



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2021 – 10:08 PM JST

PDB ID : 7DLX  
Title : crystal structure of H2AM4>Z-H2B  
Authors : Dai, L.C.; Zhou, Z.  
Deposited on : 2020-11-30  
Resolution : 2.40 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	:	2.20
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)	:	2.20

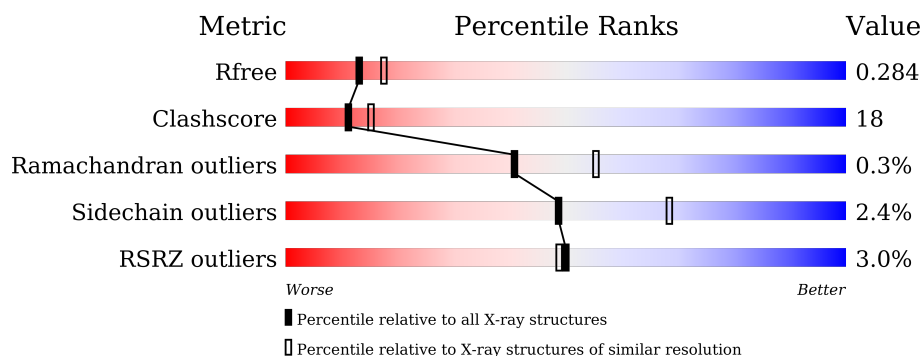
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	208	<div> <div>59%</div> <div>23%</div> <div>•</div> <div>16%</div> </div>
1	B	208	<div> <div>55%</div> <div>28%</div> <div></div> <div>17%</div> </div>
1	C	208	<div> <div>60%</div> <div>22%</div> <div>•</div> <div>16%</div> </div>
1	D	208	<div> <div>4%</div> <div>51%</div> <div>32%</div> <div>17%</div> </div>
1	E	208	<div> <div>6%</div> <div>59%</div> <div>24%</div> <div>•</div> <div>17%</div> </div>
1	F	208	<div> <div>6%</div> <div>59%</div> <div>22%</div> <div>18%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	208	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>48%</div><div>35%</div><div>17%</div></div></div>
1	H	208	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>59%</div><div>23%</div><div>17%</div></div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10856 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 Histone H2B,Histone H2A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	174	Total	C	N	O	S	0	0	0
			1357	852	250	254	1			
1	B	173	Total	C	N	O	S	0	0	0
			1348	847	249	251	1			
1	C	174	Total	C	N	O	S	0	0	0
			1357	852	250	254	1			
1	D	173	Total	C	N	O	S	0	0	0
			1353	850	249	253	1			
1	E	173	Total	C	N	O	S	0	0	0
			1353	850	249	253	1			
1	F	170	Total	C	N	O	S	0	0	0
			1325	832	246	246	1			
1	G	173	Total	C	N	O	S	0	0	0
			1353	850	249	253	1			
1	H	173	Total	C	N	O	S	0	0	0
			1353	850	249	253	1			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	MET	-	initiating methionine	UNP B3LG63
A	177	LYS	GLY	engineered mutation	UNP B3LG62
A	179	ALA	PRO	engineered mutation	UNP B3LG62
A	180	ILE	VAL	engineered mutation	UNP B3LG62
A	190	THR	ALA	engineered mutation	UNP B3LG62
A	193	VAL	ILE	engineered mutation	UNP B3LG62
B	35	MET	-	initiating methionine	UNP B3LG63
B	177	LYS	GLY	engineered mutation	UNP B3LG62
B	179	ALA	PRO	engineered mutation	UNP B3LG62
B	180	ILE	VAL	engineered mutation	UNP B3LG62
B	190	THR	ALA	engineered mutation	UNP B3LG62
B	193	VAL	ILE	engineered mutation	UNP B3LG62
C	35	MET	-	initiating methionine	UNP B3LG63

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Chain	Residue	Modelled	Actual	Comment	Reference
C	177	LYS	GLY	engineered mutation	UNP B3LG62
C	179	ALA	PRO	engineered mutation	UNP B3LG62
C	180	ILE	VAL	engineered mutation	UNP B3LG62
C	190	THR	ALA	engineered mutation	UNP B3LG62
C	193	VAL	ILE	engineered mutation	UNP B3LG62
D	35	MET	-	initiating methionine	UNP B3LG63
D	177	LYS	GLY	engineered mutation	UNP B3LG62
D	179	ALA	PRO	engineered mutation	UNP B3LG62
D	180	ILE	VAL	engineered mutation	UNP B3LG62
D	190	THR	ALA	engineered mutation	UNP B3LG62
D	193	VAL	ILE	engineered mutation	UNP B3LG62
E	35	MET	-	initiating methionine	UNP B3LG63
E	177	LYS	GLY	engineered mutation	UNP B3LG62
E	179	ALA	PRO	engineered mutation	UNP B3LG62
E	180	ILE	VAL	engineered mutation	UNP B3LG62
E	190	THR	ALA	engineered mutation	UNP B3LG62
E	193	VAL	ILE	engineered mutation	UNP B3LG62
F	35	MET	-	initiating methionine	UNP B3LG63
F	177	LYS	GLY	engineered mutation	UNP B3LG62
F	179	ALA	PRO	engineered mutation	UNP B3LG62
F	180	ILE	VAL	engineered mutation	UNP B3LG62
F	190	THR	ALA	engineered mutation	UNP B3LG62
F	193	VAL	ILE	engineered mutation	UNP B3LG62
G	35	MET	-	initiating methionine	UNP B3LG63
G	177	LYS	GLY	engineered mutation	UNP B3LG62
G	179	ALA	PRO	engineered mutation	UNP B3LG62
G	180	ILE	VAL	engineered mutation	UNP B3LG62
G	190	THR	ALA	engineered mutation	UNP B3LG62
G	193	VAL	ILE	engineered mutation	UNP B3LG62
H	35	MET	-	initiating methionine	UNP B3LG63
H	177	LYS	GLY	engineered mutation	UNP B3LG62
H	179	ALA	PRO	engineered mutation	UNP B3LG62
H	180	ILE	VAL	engineered mutation	UNP B3LG62
H	190	THR	ALA	engineered mutation	UNP B3LG62
H	193	VAL	ILE	engineered mutation	UNP B3LG62

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	10	Total O 10 10	0	0
2	B	6	Total O 6 6	0	0

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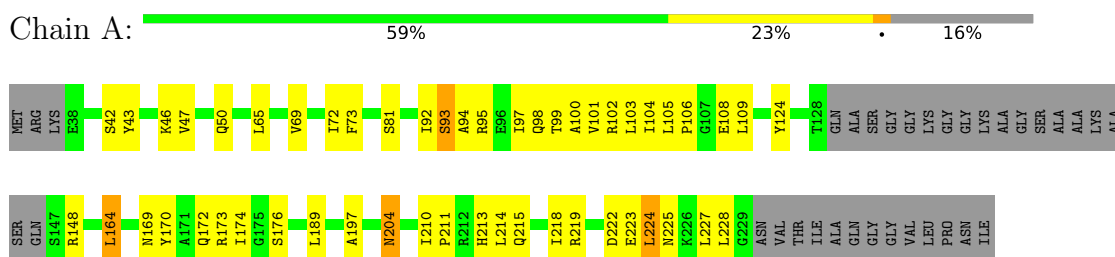
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	10	Total 10	O 10	0	0
2	D	8	Total 8	O 8	0	0
2	E	8	Total 8	O 8	0	0
2	F	4	Total 4	O 4	0	0
2	G	5	Total 5	O 5	0	0
2	H	6	Total 6	O 6	0	0

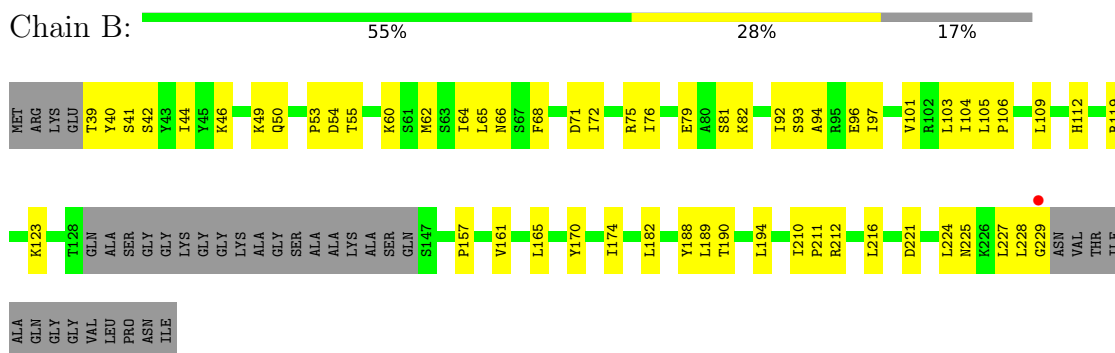
### 3 Residue-property plots

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.

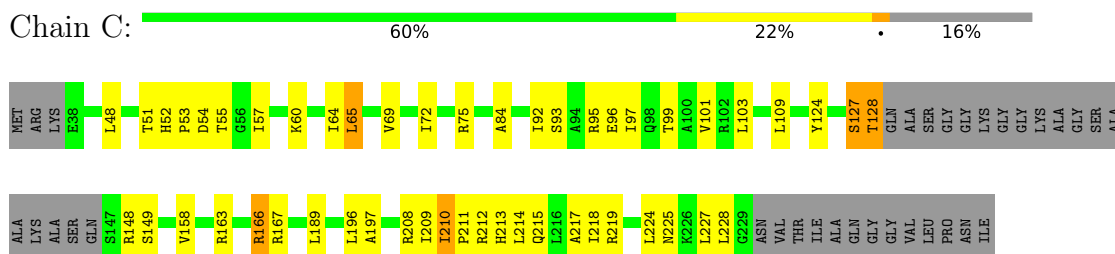
#### • Molecule 1: Histone H2B,Histone H2A



#### • Molecule 1: Histone H2B,Histone H2A

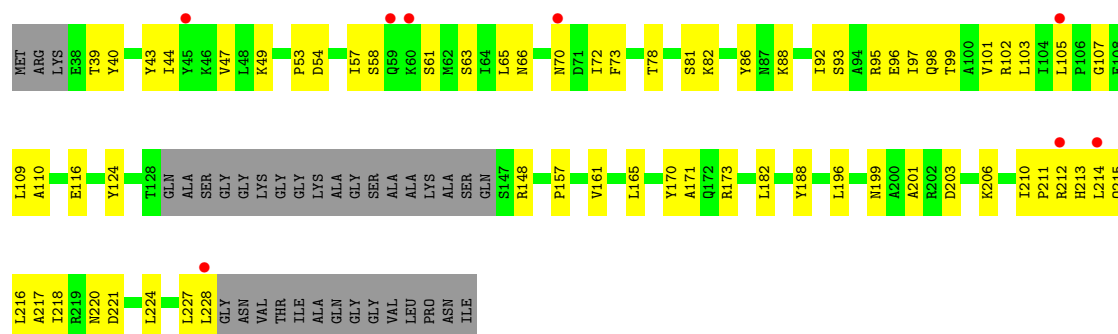


#### • Molecule 1: Histone H2B,Histone H2A

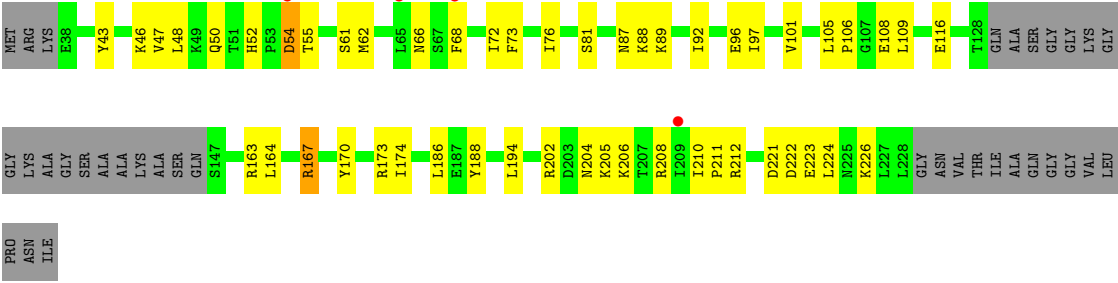


#### • Molecule 1: Histone H2B,Histone H2A









## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.58Å 73.24Å 109.68Å 90.00° 95.48° 90.00°	Depositor
Resolution (Å)	43.77 – 2.40 43.77 – 2.40	Depositor EDS
% Data completeness (in resolution range)	75.2 (43.77-2.40) 75.2 (43.77-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.27 (at 2.39Å)	Xtrriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, $R_{free}$	0.227 , 0.279 0.233 , 0.284	Depositor DCC
$R_{free}$ test set	2459 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.7	Xtrriage
Anisotropy	0.229	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 45.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10856	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.79 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7338e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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	0.81	0/1374	0.52	0/1851
1	B	0.31	0/1365	0.39	0/1839
1	C	0.48	0/1374	0.45	0/1851
1	D	0.44	0/1370	0.41	0/1846
1	E	0.28	0/1370	0.38	0/1846
1	F	0.36	0/1341	0.43	0/1806
1	G	0.39	0/1370	0.43	0/1846
1	H	0.21	0/1370	0.38	0/1846
All	All	0.45	0/10934	0.42	0/14731

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	1357	0	1412	39	0
1	B	1348	0	1406	53	0
1	C	1357	0	1412	50	0
1	D	1353	0	1409	53	0
1	E	1353	0	1409	45	0
1	F	1325	0	1387	51	0
1	G	1353	0	1409	65	0
1	H	1353	0	1409	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	10	0	0	0	0
2	B	6	0	0	1	0
2	C	10	0	0	0	0
2	D	8	0	0	0	0
2	E	8	0	0	1	0
2	F	4	0	0	0	0
2	G	5	0	0	0	0
2	H	6	0	0	0	0
All	All	10856	0	11253	394	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 18.

All (394) 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:G:52:HIS:CG	1:G:202:ARG:HH12	1.54	1.25
1:C:92:ILE:HA	1:C:96:GLU:OE1	1.45	1.16
1:D:210:ILE:HB	1:D:211:PRO:HD2	1.39	1.04
1:D:218:ILE:HD11	1:D:228:LEU:HD12	1.39	1.04
1:G:52:HIS:CG	1:G:202:ARG:NH1	2.29	1.00
1:G:198:GLY:O	1:G:202:ARG:HG3	1.61	1.00
1:F:46:LYS:O	1:F:50:GLN:HG2	1.63	0.98
1:F:43:TYR:CE1	1:F:157:PRO:HG3	2.02	0.94
1:A:224:LEU:HD22	1:A:228:LEU:HD13	1.50	0.94
1:B:41:SER:HA	1:B:62:MET:HE2	1.50	0.92
1:H:210:ILE:HG23	1:H:211:PRO:HD2	1.53	0.89
1:F:46:LYS:O	1:F:50:GLN:CG	2.21	0.88
1:F:43:TYR:CZ	1:F:157:PRO:HG2	2.08	0.88
1:F:43:TYR:CE1	1:F:157:PRO:CG	2.56	0.87
1:G:52:HIS:CD2	1:G:202:ARG:HH12	1.94	0.86
1:G:198:GLY:C	1:G:202:ARG:HE	1.81	0.83
1:F:45:TYR:CE2	1:F:49:LYS:HG3	2.15	0.82
1:G:210:ILE:HG23	1:G:211:PRO:HD2	1.62	0.81
1:B:41:SER:HA	1:B:62:MET:CE	2.12	0.79
1:C:196:LEU:HB3	1:C:217:ALA:HB1	1.67	0.77
1:F:45:TYR:CZ	1:F:49:LYS:HD2	2.20	0.76
1:A:73:PHE:CE2	1:A:164:LEU:HD23	2.21	0.76
1:F:49:LYS:HA	1:F:49:LYS:HE2	1.68	0.76
1:G:165:LEU:HB3	1:G:174:ILE:HD13	1.69	0.75
1:B:106:PRO:HD3	1:B:227:LEU:HD13	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:60:LYS:HE2	1:F:64:ILE:HD11	1.69	0.73
1:G:64:ILE:HD11	1:G:214:LEU:HD12	1.69	0.73
1:F:43:TYR:CZ	1:F:157:PRO:CG	2.71	0.72
1:B:44:ILE:HD12	1:B:62:MET:HE3	1.71	0.72
1:D:93:SER:HB3	1:D:96:GLU:OE1	1.88	0.72
1:F:43:TYR:CD1	1:F:157:PRO:HD3	2.25	0.72
1:G:39:THR:O	1:G:160:ARG:NH1	2.22	0.72
1:G:198:GLY:HA3	1:G:202:ARG:HH21	1.54	0.71
1:C:72:ILE:HD11	1:C:228:LEU:HD21	1.71	0.71
1:C:166:ARG:HH11	1:C:166:ARG:HG3	1.55	0.71
1:G:101:VAL:HG13	1:G:105:LEU:HD12	1.71	0.71
1:B:44:ILE:HB	1:B:62:MET:CE	2.21	0.70
1:A:197:ALA:HB2	1:A:214:LEU:HD23	1.73	0.70
1:B:101:VAL:HG13	1:B:105:LEU:HD12	1.72	0.70
1:G:106:PRO:CG	1:G:223:GLU:HB3	2.21	0.69
1:H:62:MET:O	1:H:66:ASN:ND2	2.24	0.69
1:G:52:HIS:CD2	1:G:202:ARG:NH1	2.57	0.69
1:A:172:GLN:O	1:A:173:ARG:HD3	1.93	0.68
1:C:210:ILE:HD12	1:C:212:ARG:H	1.58	0.68
1:D:81:SER:HB2	1:D:170:TYR:HB3	1.76	0.68
1:A:227:LEU:HD22	1:A:228:LEU:HD12	1.75	0.67
1:C:92:ILE:CA	1:C:96:GLU:OE1	2.35	0.67
1:D:212:ARG:HA	1:D:215:GLN:HG2	1.77	0.66
1:E:218:ILE:HA	1:E:224:LEU:HD12	1.77	0.66
1:F:159:GLY:O	1:F:163:ARG:HG3	1.95	0.66
1:C:210:ILE:HD11	1:C:212:ARG:CB	2.26	0.66
1:H:163:ARG:HH21	1:H:167:ARG:HH21	1.45	0.65
1:F:45:TYR:OH	1:F:49:LYS:HD2	1.96	0.64
1:D:210:ILE:HB	1:D:211:PRO:CD	2.23	0.64
1:E:218:ILE:HD13	1:E:228:LEU:HD11	1.78	0.64
1:G:93:SER:OG	1:G:95:ARG:HG2	1.98	0.64
1:A:227:LEU:HD22	1:A:228:LEU:CD1	2.27	0.64
1:G:210:ILE:CG2	1:G:211:PRO:HD2	2.28	0.64
1:E:95:ARG:NH1	2:E:301:HOH:O	2.31	0.63
1:E:90:SER:HB2	1:E:172:GLN:HB2	1.80	0.63
1:F:109:LEU:HD11	1:F:224:LEU:HD23	1.81	0.63
1:C:72:ILE:HD13	1:C:189:LEU:HD13	1.80	0.63
1:C:215:GLN:CG	1:C:219:ARG:HD3	2.29	0.63
1:D:92:ILE:HG13	1:D:171:ALA:CB	2.28	0.63
1:D:44:ILE:HG21	1:D:65:LEU:HD23	1.80	0.62
1:G:64:ILE:HD11	1:G:214:LEU:CD1	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:LEU:CB	1:C:217:ALA:HB1	2.29	0.62
1:C:215:GLN:HG2	1:C:219:ARG:HD3	1.81	0.62
1:C:215:GLN:OE1	1:C:219:ARG:NH1	2.33	0.62
1:F:46:LYS:O	1:F:50:GLN:HG3	2.00	0.61
1:B:44:ILE:HB	1:B:62:MET:HE1	1.82	0.61
1:H:48:LEU:HD13	1:H:194:LEU:HD22	1.82	0.61
1:A:124:TYR:O	1:A:124:TYR:CD1	2.53	0.61
1:H:108:GLU:HB3	1:H:223:GLU:OE1	2.00	0.61
1:D:116:GLU:HG2	1:D:188:TYR:HB2	1.83	0.61
1:F:108:GLU:N	1:F:223:GLU:OE2	2.32	0.61
1:A:124:TYR:CD1	1:A:124:TYR:C	2.73	0.61
1:C:48:LEU:HD22	1:C:57:ILE:HD11	1.83	0.61
1:E:218:ILE:HG23	1:E:224:LEU:HD12	1.83	0.61
1:G:218:ILE:HD13	1:G:228:LEU:HD12	1.82	0.61
1:D:95:ARG:NH1	1:D:95:ARG:HB2	2.16	0.60
1:F:48:LEU:HB2	1:F:194:LEU:HD13	1.83	0.60
1:B:49:LYS:HD2	1:B:53:PRO:HA	1.83	0.60
1:B:76:ILE:HA	1:B:104:ILE:CD1	2.30	0.60
1:B:76:ILE:HA	1:B:104:ILE:HD12	1.83	0.60
1:B:103:LEU:HD23	1:D:103:LEU:HD21	1.81	0.60
1:C:166:ARG:HG3	1:C:166:ARG:NH1	2.13	0.60
1:E:93:SER:OG	1:E:94:ALA:N	2.30	0.60
1:G:81:SER:HB2	1:G:170:TYR:HB3	1.82	0.60
1:B:39:THR:HG22	1:B:66:ASN:HD21	1.67	0.60
1:B:119:ARG:HH12	1:B:123:LYS:HD2	1.67	0.60
1:E:218:ILE:HD13	1:E:228:LEU:CD1	2.32	0.60
1:A:108:GLU:HB3	1:A:223:GLU:OE1	2.02	0.59
1:G:79:GLU:CB	1:G:104:ILE:HD11	2.32	0.59
1:C:197:ALA:HB2	1:C:214:LEU:HD23	1.83	0.59
1:C:127:SER:O	1:C:128:THR:C	2.39	0.59
1:A:204:ASN:O	1:A:204:ASN:ND2	2.34	0.59
1:D:220:ASN:OD1	1:D:221:ASP:N	2.36	0.59
1:G:197:ALA:CB	1:G:214:LEU:HD23	2.32	0.59
1:C:210:ILE:HD12	1:C:211:PRO:N	2.18	0.59
1:H:221:ASP:OD2	1:H:224:LEU:HG	2.03	0.59
1:H:92:ILE:HB	1:H:174:ILE:HD13	1.85	0.59
1:C:210:ILE:HD11	1:C:212:ARG:HB2	1.83	0.59
1:G:197:ALA:HB2	1:G:214:LEU:HD23	1.84	0.59
1:A:106:PRO:HG2	1:A:109:LEU:HD12	1.85	0.58
1:B:44:ILE:HB	1:B:62:MET:HE3	1.86	0.58
1:D:49:LYS:HD2	1:D:53:PRO:HA	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:46:LYS:O	1:G:50:GLN:HG3	2.02	0.58
1:G:57:ILE:HG22	1:G:209:ILE:HD12	1.85	0.58
1:G:106:PRO:HB2	1:G:223:GLU:HG2	1.86	0.58
1:E:46:LYS:O	1:E:50:GLN:HG3	2.04	0.58
1:E:201:ALA:HB2	1:E:213:HIS:ND1	2.20	0.57
1:F:165:LEU:HD11	1:F:182:LEU:HD23	1.86	0.57
1:F:211:PRO:O	1:F:215:GLN:HG2	2.03	0.57
1:H:81:SER:HB2	1:H:170:TYR:HB3	1.87	0.57
1:G:212:ARG:O	1:G:215:GLN:N	2.38	0.57
1:H:97:ILE:O	1:H:101:VAL:HG23	2.06	0.56
1:B:210:ILE:HB	1:B:211:PRO:HD2	1.87	0.56
1:C:54:ASP:OD1	1:C:55:THR:N	2.38	0.56
1:C:163:ARG:O	1:C:167:ARG:HG3	2.05	0.56
1:F:210:ILE:HB	1:F:211:PRO:HD2	1.87	0.56
1:A:227:LEU:HB3	1:A:228:LEU:HD12	1.86	0.56
1:D:105:LEU:HB3	1:D:110:ALA:HB2	1.87	0.56
1:H:55:THR:CB	1:H:202:ARG:HH21	2.19	0.56
1:H:221:ASP:HB3	1:H:224:LEU:HB2	1.88	0.56
1:F:76:ILE:HA	1:F:104:ILE:HD12	1.88	0.56
1:D:95:ARG:HB2	1:D:95:ARG:HH11	1.69	0.56
1:G:218:ILE:HD13	1:G:228:LEU:CD1	2.36	0.55
1:A:97:ILE:O	1:A:101:VAL:HG23	2.06	0.55
1:D:72:ILE:HD11	1:D:228:LEU:HD21	1.87	0.55
1:E:165:LEU:O	1:E:174:ILE:HG13	2.06	0.55
1:A:218:ILE:HG12	1:A:224:LEU:HD13	1.88	0.55
1:H:73:PHE:HD1	1:H:186:LEU:HD11	1.72	0.55
1:C:51:THR:C	1:C:53:PRO:HD3	2.27	0.55
1:C:210:ILE:O	1:C:213:HIS:N	2.40	0.55
1:H:210:ILE:CG2	1:H:211:PRO:HD2	2.32	0.54
1:B:93:SER:OG	1:B:94:ALA:N	2.35	0.54
1:G:163:ARG:HD2	1:G:167:ARG:HE	1.73	0.54
1:A:99:THR:O	1:A:103:LEU:HG	2.07	0.54
1:E:51:THR:HG23	1:E:52:HIS:HD2	1.73	0.54
1:F:51:THR:OG1	1:F:52:HIS:CE1	2.61	0.54
1:H:222:ASP:OD1	1:H:226:LYS:NZ	2.39	0.54
1:F:212:ARG:O	1:F:216:LEU:HD13	2.07	0.54
1:H:54:ASP:OD1	1:H:54:ASP:N	2.41	0.54
1:E:124:TYR:CE1	1:E:148:ARG:HG2	2.43	0.54
1:E:90:SER:HB2	1:E:172:GLN:CB	2.38	0.54
1:H:106:PRO:HG2	1:H:109:LEU:HD12	1.90	0.54
1:H:101:VAL:HG13	1:H:105:LEU:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:SER:HB2	1:A:170:TYR:HB3	1.91	0.53
1:E:51:THR:HG23	1:E:52:HIS:CD2	2.42	0.53
1:G:163:ARG:HH11	1:G:167:ARG:HE	1.54	0.53
1:G:57:ILE:HG22	1:G:209:ILE:HB	1.91	0.53
1:B:44:ILE:HG21	1:B:65:LEU:HD23	1.91	0.53
1:A:92:ILE:O	1:A:92:ILE:HG22	2.07	0.53
1:E:89:LYS:HE3	1:E:95:ARG:CZ	2.38	0.53
1:E:221:ASP:HB3	1:E:224:LEU:HB3	1.91	0.53
1:B:71:ASP:O	1:B:75:ARG:HG3	2.09	0.53
1:D:165:LEU:HD21	1:D:182:LEU:CD2	2.38	0.53
1:B:79:GLU:HB2	1:B:104:ILE:HD11	1.91	0.53
1:D:92:ILE:HG13	1:D:171:ALA:HB2	1.90	0.52
1:B:72:ILE:HD13	1:B:189:LEU:HD13	1.90	0.52
1:C:210:ILE:CD1	1:C:212:ARG:H	2.22	0.52
1:E:221:ASP:OD2	1:E:224:LEU:HB2	2.10	0.52
1:F:160:ARG:HD3	1:F:163:ARG:NH1	2.24	0.52
1:G:79:GLU:HB3	1:G:104:ILE:HD11	1.91	0.52
1:G:222:ASP:OD1	1:G:223:GLU:N	2.40	0.52
1:C:210:ILE:HB	1:C:211:PRO:HD2	1.92	0.52
1:F:45:TYR:O	1:F:49:LYS:HG2	2.10	0.52
1:A:100:ALA:O	1:A:104:ILE:HD13	2.10	0.52
1:B:42:SER:O	1:B:46:LYS:HG3	2.10	0.52
1:E:108:GLU:N	1:E:223:GLU:OE2	2.42	0.52
1:A:46:LYS:O	1:A:50:GLN:HG3	2.09	0.52
1:H:108:GLU:HB3	1:H:223:GLU:CD	2.30	0.52
1:C:75:ARG:NH2	1:C:227:LEU:HD12	2.25	0.51
1:E:172:GLN:O	1:E:173:ARG:HD3	2.09	0.51
1:D:43:TYR:CG	1:D:157:PRO:HD3	2.45	0.51
1:E:124:TYR:HE1	1:E:148:ARG:HG2	1.74	0.51
1:C:210:ILE:HD12	1:C:212:ARG:N	2.24	0.51
1:D:214:LEU:O	1:D:218:ILE:HB	2.10	0.51
1:D:43:TYR:O	1:D:47:VAL:HG23	2.10	0.51
1:F:43:TYR:CD1	1:F:157:PRO:CD	2.92	0.51
1:H:206:LYS:HE2	1:H:208:ARG:H	1.75	0.51
1:G:201:ALA:HB2	1:G:213:HIS:ND1	2.26	0.51
1:E:182:LEU:O	1:E:186:LEU:HG	2.11	0.51
1:H:92:ILE:HB	1:H:174:ILE:CD1	2.41	0.51
1:A:42:SER:O	1:A:46:LYS:HG3	2.11	0.51
1:F:72:ILE:CD1	1:F:227:LEU:HD21	2.40	0.51
1:B:165:LEU:HD11	1:B:182:LEU:HD23	1.93	0.50
1:E:60:LYS:HE2	1:E:211:PRO:HG2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:47:VAL:O	1:F:51:THR:HG22	2.10	0.50
1:A:197:ALA:CB	1:A:214:LEU:HD23	2.40	0.50
1:C:127:SER:O	1:C:128:THR:O	2.29	0.50
1:F:97:ILE:O	1:F:101:VAL:HG23	2.12	0.50
1:G:92:ILE:O	1:G:92:ILE:HG22	2.12	0.50
1:E:176:SER:O	1:E:180:ILE:HG13	2.10	0.50
1:G:124:TYR:HB2	1:G:152:ALA:HB2	1.93	0.50
1:E:108:GLU:HB3	1:E:223:GLU:OE1	2.12	0.50
1:F:57:ILE:CD1	1:F:209:ILE:HB	2.42	0.50
1:G:98:GLN:O	1:G:102:ARG:HG3	2.11	0.50
1:D:43:TYR:CE2	1:D:157:PRO:HG3	2.47	0.50
1:E:214:LEU:O	1:E:218:ILE:HG13	2.12	0.50
1:F:57:ILE:HD11	1:F:61:SER:OG	2.12	0.50
1:C:72:ILE:HD13	1:C:189:LEU:CD1	2.42	0.49
1:A:72:ILE:HD13	1:A:189:LEU:HD13	1.95	0.49
1:B:227:LEU:C	1:B:228:LEU:HD12	2.32	0.49
1:C:92:ILE:O	1:C:92:ILE:HG22	2.10	0.49
1:D:124:TYR:HE2	1:D:148:ARG:HG2	1.77	0.49
1:G:106:PRO:HG2	1:G:223:GLU:HB3	1.93	0.49
1:C:99:THR:O	1:C:103:LEU:HG	2.12	0.49
1:A:148:ARG:NH1	1:A:176:SER:OG	2.45	0.49
1:D:49:LYS:O	1:D:53:PRO:HG3	2.12	0.49
1:B:49:LYS:CD	1:B:53:PRO:HA	2.42	0.49
1:C:124:TYR:HE1	1:C:148:ARG:HG2	1.77	0.49
1:B:46:LYS:O	1:B:50:GLN:HG3	2.13	0.49
1:C:109:LEU:HD11	1:C:224:LEU:HD23	1.94	0.49
1:C:210:ILE:HD11	1:C:212:ARG:HB3	1.93	0.49
1:D:92:ILE:HG13	1:D:171:ALA:HB3	1.95	0.49
1:H:46:LYS:O	1:H:50:GLN:HG3	2.13	0.48
1:C:196:LEU:HD12	1:C:224:LEU:HD12	1.95	0.48
1:F:93:SER:N	1:F:96:GLU:OE1	2.37	0.48
1:H:108:GLU:HB3	1:H:223:GLU:OE2	2.14	0.48
1:E:95:ARG:HG3	1:E:96:GLU:N	2.28	0.48
1:G:52:HIS:CE1	1:G:202:ARG:HH12	2.30	0.48
1:G:57:ILE:HD11	1:G:62:MET:HE1	1.95	0.48
1:H:222:ASP:O	1:H:226:LYS:HG3	2.12	0.48
1:E:165:LEU:HB3	1:E:174:ILE:HG21	1.96	0.48
1:D:57:ILE:HG12	1:D:58:SER:N	2.29	0.48
1:E:60:LYS:O	1:E:64:ILE:HG13	2.13	0.48
1:B:44:ILE:CD1	1:B:62:MET:HE3	2.41	0.48
1:G:43:TYR:O	1:G:47:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ILE:CG2	1:B:194:LEU:HD11	2.43	0.48
1:B:60:LYS:O	1:B:64:ILE:HG13	2.13	0.48
1:D:49:LYS:NZ	1:D:53:PRO:O	2.25	0.48
1:F:42:SER:O	1:F:46:LYS:HG3	2.14	0.48
1:G:106:PRO:HB2	1:G:223:GLU:CG	2.44	0.48
1:B:81:SER:HB2	1:B:170:TYR:HB3	1.96	0.48
1:C:210:ILE:O	1:C:211:PRO:C	2.52	0.48
1:F:43:TYR:CE2	1:F:157:PRO:HG2	2.46	0.48
1:G:76:ILE:HA	1:G:104:ILE:CD1	2.44	0.48
1:D:40:TYR:O	1:D:44:ILE:HG13	2.14	0.47
1:G:116:GLU:HG2	1:G:188:TYR:HB2	1.95	0.47
1:H:206:LYS:NZ	1:H:208:ARG:HB3	2.28	0.47
1:B:49:LYS:NZ	1:B:55:THR:O	2.31	0.47
1:C:124:TYR:CE1	1:C:148:ARG:HG2	2.48	0.47
1:D:105:LEU:HD23	1:D:109:LEU:C	2.35	0.47
1:G:148:ARG:NH1	1:G:176:SER:OG	2.38	0.47
1:B:44:ILE:HD13	1:B:65:LEU:HG	1.95	0.47
1:B:212:ARG:O	1:B:216:LEU:HG	2.14	0.47
1:E:75:ARG:HB3	1:E:104:ILE:HD13	1.95	0.47
1:H:210:ILE:HG22	1:H:212:ARG:H	1.79	0.47
1:F:57:ILE:HD12	1:F:209:ILE:O	2.15	0.47
1:B:112:HIS:ND1	1:B:188:TYR:OH	2.44	0.47
1:C:218:ILE:O	1:C:225:ASN:HB2	2.15	0.47
1:H:106:PRO:CG	1:H:223:GLU:HB3	2.45	0.47
1:H:164:LEU:HA	1:H:167:ARG:CG	2.45	0.47
1:A:210:ILE:HG12	1:A:213:HIS:CE1	2.49	0.47
1:C:208:ARG:HD3	1:D:173:ARG:NH2	2.30	0.47
1:E:97:ILE:O	1:E:101:VAL:HG23	2.14	0.47
1:F:99:THR:O	1:F:103:LEU:HG	2.15	0.47
1:D:227:LEU:HD23	1:D:228:LEU:HG	1.95	0.47
1:C:210:ILE:HD12	1:C:210:ILE:C	2.35	0.47
1:D:196:LEU:HD12	1:D:224:LEU:HD12	1.96	0.47
1:C:84:ALA:HB2	1:C:96:GLU:CD	2.35	0.46
1:D:101:VAL:O	1:D:105:LEU:HB2	2.14	0.46
1:B:97:ILE:O	1:B:101:VAL:HG23	2.15	0.46
1:D:201:ALA:HA	1:D:213:HIS:CE1	2.51	0.46
1:D:78:THR:HG22	1:D:82:LYS:NZ	2.31	0.46
1:B:82:LYS:HB2	1:D:86:TYR:OH	2.16	0.46
1:A:73:PHE:CZ	1:A:164:LEU:HD23	2.50	0.46
1:B:44:ILE:HG23	1:B:194:LEU:HD11	1.97	0.46
1:B:68:PHE:CG	1:B:228:LEU:HD23	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:LEU:HG	1:B:228:LEU:HD12	1.98	0.46
1:B:225:ASN:OD1	1:B:229:GLY:HA3	2.16	0.46
1:H:163:ARG:NH2	1:H:167:ARG:HH21	2.11	0.46
1:A:224:LEU:HD23	1:A:224:LEU:HA	1.80	0.46
1:B:157:PRO:O	1:B:161:VAL:HG23	2.16	0.46
1:G:90:SER:HB2	1:G:172:GLN:HB2	1.98	0.46
1:A:101:VAL:HG13	1:A:105:LEU:CD1	2.46	0.46
1:D:199:ASN:O	1:D:203:ASP:N	2.49	0.46
1:G:73:PHE:HD1	1:G:186:LEU:HD11	1.81	0.46
1:A:101:VAL:HG13	1:A:105:LEU:HD12	1.98	0.45
1:E:193:VAL:HG22	1:E:224:LEU:HD21	1.97	0.45
1:H:202:ARG:C	1:H:204:ASN:H	2.19	0.45
1:F:212:ARG:HD2	1:F:216:LEU:HD13	1.98	0.45
1:A:65:LEU:O	1:A:69:VAL:HG23	2.16	0.45
1:A:93:SER:OG	1:A:94:ALA:N	2.47	0.45
1:C:60:LYS:O	1:C:64:ILE:HG13	2.15	0.45
1:C:65:LEU:O	1:C:69:VAL:HG23	2.16	0.45
1:C:84:ALA:HB2	1:C:96:GLU:OE1	2.16	0.45
1:D:124:TYR:CE2	1:D:148:ARG:HG2	2.52	0.45
1:G:93:SER:OG	1:G:96:GLU:OE1	2.32	0.45
1:H:87:ASN:O	1:H:89:LYS:HG2	2.17	0.45
1:C:65:LEU:HD12	1:C:65:LEU:HA	1.83	0.45
1:E:60:LYS:CD	1:E:211:PRO:HG2	2.46	0.45
1:B:96:GLU:N	1:B:96:GLU:OE1	2.49	0.45
1:E:92:ILE:HG13	1:E:171:ALA:HB2	1.99	0.45
1:F:160:ARG:HA	1:F:163:ARG:NH1	2.31	0.45
1:C:55:THR:CG2	1:C:209:ILE:HG13	2.46	0.45
1:H:61:SER:OG	1:H:211:PRO:HD3	2.16	0.45
1:D:93:SER:CB	1:D:96:GLU:OE1	2.60	0.44
1:D:97:ILE:O	1:D:101:VAL:HG22	2.17	0.44
1:D:215:GLN:HG3	1:D:216:LEU:N	2.32	0.44
1:G:48:LEU:HD22	1:G:57:ILE:HG23	1.99	0.44
1:D:99:THR:O	1:D:103:LEU:HG	2.17	0.44
1:E:209:ILE:HA	1:E:213:HIS:ND1	2.33	0.44
1:F:57:ILE:HD11	1:F:61:SER:CB	2.48	0.44
1:F:57:ILE:HD13	1:F:209:ILE:HB	1.99	0.44
1:D:61:SER:HB3	1:D:214:LEU:HD11	1.99	0.44
1:E:156:PHE:HB3	1:E:183:THR:HG23	1.99	0.44
1:E:209:ILE:HG23	1:E:213:HIS:HB2	1.99	0.44
1:G:202:ARG:O	1:G:205:LYS:N	2.44	0.44
1:A:210:ILE:HB	1:A:211:PRO:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:164:LEU:HD23	1:H:167:ARG:HD2	2.00	0.44
1:B:60:LYS:HD3	2:B:305:HOH:O	2.17	0.44
1:B:40:TYR:O	1:B:44:ILE:HG13	2.17	0.44
1:B:92:ILE:HD12	1:B:174:ILE:CD1	2.48	0.44
1:E:52:HIS:NE2	1:E:195:GLU:OE1	2.50	0.44
1:F:168:GLY:HA3	1:F:170:TYR:CE2	2.52	0.44
1:G:165:LEU:HB3	1:G:174:ILE:CD1	2.43	0.44
1:A:98:GLN:O	1:A:102:ARG:HG2	2.17	0.44
1:B:105:LEU:HD23	1:B:227:LEU:HD11	2.00	0.44
1:E:218:ILE:HG23	1:E:224:LEU:CD1	2.47	0.44
1:F:72:ILE:O	1:F:76:ILE:HG13	2.18	0.44
1:A:169:ASN:O	1:A:169:ASN:CG	2.55	0.44
1:F:92:ILE:O	1:F:92:ILE:HG22	2.15	0.44
1:G:43:TYR:CG	1:G:157:PRO:HD3	2.53	0.44
1:E:197:ALA:HB1	1:E:209:ILE:HG21	2.00	0.43
1:E:60:LYS:CE	1:E:211:PRO:HG2	2.47	0.43
1:E:79:GLU:O	1:E:83:LEU:HG	2.17	0.43
1:F:47:VAL:O	1:F:50:GLN:HG3	2.18	0.43
1:H:116:GLU:HG2	1:H:188:TYR:HB2	2.00	0.43
1:E:224:LEU:HD13	1:E:224:LEU:O	2.17	0.43
1:B:93:SER:O	1:B:97:ILE:HG12	2.18	0.43
1:B:119:ARG:NH1	1:B:123:LYS:HD2	2.33	0.43
1:H:72:ILE:O	1:H:76:ILE:HG13	2.18	0.43
1:F:72:ILE:HD13	1:F:227:LEU:HD21	2.01	0.43
1:G:97:ILE:O	1:G:101:VAL:HG23	2.18	0.43
1:H:68:PHE:O	1:H:72:ILE:HG12	2.18	0.43
1:D:196:LEU:HD12	1:D:224:LEU:CD1	2.49	0.43
1:E:163:ARG:HD2	1:E:167:ARG:NH1	2.33	0.43
1:A:215:GLN:HG2	1:A:219:ARG:HH12	1.83	0.43
1:D:49:LYS:CD	1:D:53:PRO:HA	2.49	0.43
1:G:48:LEU:CD2	1:G:57:ILE:HG23	2.49	0.43
1:G:93:SER:HG	1:G:95:ARG:HG2	1.83	0.43
1:H:96:GLU:OE1	1:H:96:GLU:N	2.50	0.43
1:B:221:ASP:OD2	1:B:224:LEU:HG	2.18	0.42
1:C:97:ILE:O	1:C:101:VAL:HG23	2.19	0.42
1:D:70:ASN:O	1:D:73:PHE:HB3	2.19	0.42
1:D:88:LYS:HB3	1:H:88:LYS:HZ1	1.83	0.42
1:A:106:PRO:HG3	1:A:223:GLU:O	2.20	0.42
1:B:41:SER:O	1:B:62:MET:HE1	2.19	0.42
1:C:149:SER:OG	1:C:158:VAL:HG23	2.18	0.42
1:G:108:GLU:HB3	1:G:223:GLU:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ASP:O	1:A:225:ASN:HB3	2.19	0.42
1:F:221:ASP:OD2	1:F:224:LEU:HG	2.18	0.42
1:G:42:SER:O	1:G:46:LYS:HG3	2.18	0.42
1:G:47:VAL:HA	1:G:50:GLN:CD	2.40	0.42
1:A:43:TYR:O	1:A:47:VAL:HG23	2.20	0.42
1:D:196:LEU:CB	1:D:217:ALA:HB1	2.50	0.42
1:F:43:TYR:CD1	1:F:157:PRO:CG	3.01	0.42
1:G:72:ILE:HG21	1:G:189:LEU:CD1	2.50	0.42
1:G:105:LEU:HD23	1:G:227:LEU:CD1	2.50	0.42
1:G:168:GLY:HA3	1:G:170:TYR:CE2	2.55	0.42
1:F:156:PHE:HA	1:F:157:PRO:HD3	1.75	0.42
1:B:44:ILE:HG12	1:B:190:THR:HG21	2.01	0.42
1:B:165:LEU:HD21	1:B:182:LEU:CD2	2.50	0.42
1:D:73:PHE:HE1	1:D:161:VAL:HG13	1.85	0.42
1:B:109:LEU:HD11	1:B:224:LEU:HD23	2.01	0.41
1:H:52:HIS:CD2	1:H:202:ARG:HH22	2.38	0.41
1:D:206:LYS:HE2	1:D:206:LYS:HB2	1.89	0.41
1:F:57:ILE:HD11	1:F:61:SER:HB3	2.02	0.41
1:B:93:SER:HB3	1:B:96:GLU:OE1	2.20	0.41
1:F:221:ASP:HB3	1:F:224:LEU:HB2	2.02	0.41
1:C:215:GLN:HG3	1:C:219:ARG:HD3	2.02	0.41
1:F:43:TYR:CG	1:F:157:PRO:HD3	2.55	0.41
1:D:215:GLN:O	1:D:218:ILE:HG22	2.20	0.41
1:G:105:LEU:HD23	1:G:227:LEU:HD13	2.03	0.41
1:G:192:GLU:O	1:G:195:GLU:HB3	2.21	0.41
1:H:43:TYR:O	1:H:47:VAL:HG23	2.21	0.41
1:G:57:ILE:CG2	1:G:209:ILE:HD12	2.48	0.41
1:C:52:HIS:N	1:C:53:PRO:HD3	2.36	0.41
1:C:215:GLN:O	1:C:219:ARG:HB2	2.21	0.41
1:D:98:GLN:O	1:D:102:ARG:HG3	2.21	0.41
1:G:73:PHE:HE1	1:G:161:VAL:HG13	1.86	0.41
1:H:204:ASN:O	1:H:205:LYS:HG2	2.21	0.41
1:G:68:PHE:O	1:G:72:ILE:HG12	2.21	0.41
1:D:39:THR:HA	1:D:66:ASN:HD21	1.86	0.40
1:H:173:ARG:HA	1:H:173:ARG:HD3	1.86	0.40
1:A:174:ILE:HD12	1:A:174:ILE:HG23	1.73	0.40
1:G:149:SER:OG	1:G:158:VAL:HG23	2.21	0.40
1:A:228:LEU:HD12	1:A:228:LEU:N	2.37	0.40
1:E:60:LYS:HD3	1:E:211:PRO:HG2	2.03	0.40
1:E:165:LEU:HD11	1:E:182:LEU:HD23	2.03	0.40
1:H:163:ARG:HH21	1:H:167:ARG:NH2	2.16	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	170/208 (82%)	167 (98%)	3 (2%)	0	100	100
1	B	169/208 (81%)	165 (98%)	3 (2%)	1 (1%)	25	36
1	C	170/208 (82%)	167 (98%)	3 (2%)	0	100	100
1	D	169/208 (81%)	163 (96%)	5 (3%)	1 (1%)	25	36
1	E	169/208 (81%)	162 (96%)	7 (4%)	0	100	100
1	F	166/208 (80%)	158 (95%)	6 (4%)	2 (1%)	13	19
1	G	169/208 (81%)	162 (96%)	7 (4%)	0	100	100
1	H	169/208 (81%)	161 (95%)	8 (5%)	0	100	100
All	All	1351/1664 (81%)	1305 (97%)	42 (3%)	4 (0%)	41	55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	107	GLY
1	F	51	THR
1	B	54	ASP
1	D	107	GLY

### 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	145/166 (87%)	140 (97%)	5 (3%)	37	56
1	B	144/166 (87%)	144 (100%)	0	100	100
1	C	145/166 (87%)	138 (95%)	7 (5%)	25	41
1	D	145/166 (87%)	143 (99%)	2 (1%)	67	82
1	E	145/166 (87%)	140 (97%)	5 (3%)	37	56
1	F	142/166 (86%)	139 (98%)	3 (2%)	53	72
1	G	145/166 (87%)	141 (97%)	4 (3%)	43	63
1	H	145/166 (87%)	143 (99%)	2 (1%)	67	82
All	All	1156/1328 (87%)	1128 (98%)	28 (2%)	49	68

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	SER
1	A	95	ARG
1	A	164	LEU
1	A	204	ASN
1	A	224	LEU
1	C	65	LEU
1	C	93	SER
1	C	95	ARG
1	C	127	SER
1	C	128	THR
1	C	166	ARG
1	C	210	ILE
1	D	54	ASP
1	D	63	SER
1	E	93	SER
1	E	128	THR
1	E	169	ASN
1	E	210	ILE
1	E	224	LEU
1	F	50	GLN
1	F	51	THR
1	F	169	ASN
1	G	54	ASP
1	G	65	LEU
1	G	66	ASN
1	G	169	ASN
1	H	54	ASP

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Mol	Chain	Res	Type
1	H	167	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides 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	174/208 (83%)	-0.06	0 100 100	19, 35, 57, 90	0
1	B	173/208 (83%)	0.14	1 (0%) 89 88	23, 46, 73, 107	0
1	C	174/208 (83%)	0.06	0 100 100	20, 38, 72, 108	0
1	D	173/208 (83%)	0.27	8 (4%) 32 31	23, 49, 93, 121	0
1	E	173/208 (83%)	0.39	12 (6%) 16 15	23, 47, 91, 121	0
1	F	170/208 (81%)	0.36	13 (7%) 13 12	27, 50, 113, 161	0
1	G	173/208 (83%)	0.20	4 (2%) 60 58	23, 53, 95, 128	0
1	H	173/208 (83%)	0.26	4 (2%) 60 58	26, 53, 103, 140	0
All	All	1383/1664 (83%)	0.20	42 (3%) 50 49	19, 46, 92, 161	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	44	ILE	4.6
1	F	43	TYR	4.6
1	F	49	LYS	4.5
1	D	228	LEU	4.4
1	F	42	SER	4.3
1	E	198	GLY	4.1
1	F	202	ARG	3.5
1	F	41	SER	3.4
1	E	48	LEU	3.3
1	E	205	LYS	3.2
1	G	216	LEU	3.2
1	B	229	GLY	3.1
1	H	54	ASP	3.1
1	D	45	TYR	3.0
1	D	214	LEU	3.0
1	G	212	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	64	ILE	3.0
1	E	207	THR	2.9
1	F	50	GLN	2.9
1	H	65	LEU	2.9
1	F	48	LEU	2.8
1	F	45	TYR	2.8
1	E	38	GLU	2.8
1	F	47	VAL	2.8
1	E	50	GLN	2.7
1	E	55	THR	2.7
1	E	45	TYR	2.6
1	H	68	PHE	2.5
1	D	212	ARG	2.5
1	D	60	LYS	2.5
1	G	68	PHE	2.4
1	D	105	LEU	2.3
1	F	52	HIS	2.3
1	E	208	ARG	2.3
1	E	214	LEU	2.2
1	D	70	ASN	2.2
1	F	95	ARG	2.2
1	H	209	ILE	2.1
1	F	51	THR	2.1
1	E	41	SER	2.0
1	E	57	ILE	2.0
1	D	59	GLN	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 monosaccharides 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.