 (92%)	0.18	15 (1%) 77 78	26, 44, 69, 93	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	142	TYR	8.2
1	C	142	TYR	6.1
1	G	51	ALA	5.6
1	A	141	GLN	4.4
1	E	51	ALA	4.3
2	B	153	ASP	3.9
2	B	155	ASN	3.1
2	D	155	ASN	3.1
1	G	54	GLU	3.1
1	G	53	ASP	2.5
2	F	124	ASN	2.5
1	G	50	SER	2.5
2	F	131	MET	2.1
2	H	132	ASP	2.1
2	H	135	ILE	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 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.