



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:30 PM GMT

PDB ID : 4IJS  
Title : Crystal structure of nucleocapsid protein encoded by the prototypic member of orthobunyavirus  
Authors : Li, B.B.; Wang, Q.; Lou, Z.Y.  
Deposited on : 2012-12-23  
Resolution : 3.20 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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

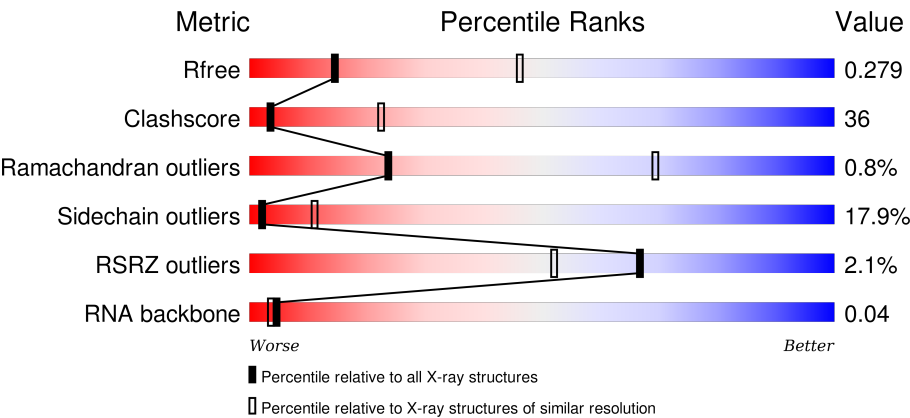
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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 <sub>free</sub>	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)
RNA backbone	2183	1079 (3.70-2.70)

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	248	<div><div></div><div>47%37%8%6%</div></div>
1	B	248	<div><div>2%</div><div>45%38%10%6%</div></div>
1	C	248	<div><div>3%</div><div>40%41%12%6%</div></div>
1	D	248	<div><div>2%</div><div>36%45%13%6%</div></div>

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Mol	Chain	Length	Quality of chain
2	E	10	<div><div></div><div></div><div></div><div></div></div> <div>10%50%30%10%</div>
2	F	10	<div><div></div><div></div><div></div><div></div></div> <div>20%50%20%10%</div>
2	G	10	<div><div></div><div></div><div></div><div></div></div> <div>10%50%30%10%</div>
2	H	10	<div><div></div><div></div><div></div><div></div></div> <div>20%70%10%</div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8298 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 Nucleoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	232	Total	C	N	O	S	0	0	0
			1865	1205	315	339	6			
1	B	232	Total	C	N	O	S	0	0	0
			1865	1205	315	339	6			
1	C	232	Total	C	N	O	S	0	0	0
			1865	1205	315	339	6			
1	D	232	Total	C	N	O	S	0	0	0
			1865	1205	315	339	6			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	MET	-	EXPRESSION TAG	UNP P16495
A	-13	ARG	-	EXPRESSION TAG	UNP P16495
A	-12	GLY	-	EXPRESSION TAG	UNP P16495
A	-11	SER	-	EXPRESSION TAG	UNP P16495
A	-10	HIS	-	EXPRESSION TAG	UNP P16495
A	-9	HIS	-	EXPRESSION TAG	UNP P16495
A	-8	HIS	-	EXPRESSION TAG	UNP P16495
A	-7	HIS	-	EXPRESSION TAG	UNP P16495
A	-6	HIS	-	EXPRESSION TAG	UNP P16495
A	-5	HIS	-	EXPRESSION TAG	UNP P16495
A	-4	GLY	-	EXPRESSION TAG	UNP P16495
A	-3	SER	-	EXPRESSION TAG	UNP P16495
A	-2	ILE	-	EXPRESSION TAG	UNP P16495
A	-1	GLU	-	EXPRESSION TAG	UNP P16495
A	0	GLY	-	EXPRESSION TAG	UNP P16495
A	1	ARG	-	EXPRESSION TAG	UNP P16495
A	83	SER	ASN	ENGINEERED MUTATION	UNP P16495
B	-14	MET	-	EXPRESSION TAG	UNP P16495
B	-13	ARG	-	EXPRESSION TAG	UNP P16495
B	-12	GLY	-	EXPRESSION TAG	UNP P16495
B	-11	SER	-	EXPRESSION TAG	UNP P16495

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	HIS	-	EXPRESSION TAG	UNP P16495
B	-9	HIS	-	EXPRESSION TAG	UNP P16495
B	-8	HIS	-	EXPRESSION TAG	UNP P16495
B	-7	HIS	-	EXPRESSION TAG	UNP P16495
B	-6	HIS	-	EXPRESSION TAG	UNP P16495
B	-5	HIS	-	EXPRESSION TAG	UNP P16495
B	-4	GLY	-	EXPRESSION TAG	UNP P16495
B	-3	SER	-	EXPRESSION TAG	UNP P16495
B	-2	ILE	-	EXPRESSION TAG	UNP P16495
B	-1	GLU	-	EXPRESSION TAG	UNP P16495
B	0	GLY	-	EXPRESSION TAG	UNP P16495
B	1	ARG	-	EXPRESSION TAG	UNP P16495
B	83	SER	ASN	ENGINEERED MUTATION	UNP P16495
C	-14	MET	-	EXPRESSION TAG	UNP P16495
C	-13	ARG	-	EXPRESSION TAG	UNP P16495
C	-12	GLY	-	EXPRESSION TAG	UNP P16495
C	-11	SER	-	EXPRESSION TAG	UNP P16495
C	-10	HIS	-	EXPRESSION TAG	UNP P16495
C	-9	HIS	-	EXPRESSION TAG	UNP P16495
C	-8	HIS	-	EXPRESSION TAG	UNP P16495
C	-7	HIS	-	EXPRESSION TAG	UNP P16495
C	-6	HIS	-	EXPRESSION TAG	UNP P16495
C	-5	HIS	-	EXPRESSION TAG	UNP P16495
C	-4	GLY	-	EXPRESSION TAG	UNP P16495
C	-3	SER	-	EXPRESSION TAG	UNP P16495
C	-2	ILE	-	EXPRESSION TAG	UNP P16495
C	-1	GLU	-	EXPRESSION TAG	UNP P16495
C	0	GLY	-	EXPRESSION TAG	UNP P16495
C	1	ARG	-	EXPRESSION TAG	UNP P16495
C	83	SER	ASN	ENGINEERED MUTATION	UNP P16495
D	-14	MET	-	EXPRESSION TAG	UNP P16495
D	-13	ARG	-	EXPRESSION TAG	UNP P16495
D	-12	GLY	-	EXPRESSION TAG	UNP P16495
D	-11	SER	-	EXPRESSION TAG	UNP P16495
D	-10	HIS	-	EXPRESSION TAG	UNP P16495
D	-9	HIS	-	EXPRESSION TAG	UNP P16495
D	-8	HIS	-	EXPRESSION TAG	UNP P16495
D	-7	HIS	-	EXPRESSION TAG	UNP P16495
D	-6	HIS	-	EXPRESSION TAG	UNP P16495
D	-5	HIS	-	EXPRESSION TAG	UNP P16495
D	-4	GLY	-	EXPRESSION TAG	UNP P16495
D	-3	SER	-	EXPRESSION TAG	UNP P16495

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	ILE	-	EXPRESSION TAG	UNP P16495
D	-1	GLU	-	EXPRESSION TAG	UNP P16495
D	0	GLY	-	EXPRESSION TAG	UNP P16495
D	1	ARG	-	EXPRESSION TAG	UNP P16495
D	83	SER	ASN	ENGINEERED MUTATION	UNP P16495

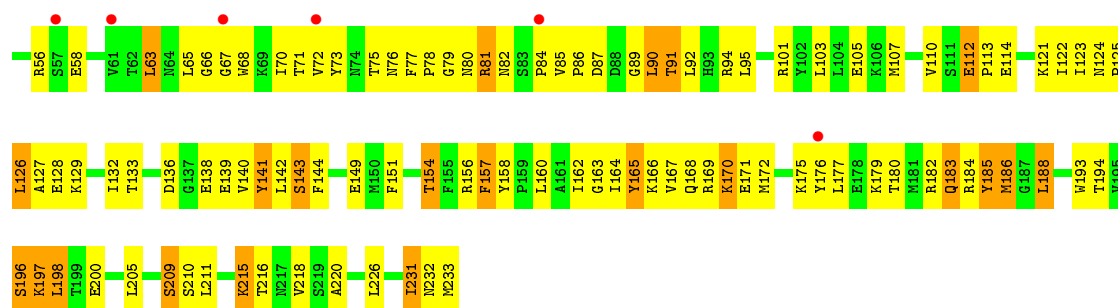
- Molecule 2 is a RNA chain called RNA (5'-R(P\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	10	Total	C	N	O	P	0	0	0
			220	100	50	60	10			
2	F	9	Total	C	N	O	P	0	0	0
			198	90	45	54	9			
2	G	9	Total	C	N	O	P	0	0	0
			198	90	45	54	9			
2	H	9	Total	C	N	O	P	0	0	0
			198	90	45	54	9			

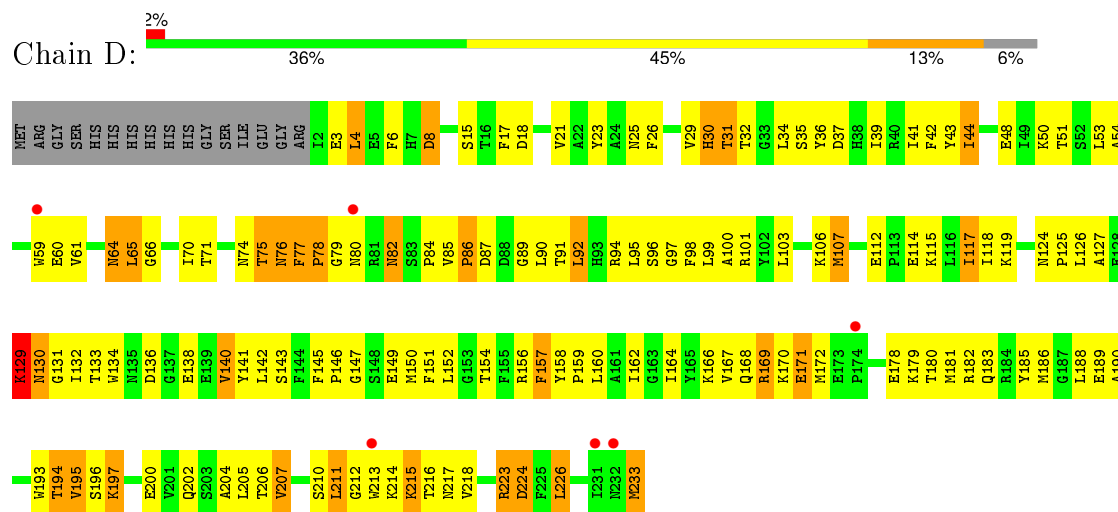
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total	O	0	0
			10	10		
3	B	6	Total	O	0	0
			6	6		
3	C	3	Total	O	0	0
			3	3		
3	D	2	Total	O	0	0
			2	2		
3	E	1	Total	O	0	0
			1	1		
3	H	2	Total	O	0	0
			2	2		

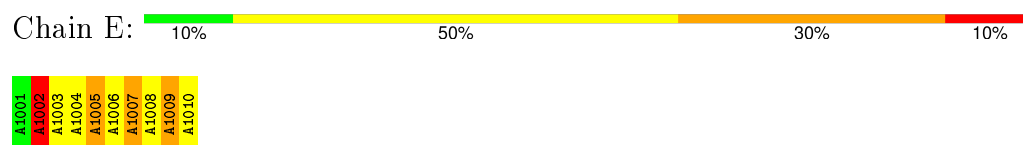




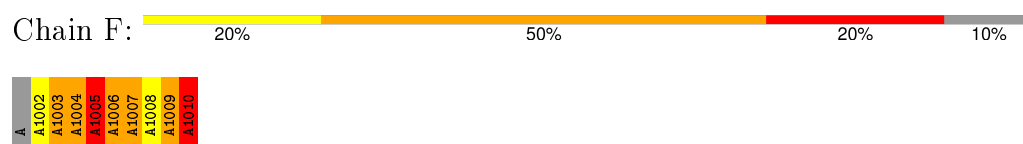
• Molecule 1: Nucleoprotein



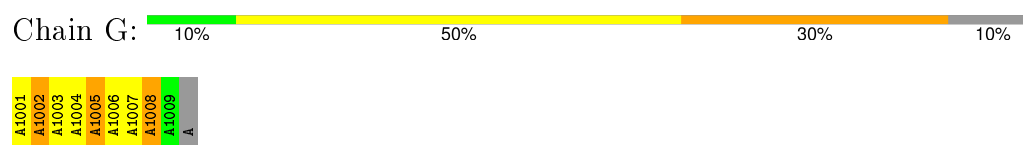
• Molecule 2: RNA (5'-R(P\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*A)-3')



• Molecule 2: RNA (5'-R(P\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*A)-3')



• Molecule 2: RNA (5'-R(P\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*A)-3')



• Molecule 2: RNA (5'-R(P\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*A)-3')





A1001
A1002
A1003
A1004
A1005
A1006
A1007
A1008
A1009
A

## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.14Å 106.14Å 485.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.75 – 3.20 47.17 – 3.19	Depositor EDS
% Data completeness (in resolution range)	90.4 (40.75-3.20) 97.5 (47.17-3.19)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.76 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.220 , 0.276 0.248 , 0.279	Depositor DCC
$R_{free}$ test set	1189 reflections (5.16%)	DCC
Wilson B-factor (Å <sup>2</sup> )	93.4	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 70.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 23462 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	8298	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.80	1/1909 (0.1%)	0.89	7/2581 (0.3%)
1	B	0.75	1/1909 (0.1%)	0.85	6/2581 (0.2%)
1	C	0.60	0/1909	0.77	3/2581 (0.1%)
1	D	0.75	1/1909 (0.1%)	0.86	5/2581 (0.2%)
2	E	1.15	2/249 (0.8%)	1.57	6/386 (1.6%)
2	F	1.01	2/224 (0.9%)	1.52	1/347 (0.3%)
2	G	0.93	1/224 (0.4%)	1.09	1/347 (0.3%)
2	H	0.65	0/224	1.09	0/347
All	All	0.76	8/8557 (0.1%)	0.92	29/11751 (0.2%)

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1005	A	N9-C4	7.59	1.42	1.37
2	E	1005	A	N9-C4	6.75	1.41	1.37
2	E	1005	A	N3-C4	6.17	1.38	1.34
1	D	78	PRO	N-CD	5.59	1.55	1.47
1	B	86	PRO	N-CD	5.44	1.55	1.47
2	F	1010	A	N9-C4	5.43	1.41	1.37
2	F	1005	A	N9-C4	5.41	1.41	1.37
1	A	78	PRO	N-CD	5.19	1.55	1.47

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	68	TRP	N-CA-C	-8.59	87.81	111.00
2	E	1007	A	O5'-P-OP1	-8.52	98.04	105.70
1	A	34	LEU	CB-CA-C	7.86	125.12	110.20
1	C	215	LYS	CB-CA-C	-6.93	96.54	110.40
1	A	34	LEU	N-CA-C	-6.68	92.95	111.00
1	D	169	ARG	N-CA-C	-6.33	93.92	111.00
1	B	63	LEU	CA-CB-CG	6.09	129.31	115.30
1	A	83	SER	C-N-CD	5.99	140.98	128.40
1	A	77	PHE	C-N-CD	5.88	140.76	128.40
1	B	67	GLY	N-CA-C	-5.85	98.47	113.10
2	E	1002	A	C8-N9-C4	5.81	108.12	105.80
1	B	85	VAL	C-N-CD	5.79	140.56	128.40
1	B	83	SER	C-N-CD	5.71	140.38	128.40
2	E	1005	A	C2-N3-C4	5.64	113.42	110.60
1	A	29	VAL	N-CA-CB	5.62	123.87	111.50
1	B	80	ASN	CB-CA-C	-5.62	99.17	110.40
1	C	34	LEU	CA-CB-CG	5.61	128.21	115.30
2	E	1005	A	N3-C4-N9	5.58	131.86	127.40
2	G	1005	A	C2-N3-C4	5.56	113.38	110.60
2	E	1005	A	C5-C6-N6	-5.53	119.27	123.70
1	C	215	LYS	N-CA-C	5.53	125.93	111.00
1	A	157	PHE	CB-CA-C	-5.51	99.39	110.40
1	D	129	LYS	N-CA-C	-5.41	96.39	111.00
1	D	170	LYS	N-CA-C	5.36	125.48	111.00
2	F	1005	A	C2-N3-C4	5.34	113.27	110.60
1	D	77	PHE	C-N-CD	5.29	139.52	128.40
1	D	170	LYS	CB-CA-C	-5.27	99.86	110.40
2	E	1005	A	N1-C6-N6	5.20	121.72	118.60
1	A	12	ASN	N-CA-C	5.01	124.54	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	33	GLY	Peptide
1	A	65	LEU	Peptide
1	B	82	ASN	Peptide
1	C	12	ASN	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	1865	0	1878	136	0
1	B	1865	0	1878	148	1
1	C	1865	0	1878	136	0
1	D	1865	0	1878	149	0
2	E	220	0	111	2	0
2	F	198	0	100	16	0
2	G	198	0	100	15	0
2	H	198	0	100	8	0
3	A	10	0	0	0	0
3	B	6	0	0	1	0
3	C	3	0	0	0	0
3	D	2	0	0	0	0
3	E	1	0	0	0	0
3	H	2	0	0	0	0
All	All	8298	0	7923	583	1

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 36.

All (583) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:PHE:CE2	1:C:185:TYR:CE1	1.94	1.55
1:C:157:PHE:CZ	1:C:185:TYR:CD1	2.01	1.47
1:D:169:ARG:NH2	1:D:215:LYS:HG2	1.08	1.39
1:D:169:ARG:NH2	1:D:215:LYS:CG	1.82	1.38
1:C:157:PHE:CE2	1:C:185:TYR:HE1	1.35	1.35
1:B:64:ASN:ND2	1:B:69:LYS:HE2	1.36	1.35
1:C:157:PHE:CD2	1:C:185:TYR:HE1	1.47	1.32
1:B:64:ASN:HD21	1:B:69:LYS:CE	1.43	1.29
1:C:157:PHE:CZ	1:C:185:TYR:HD1	1.41	1.25
1:D:215:LYS:O	1:D:216:THR:HG22	1.35	1.24
1:A:30:HIS:O	1:A:31:THR:HG22	1.38	1.23
1:B:226:LEU:O	1:B:231:ILE:O	1.61	1.18
1:B:224:ASP:O	1:B:227:ALA:N	1.81	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:TYR:OH	1:D:96:SER:O	1.67	1.13
1:A:38:HIS:HD2	1:A:68:TRP:HB3	1.17	1.06
1:C:12:ASN:HB3	1:C:13:THR:HA	1.37	1.05
1:C:157:PHE:CE1	1:C:185:TYR:HD1	1.73	1.04
1:A:58:GLU:OE1	1:A:58:GLU:N	1.89	1.04
1:A:38:HIS:CD2	1:A:68:TRP:CB	2.40	1.04
1:D:130:ASN:OD1	1:D:131:GLY:N	1.90	1.04
1:C:188:LEU:HD12	1:C:193:TRP:HB3	1.40	1.03
1:A:38:HIS:HD2	1:A:68:TRP:CB	1.69	1.03
1:C:232:ASN:ND2	1:C:233:MET:N	2.07	1.01
1:B:224:ASP:OD1	1:B:225:PHE:N	1.93	1.00
1:A:38:HIS:CD2	1:A:68:TRP:HB2	1.96	1.00
1:A:30:HIS:O	1:A:31:THR:CG2	2.10	1.00
1:B:17:PHE:HE2	1:B:94:ARG:CZ	1.74	1.00
1:D:169:ARG:HH22	1:D:215:LYS:HG3	1.25	0.99
1:C:157:PHE:CZ	1:C:185:TYR:CE1	2.37	0.98
1:D:169:ARG:HH22	1:D:215:LYS:CG	1.54	0.97
1:D:207:VAL:O	1:D:210:SER:OG	1.82	0.95
1:A:200:GLU:OE1	1:A:200:GLU:N	2.01	0.94
1:C:185:TYR:HD2	1:C:186:MET:HB2	1.32	0.94
1:D:75:THR:O	1:D:80:ASN:HB3	1.64	0.94
1:D:215:LYS:O	1:D:216:THR:CG2	2.14	0.94
1:A:38:HIS:CD2	1:A:68:TRP:HB3	2.02	0.93
1:B:92:LEU:HD23	1:B:92:LEU:H	1.32	0.93
1:B:17:PHE:CE2	1:B:94:ARG:NH1	2.38	0.91
1:A:35:SER:CB	1:A:38:HIS:ND1	2.33	0.91
1:C:157:PHE:CD2	1:C:185:TYR:CE1	2.39	0.90
1:B:17:PHE:CE2	1:B:94:ARG:CZ	2.55	0.89
1:B:182:ARG:NH1	2:F:1003:A:OP2	2.04	0.88
1:C:157:PHE:CE1	1:C:185:TYR:CD1	2.55	0.88
1:C:81:ARG:NH2	2:G:1001:A:N6	2.22	0.87
1:C:196:SER:OG	1:C:197:LYS:CD	2.24	0.86
1:C:185:TYR:CD2	1:C:186:MET:HB2	2.12	0.85
1:D:96:SER:HB3	1:D:146:PRO:O	1.75	0.84
1:C:4:LEU:H	1:C:4:LEU:HD22	1.43	0.84
1:D:188:LEU:O	1:D:193:TRP:HD1	1.62	0.83
1:C:3:GLU:HG2	1:C:4:LEU:CD1	2.09	0.82
1:C:81:ARG:NH2	2:G:1001:A:H61	1.78	0.82
1:B:222:ALA:O	1:B:226:LEU:HD23	1.80	0.82
1:A:57:SER:N	1:A:58:GLU:OE1	2.12	0.82
1:C:81:ARG:HH22	2:G:1001:A:N6	1.77	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:ASP:CG	1:D:211:LEU:HD11	2.00	0.82
1:B:227:ALA:O	1:B:229:PHE:N	2.12	0.81
1:A:63:LEU:CD1	1:A:65:LEU:HD21	2.11	0.81
1:A:13:THR:HB	1:C:67:GLY:N	1.94	0.81
1:B:72:VAL:HG12	1:B:90:LEU:HD11	1.60	0.81
1:C:196:SER:OG	1:C:197:LYS:HD2	1.82	0.80
1:A:198:LEU:O	1:A:198:LEU:HD12	1.81	0.80
1:B:226:LEU:C	1:B:231:ILE:O	2.22	0.78
1:A:34:LEU:HD12	1:A:35:SER:N	1.99	0.78
1:C:3:GLU:CB	1:C:4:LEU:HD13	2.13	0.78
1:C:129:LYS:HG3	2:G:1008:A:H5"	1.64	0.78
1:A:80:ASN:CG	1:A:82:ASN:H	1.87	0.78
1:D:129:LYS:HD3	1:D:130:ASN:N	1.99	0.78
1:C:22:ALA:HB2	1:C:87:ASP:HB2	1.66	0.78
1:D:156:ARG:O	1:D:157:PHE:HB2	1.82	0.77
1:A:30:HIS:HB3	1:A:68:TRP:HH2	1.49	0.77
1:A:35:SER:CB	1:A:38:HIS:CE1	2.66	0.77
1:D:89:GLY:O	1:D:94:ARG:NH1	2.18	0.77
1:A:166:LYS:HD2	1:A:172:MET:HE3	1.66	0.76
1:D:169:ARG:HH21	1:D:215:LYS:CG	1.68	0.76
1:B:80:ASN:O	1:B:81:ARG:HG2	1.85	0.76
1:C:185:TYR:O	1:C:188:LEU:HG	1.85	0.76
1:B:17:PHE:O	1:B:19:PRO:HD3	1.86	0.76
1:D:215:LYS:C	1:D:216:THR:HG22	2.06	0.75
1:C:128:GLU:OE1	1:C:133:THR:HG22	1.87	0.75
1:D:64:ASN:ND2	1:D:66:GLY:O	2.20	0.75
1:D:125:PRO:O	1:D:129:LYS:HB2	1.86	0.75
1:C:232:ASN:HD22	1:C:233:MET:N	1.83	0.75
1:D:166:LYS:HB3	1:D:172:MET:HB2	1.68	0.74
1:C:3:GLU:HB3	1:C:4:LEU:HD13	1.67	0.74
1:A:80:ASN:OD1	1:A:82:ASN:N	2.21	0.74
1:A:80:ASN:HB2	1:A:82:ASN:N	2.02	0.74
1:D:42:PHE:HB2	1:D:65:LEU:HD13	1.68	0.74
1:C:188:LEU:CD1	1:C:193:TRP:HB3	2.16	0.74
1:B:64:ASN:HD21	1:B:69:LYS:HE2	0.60	0.74
1:D:124:ASN:HB3	1:D:145:PHE:CE1	2.22	0.74
1:D:185:TYR:O	1:D:186:MET:HG2	1.87	0.73
1:D:211:LEU:O	1:D:213:TRP:HB2	1.89	0.73
1:A:13:THR:OG1	1:A:14:SER:N	2.22	0.73
1:A:91:THR:HB	1:A:94:ARG:HG3	1.70	0.73
1:A:103:LEU:HD22	1:A:118:ILE:HD11	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:PRO:HB2	1:B:87:ASP:OD1	1.88	0.72
1:A:80:ASN:HB2	1:A:82:ASN:H	1.55	0.72
1:C:4:LEU:HD13	1:C:4:LEU:N	2.04	0.72
1:A:41:ILE:HG21	1:A:65:LEU:HB2	1.71	0.72
1:A:80:ASN:CB	1:A:82:ASN:H	2.03	0.71
1:D:212:GLY:HA2	1:D:213:TRP:HB2	1.72	0.71
1:B:64:ASN:ND2	1:B:69:LYS:HG2	2.05	0.71
1:B:64:ASN:CG	1:B:69:LYS:HG2	2.11	0.71
1:B:92:LEU:HD23	1:B:92:LEU:N	2.04	0.71
1:D:112:GLU:OE2	1:D:115:LYS:NZ	2.24	0.71
1:C:164:ILE:O	1:C:168:GLN:HG3	1.91	0.71
1:B:226:LEU:HD22	1:B:226:LEU:N	2.05	0.71
1:A:28:ARG:HG3	1:A:29:VAL:H	1.55	0.70
1:B:92:LEU:CD2	1:B:92:LEU:H	2.02	0.70
1:A:79:GLY:HA3	1:A:81:ARG:HG2	1.73	0.70
1:B:17:PHE:CD2	1:B:86:PRO:O	2.44	0.70
1:C:164:ILE:O	1:C:168:GLN:CG	2.40	0.70
1:C:157:PHE:CE2	1:C:185:TYR:CD1	2.42	0.70
1:B:13:THR:OG1	1:B:14:SER:N	2.23	0.69
1:B:218:VAL:HG21	1:B:233:MET:HB3	1.73	0.69
1:A:34:LEU:HD12	1:A:35:SER:H	1.55	0.69
1:D:127:ALA:HB1	1:D:132:ILE:HB	1.73	0.69
1:B:90:LEU:C	1:B:90:LEU:HD12	2.13	0.69
1:A:63:LEU:HD12	1:A:65:LEU:HD21	1.74	0.69
1:A:41:ILE:CG2	1:A:65:LEU:HB2	2.22	0.69
1:B:179:LYS:O	1:B:183:GLN:NE2	2.25	0.69
1:D:97:GLY:O	1:D:100:ALA:N	2.25	0.68
1:A:13:THR:HB	1:C:67:GLY:CA	2.23	0.68
1:B:223:ARG:CB	1:B:223:ARG:HH11	2.06	0.68
1:A:80:ASN:H	1:A:80:ASN:ND2	1.89	0.68
1:B:17:PHE:CZ	1:B:94:ARG:NH1	2.62	0.68
1:D:129:LYS:HD3	1:D:129:LYS:C	2.13	0.67
1:B:224:ASP:O	1:B:227:ALA:CA	2.42	0.67
1:D:124:ASN:HB3	1:D:145:PHE:HE1	1.59	0.67
1:B:31:THR:HG21	1:B:102:TYR:CE1	2.30	0.67
1:A:54:ALA:HA	1:A:77:PHE:HA	1.75	0.67
1:C:3:GLU:HG2	1:C:4:LEU:HD13	1.75	0.67
1:B:101:ARG:NH1	1:B:105:GLU:OE2	2.26	0.67
1:C:124:ASN:HB3	1:C:141:TYR:CE1	2.30	0.67
1:A:28:ARG:HG3	1:A:29:VAL:N	2.10	0.66
1:B:226:LEU:HG	1:B:233:MET:HG2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:THR:CG2	1:B:94:ARG:HG3	2.26	0.66
1:B:64:ASN:ND2	1:B:69:LYS:CE	2.23	0.66
1:A:166:LYS:HD2	1:A:172:MET:CE	2.25	0.66
1:D:143:SER:OG	1:D:159:PRO:HD3	1.95	0.65
1:C:3:GLU:CG	1:C:4:LEU:HD13	2.26	0.65
1:B:64:ASN:HD21	1:B:69:LYS:CD	2.08	0.65
2:F:1003:A:H2'	2:F:1004:A:C8	2.30	0.65
1:A:217:ASN:OD1	1:A:217:ASN:N	2.30	0.65
1:C:81:ARG:HH22	2:G:1001:A:H61	1.39	0.65
1:B:224:ASP:O	1:B:227:ALA:HB3	1.97	0.65
1:A:80:ASN:N	1:A:81:ARG:HA	2.11	0.65
1:C:232:ASN:ND2	1:C:233:MET:CA	2.59	0.65
1:C:197:LYS:HD2	1:C:197:LYS:N	2.10	0.65
1:D:169:ARG:NH2	1:D:215:LYS:HG3	1.87	0.64
1:C:124:ASN:HB3	1:C:141:TYR:HE1	1.61	0.64
1:B:227:ALA:O	1:B:228:LYS:C	2.30	0.64
1:C:198:LEU:HD12	1:C:198:LEU:O	1.96	0.64
1:D:23:TYR:CZ	1:D:101:ARG:HG2	2.33	0.64
1:D:168:GLN:OE1	1:D:168:GLN:HA	1.97	0.64
1:D:149:GLU:O	1:D:183:GLN:HG3	1.97	0.64
1:C:226:LEU:CD1	1:C:233:MET:HG3	2.27	0.64
1:C:3:GLU:HG2	1:C:4:LEU:HD12	1.78	0.64
1:D:79:GLY:O	1:D:82:ASN:ND2	2.30	0.63
1:D:134:TRP:CH2	1:D:142:LEU:HD11	2.33	0.63
1:B:17:PHE:HE2	1:B:94:ARG:NH2	1.95	0.63
1:A:79:GLY:O	1:A:81:ARG:HG3	1.98	0.63
1:A:107:MET:HE2	1:A:138:GLU:HG2	1.80	0.63
1:D:6:PHE:CZ	1:D:8:ASP:HB2	2.34	0.63
1:C:112:GLU:N	1:C:113:PRO:HD2	2.12	0.63
1:B:91:THR:OG1	1:B:92:LEU:HD23	1.99	0.63
1:B:80:ASN:C	1:B:80:ASN:OD1	2.36	0.63
1:C:47:ARG:HD3	2:G:1008:A:C8	2.34	0.63
1:C:13:THR:OG1	1:C:14:SER:N	2.31	0.62
1:D:190:ALA:O	1:D:194:THR:HG22	1.99	0.62
1:A:31:THR:OG1	1:A:34:LEU:HB3	1.99	0.62
1:C:139:GLU:OE1	1:C:139:GLU:N	2.33	0.62
1:B:56:ARG:CG	1:B:56:ARG:HH11	2.11	0.62
1:B:224:ASP:C	1:B:227:ALA:H	1.99	0.62
1:C:232:ASN:ND2	1:C:233:MET:H	1.96	0.62
1:C:34:LEU:HB3	1:C:68:TRP:CZ3	2.35	0.62
1:A:47:ARG:O	1:A:51:THR:HG23	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:THR:HB	1:C:67:GLY:HA3	1.82	0.61
1:A:41:ILE:HG21	1:A:65:LEU:CB	2.29	0.61
1:A:63:LEU:HD13	1:A:65:LEU:HD21	1.81	0.61
1:C:16:THR:HG22	1:C:16:THR:O	2.01	0.61
1:A:149:GLU:O	1:A:183:GLN:HG3	2.00	0.61
1:D:29:VAL:HG12	1:D:30:HIS:ND1	2.16	0.60
1:A:199:THR:O	1:A:200:GLU:C	2.37	0.60
1:D:197:LYS:HG3	1:D:200:GLU:OE1	2.01	0.60
1:C:176:TYR:HE1	2:G:1005:A:N1	1.99	0.60
2:F:1003:A:H2'	2:F:1004:A:H8	1.65	0.60
1:A:172:MET:HG2	1:A:173:GLU:O	2.02	0.60
1:B:158:TYR:O	1:B:162:ILE:HG13	2.01	0.60
1:B:66:GLY:N	1:B:67:GLY:HA2	2.17	0.60
1:B:125:PRO:HB2	2:F:1008:A:H1'	1.82	0.60
1:B:149:GLU:HG3	1:B:180:THR:HB	1.83	0.60
1:A:31:THR:OG1	1:A:34:LEU:HD23	2.02	0.60
1:D:134:TRP:NE1	1:D:141:TYR:HE2	2.00	0.60
1:D:29:VAL:O	1:D:31:THR:N	2.32	0.60
1:B:91:THR:HG22	1:B:94:ARG:HG3	1.84	0.59
1:D:211:LEU:HB3	1:D:213:TRP:HD1	1.65	0.59
1:B:31:THR:O	1:B:31:THR:HG22	2.02	0.59
1:B:224:ASP:O	1:B:227:ALA:CB	2.50	0.59
1:D:125:PRO:O	1:D:129:LYS:CB	2.50	0.59
1:C:232:ASN:HD22	1:C:233:MET:CA	2.16	0.59
1:D:147:GLY:O	1:D:150:MET:HG2	2.03	0.59
1:C:163:GLY:O	1:C:167:VAL:HG23	2.03	0.59
1:D:188:LEU:O	1:D:193:TRP:CD1	2.51	0.59
1:D:30:HIS:HB3	1:D:70:ILE:HD11	1.85	0.59
1:D:114:GLU:HA	1:D:117:ILE:HD11	1.84	0.59
1:D:97:GLY:O	1:D:100:ALA:HB3	2.02	0.58
2:H:1002:A:O2'	2:H:1003:A:OP1	2.20	0.58
1:C:166:LYS:HB3	1:C:172:MET:HB3	1.83	0.58
1:A:175:LYS:O	1:A:178:GLU:HG2	2.03	0.58
1:D:84:PRO:O	1:D:85:VAL:C	2.41	0.58
1:D:54:ALA:HA	1:D:77:PHE:HA	1.85	0.58
1:D:129:LYS:HE3	1:D:217:ASN:OD1	2.03	0.58
1:C:3:GLU:HB3	1:C:4:LEU:CD1	2.34	0.58
1:A:79:GLY:CA	1:A:81:ARG:HG2	2.34	0.58
1:B:80:ASN:O	1:B:81:ARG:CG	2.50	0.58
1:B:56:ARG:HG3	1:B:56:ARG:HH11	1.69	0.58
1:A:90:LEU:HD23	1:A:95:LEU:HD13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:TYR:HE2	1:C:209:SER:HA	1.69	0.58
1:B:56:ARG:NH1	1:B:56:ARG:HG3	2.17	0.58
1:C:179:LYS:O	1:C:182:ARG:HB2	2.03	0.57
1:D:216:THR:HG23	1:D:218:VAL:HG22	1.87	0.57
1:A:91:THR:HG22	1:A:93:HIS:H	1.69	0.57
1:D:224:ASP:OD1	1:D:224:ASP:N	2.35	0.57
1:C:17:PHE:CE2	1:C:19:PRO:HG3	2.40	0.57
1:C:45:LYS:O	1:C:49:ILE:HG13	2.04	0.57
1:A:30:HIS:C	1:A:31:THR:HG22	2.20	0.57
1:C:218:VAL:HG11	1:C:233:MET:HE2	1.87	0.57
1:B:46:GLY:HA2	1:B:49:ILE:HB	1.86	0.57
1:A:199:THR:O	1:A:202:GLN:N	2.38	0.57
1:C:91:THR:HG23	1:C:94:ARG:H	1.70	0.57
1:D:82:ASN:OD1	1:D:82:ASN:N	2.33	0.56
1:D:134:TRP:NE1	1:D:141:TYR:CE2	2.73	0.56
1:B:180:THR:O	1:B:183:GLN:HG2	2.04	0.56
1:B:227:ALA:C	1:B:229:PHE:H	2.08	0.56
1:B:65:LEU:N	1:B:68:TRP:O	2.37	0.56
1:D:166:LYS:HG3	1:D:213:TRP:HH2	1.71	0.56
1:A:77:PHE:O	1:A:80:ASN:HA	2.06	0.56
1:C:91:THR:OG1	1:C:92:LEU:N	2.37	0.56
1:C:158:TYR:O	1:C:162:ILE:HG13	2.05	0.56
1:D:204:ALA:O	1:D:207:VAL:HG12	2.05	0.56
1:D:18:ASP:O	1:D:21:VAL:HG22	2.06	0.56
1:A:31:THR:CB	1:A:34:LEU:HD23	2.36	0.56
1:B:223:ARG:CG	1:B:223:ARG:HH11	2.19	0.56
1:B:225:PHE:O	1:B:229:PHE:HD1	1.89	0.56
1:B:222:ALA:O	1:B:226:LEU:CD2	2.53	0.55
1:B:80:ASN:OD1	1:B:81:ARG:HB3	2.06	0.55
1:D:179:LYS:NZ	2:H:1005:A:N7	2.54	0.55
1:C:72:VAL:HG12	1:C:90:LEU:HD23	1.88	0.55
1:D:214:LYS:HB3	1:D:223:ARG:HD3	1.88	0.55
1:A:78:PRO:HA	1:A:79:GLY:C	2.27	0.55
1:C:232:ASN:ND2	1:C:233:MET:HA	2.21	0.55
1:B:42:PHE:CD2	1:B:99:LEU:HD12	2.42	0.55
1:A:165:TYR:CE2	1:A:209:SER:HA	2.42	0.55
1:D:80:ASN:HA	1:D:82:ASN:OD1	2.07	0.55
1:D:134:TRP:CD1	1:D:141:TYR:CE2	2.94	0.55
1:B:59:TRP:CZ3	1:B:75:THR:HG23	2.42	0.55
1:C:196:SER:OG	1:C:197:LYS:HD3	2.06	0.55
1:B:127:ALA:HB2	1:B:144:PHE:CG	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:SER:OG	1:D:159:PRO:CD	2.54	0.54
1:D:76:ASN:OD1	1:D:76:ASN:N	2.41	0.54
1:C:25:ASN:O	1:C:29:VAL:HG12	2.07	0.54
1:D:17:PHE:HD2	2:H:1003:A:H5''	1.71	0.54
1:B:112:GLU:OE1	1:B:115:LYS:NZ	2.35	0.54
1:B:62:THR:HA	1:B:71:THR:HA	1.90	0.54
1:D:212:GLY:CA	1:D:213:TRP:HB2	2.38	0.54
1:D:216:THR:CG2	1:D:233:MET:O	2.56	0.54
1:B:129:LYS:HB2	2:F:1009:A:H5''	1.88	0.54
1:A:59:TRP:CZ2	1:A:73:TYR:HD2	2.26	0.54
1:C:18:ASP:OD1	1:C:21:VAL:HG23	2.08	0.54
1:C:73:TYR:CE1	1:C:89:GLY:HA2	2.42	0.54
1:A:31:THR:OG1	1:A:34:LEU:CB	2.56	0.54
1:C:226:LEU:HD12	1:C:233:MET:HG3	1.90	0.54
1:A:215:LYS:O	1:A:223:ARG:NH2	2.41	0.54
1:C:167:VAL:HG21	1:C:177:LEU:HD22	1.89	0.54
1:D:211:LEU:CB	1:D:213:TRP:HD1	2.21	0.53
1:B:59:TRP:CZ3	1:B:73:TYR:HB3	2.43	0.53
1:D:130:ASN:CG	1:D:131:GLY:N	2.58	0.53
1:C:226:LEU:HD13	1:C:233:MET:HG3	1.89	0.53
1:C:156:ARG:O	1:C:157:PHE:HB2	2.07	0.53
1:B:65:LEU:HD23	1:B:68:TRP:CE3	2.43	0.53
1:B:91:THR:HG23	1:B:94:ARG:HG3	1.90	0.53
1:C:107:MET:HA	1:C:110:VAL:HG22	1.90	0.53
1:D:169:ARG:HH21	1:D:215:LYS:HG2	0.71	0.53
1:D:29:VAL:CG1	1:D:30:HIS:ND1	2.72	0.53
1:B:226:LEU:N	1:B:226:LEU:CD2	2.72	0.53
1:D:179:LYS:HG2	1:D:182:ARG:HH12	1.73	0.53
1:B:64:ASN:ND2	1:B:69:LYS:CG	2.71	0.53
1:A:37:ASP:O	1:A:41:ILE:HD13	2.08	0.53
1:D:126:LEU:O	1:D:129:LYS:HB3	2.08	0.52
1:B:190:ALA:HA	1:B:193:TRP:NE1	2.24	0.52
1:C:132:ILE:HD12	1:C:211:LEU:HD13	1.91	0.52
1:B:29:VAL:HG23	1:B:30:HIS:ND1	2.25	0.52
1:A:111:SER:OG	1:A:113:PRO:HD2	2.10	0.52
1:B:64:ASN:CG	1:B:69:LYS:HE2	2.18	0.52
1:C:164:ILE:O	1:C:168:GLN:HG2	2.09	0.52
2:F:1006:A:O2'	2:F:1007:A:OP1	2.23	0.52
1:D:168:GLN:O	1:D:169:ARG:HG2	2.09	0.52
1:A:129:LYS:HZ1	1:A:215:LYS:HE3	1.74	0.52
1:B:223:ARG:HD3	1:B:233:MET:C	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:LYS:O	1:C:31:THR:OG1	2.25	0.52
1:B:65:LEU:HD23	1:B:68:TRP:HE3	1.75	0.52
1:B:223:ARG:CG	1:B:223:ARG:NH1	2.73	0.52
1:B:87:ASP:N	1:B:87:ASP:OD1	2.42	0.52
1:D:140:VAL:HG22	1:D:158:TYR:CE2	2.45	0.52
1:D:98:PHE:CD1	1:D:98:PHE:N	2.78	0.52
1:A:158:TYR:O	1:A:162:ILE:HG13	2.10	0.52
1:B:220:ALA:HA	1:B:223:ARG:HG3	1.91	0.51
1:D:142:LEU:HG	1:D:145:PHE:HE2	1.75	0.51
1:D:98:PHE:HD1	1:D:98:PHE:N	2.09	0.51
1:D:114:GLU:O	1:D:118:ILE:HG13	2.10	0.51
1:A:31:THR:HB	1:A:34:LEU:HD23	1.91	0.51
1:A:53:LEU:HD21	1:A:61:VAL:HG11	1.91	0.51
1:A:65:LEU:O	1:A:68:TRP:HB3	2.10	0.51
1:A:59:TRP:CH2	1:A:73:TYR:CD2	2.99	0.51
1:D:132:ILE:N	1:D:132:ILE:HD13	2.24	0.51
1:B:85:VAL:HG11	1:B:88:ASP:HB2	1.91	0.51
1:C:77:PHE:O	1:C:79:GLY:N	2.44	0.51
1:C:3:GLU:CG	1:C:4:LEU:CD1	2.85	0.51
1:D:151:PHE:HB3	1:D:154:THR:OG1	2.11	0.51
1:A:132:ILE:HD12	1:A:211:LEU:HD13	1.93	0.51
1:D:91:THR:HG22	1:D:92:LEU:N	2.26	0.51
1:C:226:LEU:HB3	1:C:231:ILE:HB	1.93	0.51
1:A:199:THR:O	1:A:203:SER:N	2.44	0.51
1:D:25:ASN:OD1	1:D:26:PHE:N	2.43	0.51
1:B:64:ASN:CG	1:B:69:LYS:CG	2.80	0.51
1:B:68:TRP:CZ3	1:B:70:ILE:HG21	2.46	0.50
1:A:107:MET:SD	1:A:118:ILE:HD13	2.51	0.50
1:A:31:THR:HB	1:A:34:LEU:CD2	2.42	0.50
2:G:1001:A:O2'	2:G:1003:A:OP2	2.25	0.50
1:D:166:LYS:HG2	1:D:171:GLU:HB3	1.91	0.50
1:C:128:GLU:OE1	1:C:133:THR:CG2	2.59	0.50
1:A:63:LEU:HD13	1:A:65:LEU:CD2	2.40	0.50
1:B:17:PHE:CD1	1:B:17:PHE:C	2.85	0.50
1:B:91:THR:H	1:B:94:ARG:HG3	1.76	0.50
1:B:64:ASN:HA	1:B:68:TRP:O	2.11	0.50
1:D:140:VAL:HG13	1:D:158:TYR:HD2	1.77	0.50
1:B:123:ILE:O	1:B:125:PRO:HD3	2.12	0.50
1:B:17:PHE:O	1:B:17:PHE:HD1	1.95	0.50
1:D:107:MET:HG2	1:D:115:LYS:HD2	1.92	0.50
1:C:103:LEU:HD23	1:C:142:LEU:HD21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:TYR:C	1:C:185:TYR:CD2	2.85	0.50
1:A:31:THR:CB	1:A:34:LEU:CD2	2.90	0.50
1:A:158:TYR:N	1:A:159:PRO:CD	2.75	0.50
1:D:212:GLY:HA2	1:D:213:TRP:CB	2.41	0.49
1:D:53:LEU:CD2	1:D:61:VAL:HG11	2.43	0.49
1:D:179:LYS:NZ	2:H:1005:A:H62	2.10	0.49
1:B:204:ALA:O	1:B:208:VAL:HG23	2.12	0.49
1:C:232:ASN:CG	1:C:233:MET:N	2.60	0.49
1:D:136:ASP:OD2	1:D:211:LEU:CD1	2.60	0.49
1:D:119:LYS:HG2	1:D:134:TRP:CD2	2.47	0.49
1:D:30:HIS:ND1	1:D:30:HIS:N	2.60	0.49
1:A:62:THR:HB	1:A:71:THR:OG1	2.13	0.49
1:B:225:PHE:CD1	1:B:225:PHE:C	2.85	0.49
1:B:19:PRO:HB3	1:B:150:MET:CE	2.42	0.49
1:C:176:TYR:HE1	2:G:1005:A:C2	2.29	0.49
1:C:200:GLU:N	1:C:200:GLU:OE1	2.37	0.49
1:D:167:VAL:HG12	1:D:168:GLN:N	2.28	0.49
1:A:29:VAL:HG22	1:A:30:HIS:CE1	2.48	0.49
1:B:127:ALA:HB1	1:B:132:ILE:HB	1.94	0.49
1:C:185:TYR:C	1:C:185:TYR:HD2	2.16	0.48
1:A:104:LEU:HD13	1:A:142:LEU:HD12	1.95	0.48
1:B:64:ASN:ND2	1:B:69:LYS:CD	2.73	0.48
1:C:86:PRO:HA	1:C:87:ASP:HA	1.53	0.48
1:D:34:LEU:HD22	1:D:39:ILE:HG12	1.95	0.48
1:B:168:GLN:C	1:B:170:LYS:H	2.17	0.48
1:A:30:HIS:HB3	1:A:68:TRP:CH2	2.39	0.48
1:D:96:SER:OG	1:D:146:PRO:HD2	2.13	0.48
1:A:74:ASN:OD1	1:A:77:PHE:CB	2.61	0.48
1:B:23:TYR:CD2	1:B:101:ARG:HD3	2.49	0.48
2:F:1009:A:N1	2:F:1010:A:N6	2.59	0.48
1:C:140:VAL:HG11	1:C:211:LEU:HD11	1.96	0.48
1:D:25:ASN:O	1:D:29:VAL:HG23	2.13	0.48
1:B:175:LYS:C	1:B:177:LEU:H	2.17	0.48
1:B:144:PHE:CE1	1:B:162:ILE:HD13	2.49	0.48
1:C:53:LEU:HD13	1:C:92:LEU:HD11	1.96	0.48
1:A:43:TYR:OH	1:A:96:SER:O	2.27	0.48
1:C:85:VAL:HG23	1:C:89:GLY:N	2.28	0.48
1:D:160:LEU:O	1:D:164:ILE:HG13	2.14	0.48
1:B:165:TYR:HB2	1:B:205:LEU:HD11	1.95	0.48
1:D:216:THR:HG21	1:D:233:MET:C	2.34	0.48
1:B:224:ASP:OD1	1:B:225:PHE:CA	2.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:PHE:HD1	1:B:17:PHE:C	2.17	0.48
1:D:17:PHE:CZ	1:D:150:MET:HE1	2.48	0.48
1:B:175:LYS:O	1:B:178:GLU:HG2	2.14	0.48
1:D:149:GLU:HB2	1:D:180:THR:HG23	1.95	0.48
1:C:80:ASN:O	1:C:82:ASN:N	2.47	0.48
1:A:47:ARG:NH1	1:A:50:LYS:HE2	2.29	0.47
1:A:104:LEU:O	1:A:108:LEU:HG	2.13	0.47
1:A:193:TRP:O	1:A:197:LYS:HB2	2.13	0.47
1:A:56:ARG:CZ	1:A:58:GLU:OE2	2.62	0.47
1:B:73:TYR:CZ	1:B:85:VAL:HG21	2.49	0.47
1:A:63:LEU:CD1	1:A:65:LEU:CD2	2.88	0.47
1:B:56:ARG:NH1	1:B:56:ARG:CG	2.72	0.47
1:C:34:LEU:HD13	1:C:39:ILE:HD11	1.97	0.47
1:C:34:LEU:HB3	1:C:68:TRP:CE3	2.49	0.47
1:A:184:ARG:HD3	2:E:1002:A:N3	2.30	0.47
2:F:1004:A:N3	2:F:1005:A:N7	2.63	0.47
1:C:165:TYR:C	1:C:165:TYR:CD1	2.87	0.47
1:D:18:ASP:HB3	1:D:21:VAL:HG22	1.97	0.47
1:B:26:PHE:O	1:B:30:HIS:HB2	2.15	0.47
1:A:29:VAL:HG22	1:A:30:HIS:CD2	2.50	0.47
1:D:136:ASP:CG	1:D:211:LEU:CD1	2.79	0.47
1:D:190:ALA:HA	1:D:193:TRP:NE1	2.30	0.47
1:C:129:LYS:HG3	2:G:1008:A:C5'	2.41	0.47
1:A:114:GLU:HA	1:A:117:ILE:HG23	1.96	0.47
1:B:203:SER:O	1:B:207:VAL:HG23	2.14	0.47
1:A:28:ARG:O	1:A:29:VAL:C	2.53	0.47
1:A:59:TRP:CH2	1:A:73:TYR:HD2	2.34	0.47
1:C:170:LYS:HE3	1:C:170:LYS:HB2	1.70	0.47
1:A:169:ARG:O	1:A:170:LYS:HB2	2.13	0.47
1:A:59:TRP:HD1	1:A:74:ASN:O	1.98	0.46
1:D:142:LEU:HG	1:D:145:PHE:CE2	2.50	0.46
1:D:152:LEU:HD23	1:D:159:PRO:HG2	1.97	0.46
1:D:160:LEU:HD11	1:D:181:MET:CE	2.46	0.46
1:C:139:GLU:O	1:C:143:SER:HB2	2.15	0.46
1:A:90:LEU:CD2	1:A:95:LEU:HD13	2.45	0.46
1:A:85:VAL:HG12	1:A:89:GLY:HA3	1.97	0.46
1:B:156:ARG:O	1:B:157:PHE:HB2	2.16	0.46
1:C:233:MET:HB3	1:C:233:MET:HE3	1.80	0.46
1:A:180:THR:O	1:A:183:GLN:HB2	2.15	0.46
1:A:59:TRP:O	1:A:59:TRP:CG	2.68	0.46
1:C:127:ALA:HB2	1:C:144:PHE:CG	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:ALA:C	1:B:229:PHE:N	2.55	0.46
1:D:131:GLY:C	1:D:132:ILE:HD13	2.36	0.46
1:D:188:LEU:O	1:D:189:GLU:C	2.54	0.46
1:A:179:LYS:HA	1:A:182:ARG:NH2	2.31	0.46
1:B:107:MET:HA	1:B:110:VAL:HG12	1.98	0.46
2:H:1006:A:H2'	2:H:1007:A:H8	1.79	0.46
1:C:63:LEU:HB2	1:C:70:ILE:O	2.16	0.46
1:B:72:VAL:HG12	1:B:90:LEU:CD1	2.39	0.46
1:A:68:TRP:CZ2	1:A:70:ILE:HD13	2.51	0.46
1:A:117:ILE:O	1:A:121:LYS:HG3	2.15	0.46
1:D:35:SER:O	1:D:39:ILE:HG13	2.16	0.46
1:A:59:TRP:CZ2	1:A:73:TYR:CD2	3.03	0.46
1:A:81:ARG:O	1:A:83:SER:N	2.49	0.46
1:D:59:TRP:CG	1:D:59:TRP:O	2.69	0.46
1:D:226:LEU:HD23	1:D:233:MET:SD	2.56	0.45
1:A:28:ARG:CG	1:A:29:VAL:N	2.77	0.45
1:B:216:THR:HG22	1:B:218:VAL:HG13	1.99	0.45
1:C:136:ASP:HB3	1:C:211:LEU:HD22	1.98	0.45
1:D:41:ILE:HA	1:D:44:ILE:HG22	1.98	0.45
1:D:132:ILE:C	1:D:133:THR:HG23	2.36	0.45
1:A:203:SER:O	1:A:206:THR:OG1	2.28	0.45
1:A:50:LYS:HG3	1:A:76:ASN:HD22	1.81	0.45
1:C:184:ARG:NE	2:G:1002:A:C2	2.84	0.45
3:B:303:HOH:O	2:F:1007:A:H2	1.98	0.45
1:D:95:LEU:O	1:D:99:LEU:HD12	2.17	0.45
1:C:149:GLU:O	1:C:183:GLN:HG2	2.16	0.45
1:B:226:LEU:O	1:B:231:ILE:C	2.46	0.45
1:D:216:THR:HG22	1:D:233:MET:O	2.16	0.45
1:D:89:GLY:O	1:D:94:ARG:HD2	2.17	0.45
1:D:94:ARG:O	1:D:98:PHE:CD1	2.70	0.45
1:C:76:ASN:ND2	2:G:1005:A:H5'	2.32	0.45
1:B:217:ASN:HB3	2:F:1010:A:H5'	1.99	0.45
1:B:226:LEU:HB3	1:B:231:ILE:HB	1.97	0.45
1:B:225:PHE:O	1:B:229:PHE:CD1	2.68	0.45
1:C:66:GLY:HA2	1:C:67:GLY:HA2	1.54	0.45
1:B:59:TRP:O	1:B:59:TRP:CG	2.70	0.45
1:B:112:GLU:N	1:B:113:PRO:HD2	2.31	0.45
1:C:180:THR:O	1:C:183:GLN:HB2	2.16	0.45
1:A:232:ASN:O	1:A:233:MET:HB2	2.17	0.45
1:D:48:GLU:O	1:D:51:THR:N	2.50	0.45
1:B:225:PHE:O	1:B:225:PHE:CD1	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:LEU:CD1	1:B:90:LEU:C	2.85	0.44
1:B:56:ARG:CB	1:B:56:ARG:HH11	2.30	0.44
1:A:79:GLY:C	1:A:81:ARG:CG	2.85	0.44
1:B:29:VAL:HG23	1:B:30:HIS:CE1	2.53	0.44
1:D:216:THR:HG21	1:D:233:MET:O	2.18	0.44
1:B:17:PHE:CD1	1:B:17:PHE:O	2.70	0.44
1:A:28:ARG:CG	1:A:29:VAL:H	2.25	0.44
1:B:16:THR:O	1:B:87:ASP:OD1	2.35	0.44
1:D:136:ASP:OD2	1:D:211:LEU:HD11	2.15	0.44
1:A:190:ALA:HA	1:A:193:TRP:CD1	2.52	0.44
1:D:59:TRP:HA	1:D:74:ASN:HB3	1.97	0.44
1:C:56:ARG:O	1:C:58:GLU:HG2	2.17	0.44
1:C:2:ILE:HG23	1:C:3:GLU:HB2	2.00	0.44
1:C:126:LEU:HA	1:C:126:LEU:HD13	1.83	0.44
1:C:20:GLU:CD	1:C:101:ARG:HH12	2.21	0.44
1:C:151:PHE:HB3	1:C:154:THR:HG23	2.00	0.44
1:A:91:THR:HG22	1:A:93:HIS:N	2.31	0.44
1:B:62:THR:OG1	1:B:71:THR:HB	2.17	0.44
1:D:167:VAL:O	1:D:168:GLN:CB	2.64	0.44
1:A:76:ASN:OD1	1:A:76:ASN:N	2.49	0.44
1:B:168:GLN:C	1:B:170:LYS:N	2.71	0.44
1:B:168:GLN:O	1:B:170:LYS:N	2.51	0.44
1:D:37:ASP:O	1:D:41:ILE:HG13	2.17	0.44
1:D:127:ALA:O	1:D:129:LYS:O	2.35	0.44
1:D:103:LEU:HA	1:D:103:LEU:HD23	1.81	0.44
1:A:200:GLU:O	1:A:201:VAL:C	2.56	0.43
1:C:81:ARG:HD3	1:C:81:ARG:O	2.18	0.43
1:D:166:LYS:HD3	1:D:172:MET:HG3	2.00	0.43
1:D:29:VAL:C	1:D:31:THR:N	2.71	0.43
1:B:44:ILE:HD11	2:F:1009:A:N6	2.32	0.43
1:A:41:ILE:CG2	1:A:65:LEU:CB	2.92	0.43
1:A:47:ARG:HH11	1:A:50:LYS:HE2	1.82	0.43
1:A:175:LYS:HE3	1:A:175:LYS:HB2	1.76	0.43
1:B:85:VAL:HB	1:B:89:GLY:H	1.83	0.43
1:C:56:ARG:CZ	1:C:56:ARG:HA	2.48	0.43
1:A:162:ILE:HG22	1:A:166:LYS:HE3	2.00	0.43
1:D:214:LYS:HG3	1:D:223:ARG:NH1	2.33	0.43
1:C:132:ILE:HG21	1:C:144:PHE:CE1	2.54	0.43
1:B:176:TYR:OH	2:F:1006:A:H1'	2.19	0.43
1:B:207:VAL:O	1:B:210:SER:HB3	2.18	0.43
1:B:224:ASP:CG	1:B:225:PHE:N	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:LEU:HD12	1:C:177:LEU:HA	1.84	0.43
1:C:103:LEU:HD21	1:C:122:ILE:HG21	2.00	0.43
1:C:157:PHE:HZ	1:C:185:TYR:CD1	2.12	0.43
1:C:185:TYR:HE2	1:C:186:MET:SD	2.42	0.43
1:D:90:LEU:HD12	1:D:95:LEU:HD13	2.00	0.43
1:D:134:TRP:CE2	1:D:141:TYR:CE2	3.07	0.43
1:A:214:LYS:HG2	1:A:214:LYS:O	2.19	0.43
1:D:216:THR:OG1	1:D:216:THR:O	2.30	0.42
1:D:107:MET:HE3	1:D:138:GLU:HG2	2.01	0.42
1:D:195:VAL:O	1:D:197:LYS:N	2.51	0.42
2:G:1005:A:N3	2:G:1005:A:H2'	2.34	0.42
1:A:168:GLN:C	1:A:170:LYS:H	2.21	0.42
1:B:223:ARG:HB3	1:B:223:ARG:HH11	1.79	0.42
1:A:114:GLU:O	1:A:118:ILE:HG22	2.19	0.42
1:B:110:VAL:CG2	1:B:114:GLU:CD	2.87	0.42
2:H:1006:A:H2'	2:H:1007:A:C8	2.53	0.42
1:A:142:LEU:HD23	1:A:142:LEU:HA	1.77	0.42
1:B:226:LEU:HD22	1:B:226:LEU:H	1.80	0.42
2:F:1004:A:H2'	2:F:1005:A:C8	2.55	0.42
1:B:42:PHE:HE2	1:B:96:SER:HA	1.85	0.42
2:E:1009:A:N3	2:E:1009:A:H2'	2.35	0.42
1:D:36:TYR:OH	1:D:106:LYS:HG2	2.20	0.42
1:A:31:THR:HA	1:A:34:LEU:HB2	2.02	0.42
1:A:79:GLY:C	1:A:81:ARG:HG2	2.39	0.42
1:A:62:THR:HA	1:A:71:THR:HA	2.01	0.42
1:C:129:LYS:HE3	2:G:1008:A:OP1	2.20	0.42
1:C:49:ILE:O	1:C:52:SER:HB3	2.19	0.42
1:D:156:ARG:HB2	1:D:158:TYR:CD1	2.55	0.42
1:C:80:ASN:C	1:C:82:ASN:H	2.22	0.42
1:C:40:ARG:HD2	1:C:121:LYS:O	2.20	0.42
1:B:10:ALA:O	1:B:11:ALA:C	2.58	0.42
1:C:156:ARG:NH1	1:C:158:TYR:OH	2.52	0.42
1:B:70:ILE:CD1	1:B:90:LEU:HD21	2.50	0.42
1:C:29:VAL:HG13	1:C:30:HIS:CE1	2.55	0.42
1:B:107:MET:HG2	1:B:115:LYS:HG2	2.01	0.42
1:D:117:ILE:H	1:D:117:ILE:HG13	1.34	0.42
1:B:165:TYR:HB2	1:B:205:LEU:CD1	2.50	0.42
1:A:115:LYS:O	1:A:119:LYS:HG3	2.20	0.42
1:B:92:LEU:HG	1:B:93:HIS:N	2.35	0.41
1:B:61:VAL:CG2	1:B:62:THR:N	2.82	0.41
1:A:80:ASN:HB2	1:A:81:ARG:CA	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:LEU:O	1:A:74:ASN:ND2	2.41	0.41
1:B:110:VAL:HG22	1:B:114:GLU:HB3	2.02	0.41
1:D:129:LYS:CD	1:D:129:LYS:C	2.85	0.41
1:D:97:GLY:O	1:D:100:ALA:CB	2.67	0.41
1:C:175:LYS:C	1:C:177:LEU:H	2.23	0.41
2:F:1009:A:C6	2:F:1010:A:N6	2.88	0.41
1:D:3:GLU:HG2	1:D:4:LEU:N	2.35	0.41
1:A:81:ARG:C	1:A:83:SER:N	2.73	0.41
1:A:29:VAL:HG22	1:A:30:HIS:NE2	2.35	0.41
1:C:84:PRO:O	1:C:86:PRO:HD3	2.20	0.41
1:C:47:ARG:HG3	1:C:50:LYS:NZ	2.35	0.41
2:F:1010:A:C8	2:F:1010:A:OP2	2.73	0.41
1:D:50:LYS:HD3	2:H:1008:A:N6	2.35	0.41
1:D:132:ILE:C	1:D:133:THR:CG2	2.89	0.41
1:B:114:GLU:HA	1:B:117:ILE:HG22	2.02	0.41
1:D:53:LEU:HD21	1:D:61:VAL:HG11	2.03	0.41
1:C:80:ASN:C	1:C:82:ASN:N	2.74	0.41
1:B:184:ARG:HG3	2:F:1002:A:N3	2.36	0.41
1:D:100:ALA:O	1:D:142:LEU:HD23	2.21	0.41
1:B:59:TRP:HZ3	1:B:75:THR:HG23	1.86	0.41
1:B:61:VAL:HG22	1:B:62:THR:N	2.36	0.41
1:B:172:MET:CE	1:B:176:TYR:HB2	2.51	0.41
1:C:122:ILE:HD13	1:C:122:ILE:HA	1.93	0.41
1:D:86:PRO:HB2	1:D:87:ASP:H	1.61	0.41
1:D:188:LEU:HB3	1:D:193:TRP:HB3	2.03	0.40
1:A:53:LEU:HD23	1:A:74:ASN:HD22	1.85	0.40
1:C:124:ASN:HA	1:C:125:PRO:HD2	1.73	0.40
1:A:227:ALA:C	1:A:229:PHE:H	2.24	0.40
1:A:39:ILE:HG22	1:A:122:ILE:HD12	2.03	0.40
1:D:134:TRP:CE2	1:D:141:TYR:CD2	3.09	0.40
1:A:215:LYS:HE3	1:A:215:LYS:HB2	1.85	0.40
1:A:185:TYR:O	1:A:188:LEU:HD12	2.22	0.40
1:C:197:LYS:O	1:C:198:LEU:C	2.60	0.40
2:G:1001:A:C8	2:G:1003:A:N7	2.89	0.40
2:H:1003:A:H2'	2:H:1004:A:H8	1.86	0.40
1:B:193:TRP:CE3	1:B:194:THR:HA	2.57	0.40
1:C:160:LEU:O	1:C:160:LEU:HD12	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:PRO:O	1:B:233:MET:CE[3_545]	1.93	0.27

## 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	230/248 (93%)	203 (88%)	24 (10%)	3 (1%)	15	59
1	B	230/248 (93%)	203 (88%)	26 (11%)	1 (0%)	39	80
1	C	230/248 (93%)	205 (89%)	23 (10%)	2 (1%)	21	67
1	D	230/248 (93%)	194 (84%)	35 (15%)	1 (0%)	39	80
All	All	920/992 (93%)	805 (88%)	108 (12%)	7 (1%)	24	69

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	ASN
1	B	169	ARG
1	C	78	PRO
1	A	228	LYS
1	C	220	ALA
1	D	86	PRO
1	A	78	PRO

### 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	200/215 (93%)	174 (87%)	26 (13%)	5	24
1	B	200/215 (93%)	167 (84%)	33 (16%)	3	13
1	C	200/215 (93%)	155 (78%)	45 (22%)	1	5
1	D	200/215 (93%)	161 (80%)	39 (20%)	2	9
All	All	800/860 (93%)	657 (82%)	143 (18%)	2	11

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	16	THR
1	A	21	VAL
1	A	27	LYS
1	A	29	VAL
1	A	34	LEU
1	A	57	SER
1	A	60	GLU
1	A	62	THR
1	A	63	LEU
1	A	65	LEU
1	A	76	ASN
1	A	80	ASN
1	A	115	LYS
1	A	117	ILE
1	A	154	THR
1	A	169	ARG
1	A	170	LYS
1	A	186	MET
1	A	198	LEU
1	A	203	SER
1	A	206	THR
1	A	210	SER
1	A	214	LYS
1	A	215	LYS
1	A	217	ASN
1	B	16	THR
1	B	17	PHE
1	B	34	LEU
1	B	37	ASP
1	B	53	LEU
1	B	56	ARG
1	B	57	SER

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Mol	Chain	Res	Type
1	B	63	LEU
1	B	65	LEU
1	B	70	ILE
1	B	71	THR
1	B	75	THR
1	B	83	SER
1	B	87	ASP
1	B	91	THR
1	B	92	LEU
1	B	106	LYS
1	B	107	MET
1	B	129	LYS
1	B	149	GLU
1	B	154	THR
1	B	160	LEU
1	B	169	ARG
1	B	179	LYS
1	B	180	THR
1	B	181	MET
1	B	195	VAL
1	B	202	GLN
1	B	203	SER
1	B	209	SER
1	B	223	ARG
1	B	232	ASN
1	B	233	MET
1	C	3	GLU
1	C	4	LEU
1	C	9	VAL
1	C	12	ASN
1	C	13	THR
1	C	20	GLU
1	C	29	VAL
1	C	31	THR
1	C	36	TYR
1	C	63	LEU
1	C	65	LEU
1	C	71	THR
1	C	75	THR
1	C	81	ARG
1	C	90	LEU
1	C	91	THR

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Mol	Chain	Res	Type
1	C	95	LEU
1	C	105	GLU
1	C	112	GLU
1	C	114	GLU
1	C	123	ILE
1	C	126	LEU
1	C	138	GLU
1	C	141	TYR
1	C	143	SER
1	C	154	THR
1	C	157	PHE
1	C	165	TYR
1	C	169	ARG
1	C	170	LYS
1	C	171	GLU
1	C	183	GLN
1	C	185	TYR
1	C	186	MET
1	C	188	LEU
1	C	194	THR
1	C	196	SER
1	C	197	LYS
1	C	198	LEU
1	C	205	LEU
1	C	209	SER
1	C	210	SER
1	C	215	LYS
1	C	216	THR
1	C	231	ILE
1	D	4	LEU
1	D	8	ASP
1	D	15	SER
1	D	30	HIS
1	D	31	THR
1	D	32	THR
1	D	44	ILE
1	D	60	GLU
1	D	64	ASN
1	D	65	LEU
1	D	71	THR
1	D	75	THR
1	D	76	ASN

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Mol	Chain	Res	Type
1	D	78	PRO
1	D	82	ASN
1	D	92	LEU
1	D	107	MET
1	D	117	ILE
1	D	129	LYS
1	D	130	ASN
1	D	140	VAL
1	D	157	PHE
1	D	162	ILE
1	D	171	GLU
1	D	178	GLU
1	D	194	THR
1	D	195	VAL
1	D	196	SER
1	D	197	LYS
1	D	202	GLN
1	D	205	LEU
1	D	206	THR
1	D	207	VAL
1	D	211	LEU
1	D	215	LYS
1	D	223	ARG
1	D	224	ASP
1	D	226	LEU
1	D	233	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	ASN
1	B	12	ASN
1	B	64	ASN
1	C	76	ASN
1	C	232	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	E	9/10 (90%)	9 (100%)	1 (11%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	F	8/10 (80%)	7 (87%)	2 (25%)
2	G	8/10 (80%)	5 (62%)	0
2	H	8/10 (80%)	6 (75%)	1 (12%)
All	All	33/40 (82%)	27 (81%)	4 (12%)

All (27) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	E	1002	A
2	E	1003	A
2	E	1004	A
2	E	1005	A
2	E	1006	A
2	E	1007	A
2	E	1008	A
2	E	1009	A
2	E	1010	A
2	F	1003	A
2	F	1004	A
2	F	1005	A
2	F	1006	A
2	F	1007	A
2	F	1009	A
2	F	1010	A
2	G	1002	A
2	G	1004	A
2	G	1006	A
2	G	1007	A
2	G	1008	A
2	H	1003	A
2	H	1004	A
2	H	1005	A
2	H	1006	A
2	H	1007	A
2	H	1008	A

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	E	1002	A
2	F	1005	A
2	F	1006	A

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Mol	Chain	Res	Type
2	H	1002	A

## 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	232/248 (93%)	-0.04	1 (0%) 93 90	26, 50, 78, 101	0
1	B	232/248 (93%)	0.06	6 (2%) 59 45	25, 62, 90, 122	0
1	C	232/248 (93%)	0.07	7 (3%) 54 39	23, 76, 104, 127	0
1	D	232/248 (93%)	0.10	6 (2%) 59 45	27, 69, 103, 125	0
2	E	10/10 (100%)	0.19	0 100 100	52, 75, 84, 95	0
2	F	9/10 (90%)	0.28	0 100 100	75, 86, 96, 106	0
2	G	9/10 (90%)	0.04	0 100 100	86, 96, 108, 111	0
2	H	9/10 (90%)	0.26	0 100 100	83, 100, 114, 120	0
All	All	965/1032 (93%)	0.05	20 (2%) 67 52	23, 66, 101, 127	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	67	GLY	4.3
1	D	213	TRP	3.5
1	B	12	ASN	3.4
1	D	232	ASN	3.3
1	B	86	PRO	3.0
1	C	72	VAL	2.9
1	C	84	PRO	2.9
1	B	59	TRP	2.8
1	B	60	GLU	2.8
1	D	231	ILE	2.7
1	C	57	SER	2.5
1	B	15	SER	2.5
1	A	83	SER	2.4
1	D	174	PRO	2.4
1	C	61	VAL	2.4
1	D	59	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	80	ASN	2.2
1	C	176	TYR	2.1
1	C	6	PHE	2.1
1	B	75	THR	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.