



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 6, 2017 – 11:44 PM EDT

PDB ID : 5JK7  
Title : The X-ray structure of the DDB1-DCAF1-Vpr-UNG2 complex  
Authors : Calero, G.; Ahn, J.; Wu, Y.  
Deposited on : unknown  
Resolution : 3.49 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 : rb-20029824  
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) : rb-20029824

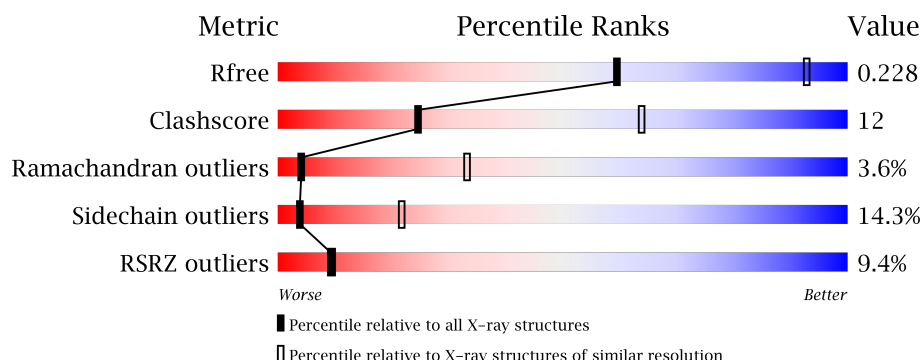
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.49 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	1195 (3.60-3.40)
Clashscore	112137	1322 (3.60-3.40)
Ramachandran outliers	110173	1283 (3.60-3.40)
Sidechain outliers	110143	1284 (3.60-3.40)
RSRZ outliers	101464	1226 (3.60-3.40)

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 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	1140	<div> <div>3%</div> <div> <div></div> <div>66%</div> <div>29%</div> <div>5%</div> </div> </div>
1	B	1140	<div> <div>24%</div> <div> <div></div> <div>70%</div> <div>26%</div> </div> </div>
2	C	361	<div> <div>%</div> <div> <div></div> <div>49%</div> <div>33%</div> <div>9%</div> <div>8%</div> </div> </div>
2	E	361	<div> <div>2%</div> <div> <div></div> <div>53%</div> <div>31%</div> <div>7%</div> <div>8%</div> </div> </div>
3	D	222	<div> <div>3%</div> <div> <div></div> <div>69%</div> <div>26%</div> <div>5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	G	222	 67% 28% 5%
4	F	96	 25% 27% 19% 6% 23%
4	H	96	 31% 29% 9% 7% 23%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27684 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 damage-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1133	Total	C	N	O	S	0	0	0
			8865	5619	1486	1711	49			
1	B	1133	Total	C	N	O	S	0	0	0
			8703	5541	1450	1663	49			

- Molecule 2 is a protein called Protein VPRBP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	331	Total	C	N	O	S	0	0	0
			2635	1666	457	494	18			
2	E	331	Total	C	N	O	S	0	0	0
			2635	1666	457	494	18			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1044	ALA	-	expression tag	UNP Q9Y4B6
C	1397	LEU	-	expression tag	UNP Q9Y4B6
C	1398	GLU	-	expression tag	UNP Q9Y4B6
C	1399	HIS	-	expression tag	UNP Q9Y4B6
C	1400	HIS	-	expression tag	UNP Q9Y4B6
C	1401	HIS	-	expression tag	UNP Q9Y4B6
C	1402	HIS	-	expression tag	UNP Q9Y4B6
C	1403	HIS	-	expression tag	UNP Q9Y4B6
C	1404	HIS	-	expression tag	UNP Q9Y4B6
E	1044	ALA	-	expression tag	UNP Q9Y4B6
E	1397	LEU	-	expression tag	UNP Q9Y4B6
E	1398	GLU	-	expression tag	UNP Q9Y4B6
E	1399	HIS	-	expression tag	UNP Q9Y4B6
E	1400	HIS	-	expression tag	UNP Q9Y4B6
E	1401	HIS	-	expression tag	UNP Q9Y4B6
E	1402	HIS	-	expression tag	UNP Q9Y4B6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1403	HIS	-	expression tag	UNP Q9Y4B6
E	1404	HIS	-	expression tag	UNP Q9Y4B6

- Molecule 3 is a protein called Uracil-DNA glycosylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	221	Total	C	N	O	S	0	0	0
			1791	1158	316	312	5			
3	G	221	Total	C	N	O	S	0	0	0
			1791	1158	316	312	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	83	VAL	-	expression tag	UNP P13051
D	84	PHE	-	expression tag	UNP P13051
G	83	VAL	-	expression tag	UNP P13051
G	84	PHE	-	expression tag	UNP P13051

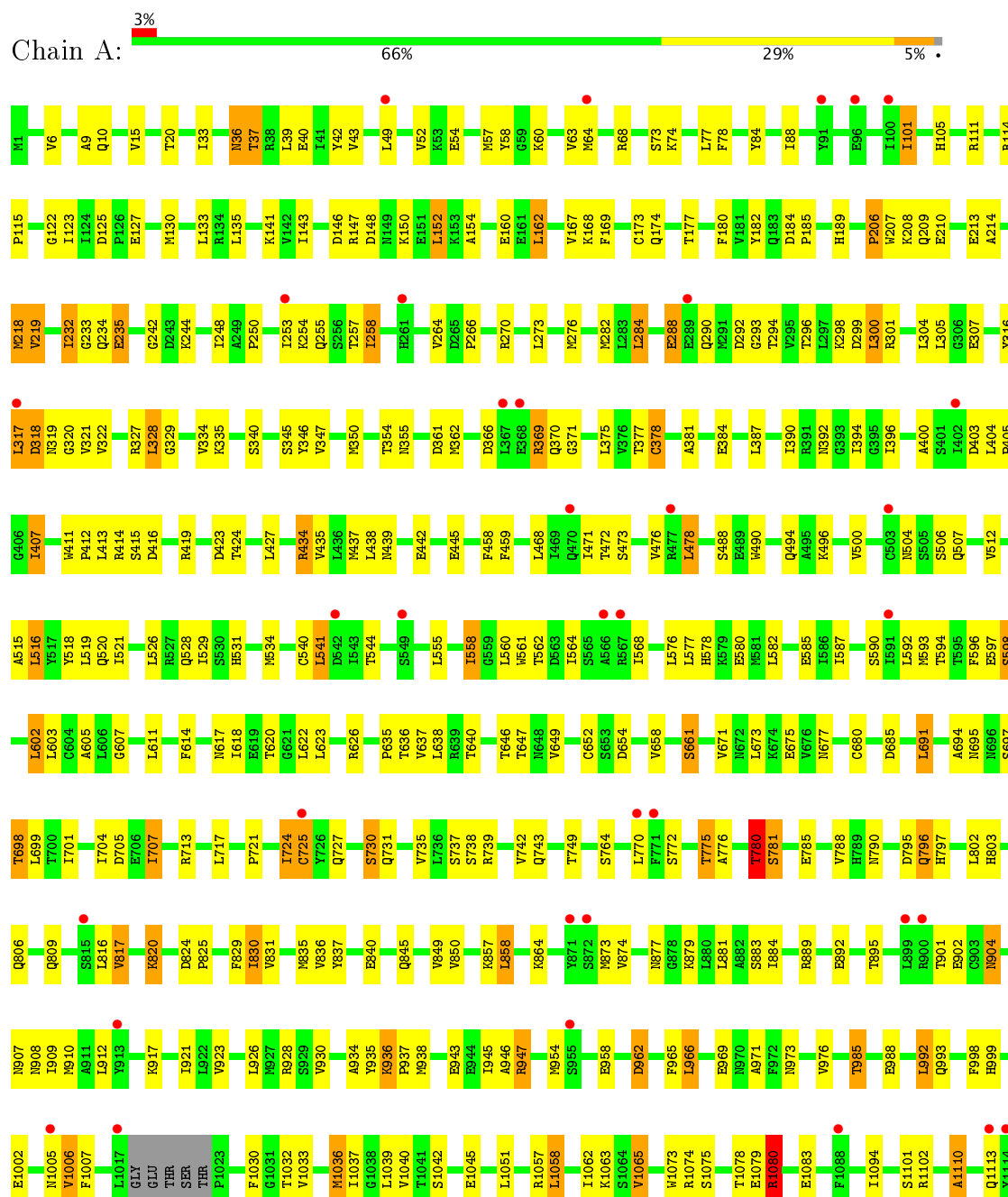
- Molecule 4 is a protein called Protein Vpr.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	74	Total	C	N	O	S	0	0	0
			632	409	109	113	1			
4	H	74	Total	C	N	O	S	0	0	0
			632	409	109	113	1			

### 3 Residue-property plots

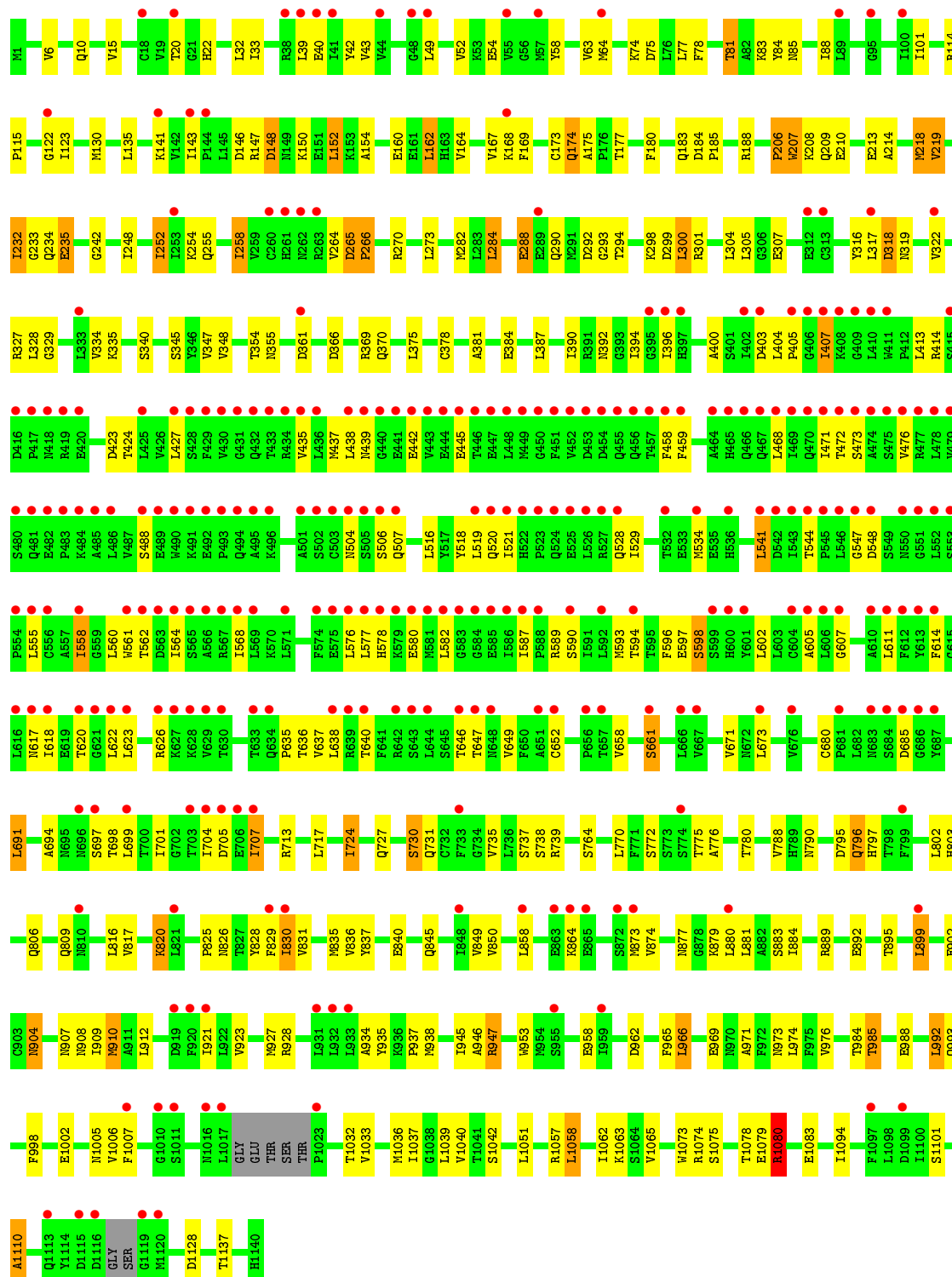
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA damage-binding protein 1

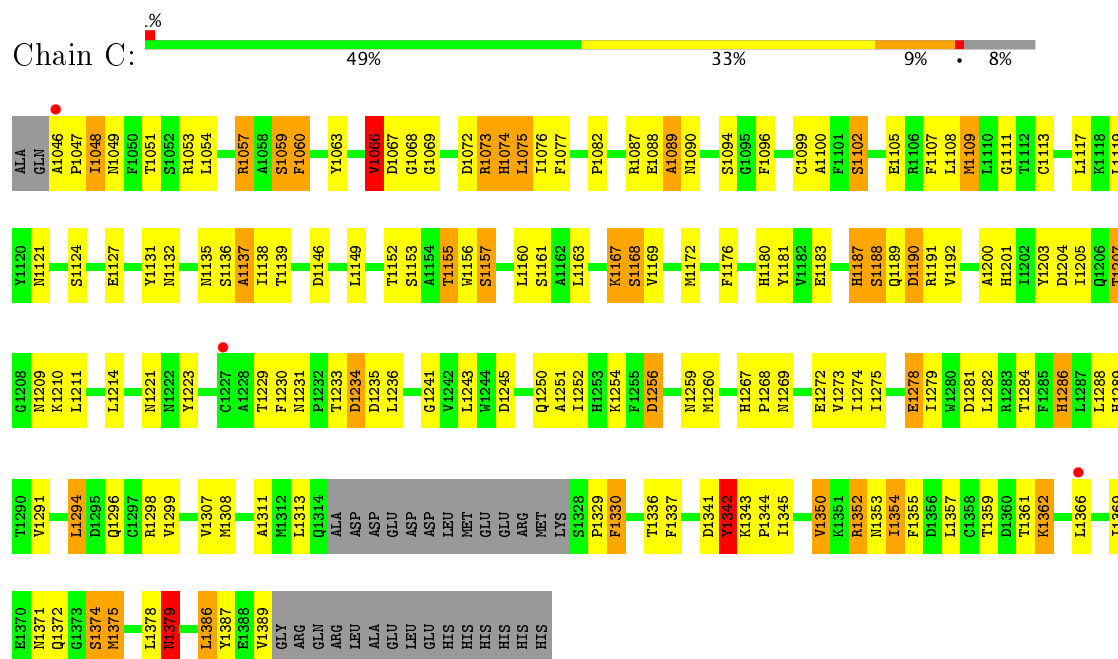




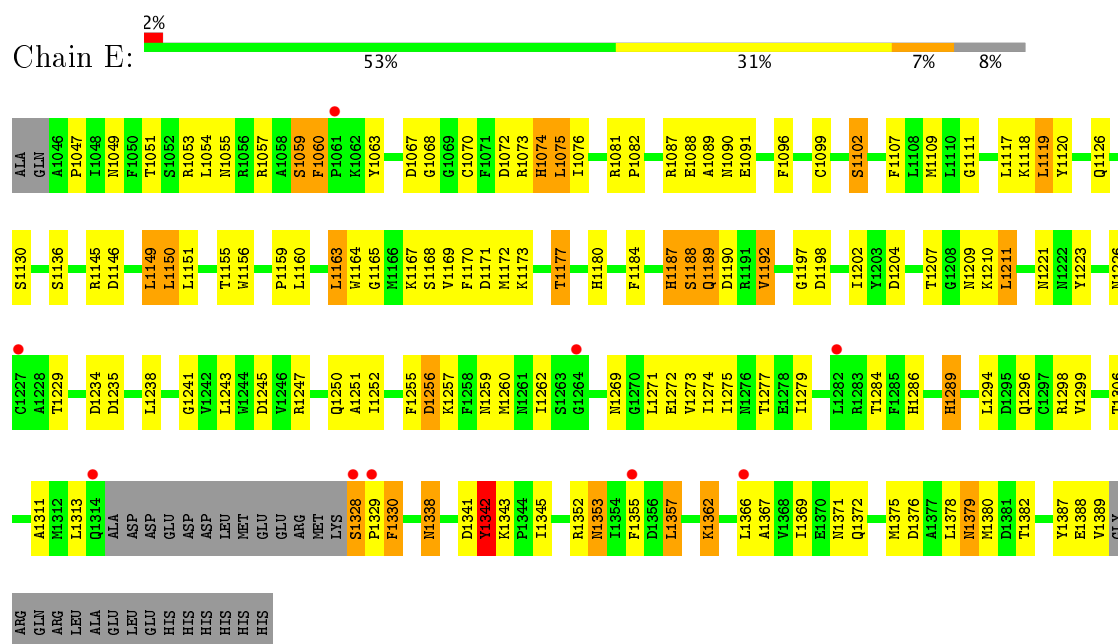
• Molecule 1: DNA damage-binding protein 1



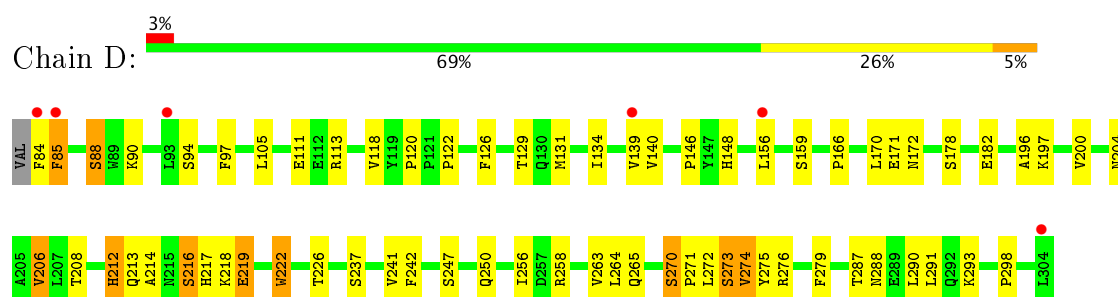
- Molecule 2: Protein VPRBP



- Molecule 2: Protein VPRBP

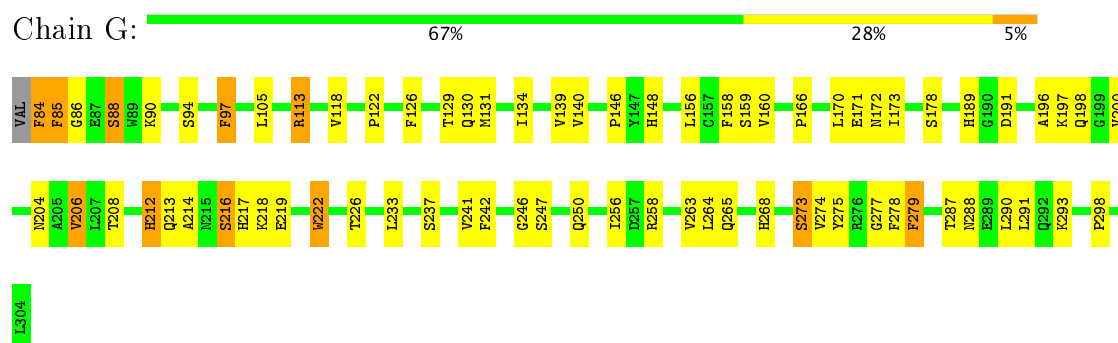


- Molecule 3: Uracil-DNA glycosylase

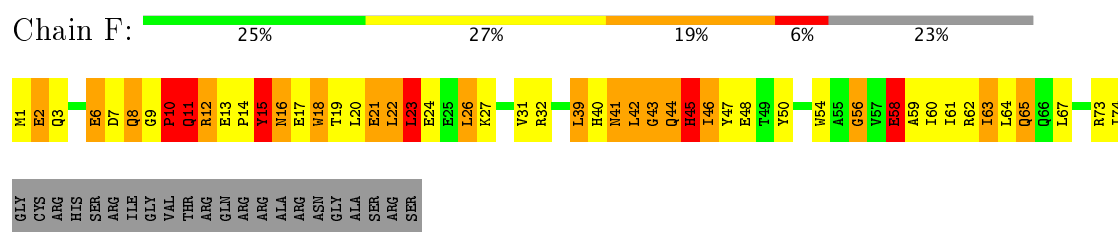




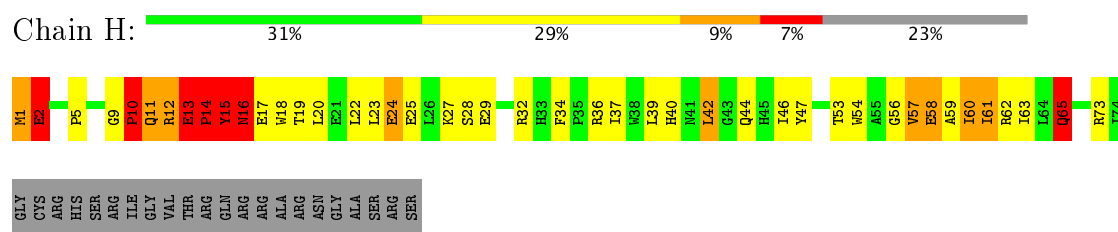
- Molecule 3: Uracil-DNA glycosylase



- Molecule 4: Protein Vpr



- Molecule 4: Protein Vpr



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.90Å 128.20Å 129.20Å 75.11° 89.44° 65.37°	Depositor
Resolution (Å)	40.30 – 3.49 39.69 – 3.49	Depositor EDS
% Data completeness (in resolution range)	90.6 (40.30-3.49) 86.2 (39.69-3.49)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.98 (at 3.48Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, $R_{free}$	0.176 , 0.206 0.197 , 0.228	Depositor DCC
$R_{free}$ test set	2464 reflections (3.19%)	DCC
Wilson B-factor (Å <sup>2</sup> )	144.6	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 155.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	27684	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	193.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.50	0/9028	0.79	0/12226
1	B	0.49	0/8864	0.78	2/12030 (0.0%)
2	C	0.61	1/2698 (0.0%)	0.92	1/3655 (0.0%)
2	E	0.56	0/2698	0.88	1/3655 (0.0%)
3	D	0.54	0/1852	0.80	1/2511 (0.0%)
3	G	0.51	0/1852	0.77	0/2511
4	F	1.71	13/651 (2.0%)	1.59	15/885 (1.7%)
4	H	1.76	19/651 (2.9%)	1.54	14/885 (1.6%)
All	All	0.63	33/28294 (0.1%)	0.86	34/38358 (0.1%)

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
4	F	0	2
4	H	0	3
All	All	0	5

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	25	GLU	C-O	-10.61	1.03	1.23
4	F	43	GLY	C-O	-10.24	1.07	1.23
4	H	58	GLU	C-O	-8.86	1.06	1.23
4	H	2	GLU	CD-OE2	-8.84	1.16	1.25
4	F	18	TRP	CE3-CZ3	-7.51	1.25	1.38
4	F	43	GLY	CA-C	-7.44	1.40	1.51
4	F	9	GLY	C-O	-7.22	1.12	1.23
4	F	22	LEU	C-O	-7.21	1.09	1.23
4	H	25	GLU	CA-C	-7.00	1.34	1.52
4	H	25	GLU	CD-OE1	-6.65	1.18	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	59	ALA	C-O	-6.42	1.11	1.23
4	F	18	TRP	CE2-CZ2	-6.27	1.29	1.39
4	H	2	GLU	C-O	-6.23	1.11	1.23
4	H	2	GLU	CG-CD	-6.23	1.42	1.51
4	F	58	GLU	CA-CB	-6.22	1.40	1.53
4	H	60	ILE	C-O	-6.02	1.11	1.23
4	F	56	GLY	C-O	-6.01	1.14	1.23
4	H	59	ALA	CA-CB	-5.86	1.40	1.52
4	H	61	ILE	C-O	-5.85	1.12	1.23
4	H	42	LEU	C-O	-5.62	1.12	1.23
4	H	14	PRO	N-CD	5.47	1.55	1.47
4	H	58	GLU	CA-CB	-5.44	1.42	1.53
4	H	15	TYR	CG-CD1	-5.43	1.32	1.39
2	C	1389	VAL	CA-C	5.27	1.66	1.52
4	F	18	TRP	CD2-CE2	-5.26	1.35	1.41
4	F	23	LEU	C-O	-5.22	1.13	1.23
4	F	45	HIS	C-O	-5.21	1.13	1.23
4	H	14	PRO	C-O	-5.17	1.12	1.23
4	H	13	GLU	CD-OE2	-5.11	1.20	1.25
4	F	11	GLN	CA-C	-5.11	1.39	1.52
4	H	59	ALA	CA-C	-5.07	1.39	1.52
4	H	15	TYR	CE2-CZ	-5.06	1.31	1.38
4	F	19	THR	C-O	-5.03	1.13	1.23

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	61	ILE	CG1-CB-CG2	-10.76	87.73	111.40
4	F	39	LEU	CB-CG-CD1	-10.14	93.76	111.00
4	F	42	LEU	CB-CG-CD1	-10.13	93.77	111.00
4	H	42	LEU	CA-CB-CG	9.92	138.12	115.30
4	H	12	ARG	NE-CZ-NH2	-9.14	115.73	120.30
4	F	39	LEU	CB-CG-CD2	-8.78	96.08	111.00
4	F	10	PRO	N-CA-C	8.27	133.59	112.10
4	F	42	LEU	CA-CB-CG	8.10	133.94	115.30
4	F	10	PRO	CA-N-CD	-7.99	100.32	111.50
4	F	23	LEU	CB-CG-CD1	7.77	124.21	111.00
4	F	9	GLY	N-CA-C	-7.65	93.98	113.10
4	F	24	GLU	OE1-CD-OE2	-7.49	114.31	123.30
2	C	1059	SER	C-N-CA	7.25	139.81	121.70
4	H	25	GLU	CB-CA-C	-7.21	95.98	110.40
2	E	1059	SER	C-N-CA	7.05	139.33	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	32	ARG	NE-CZ-NH2	6.94	123.77	120.30
4	H	42	LEU	CB-CG-CD2	-6.85	99.36	111.00
4	H	65	GLN	CA-CB-CG	6.68	128.11	113.40
4	F	42	LEU	CB-CA-C	-6.28	98.27	110.20
4	H	12	ARG	N-CA-C	6.25	127.89	111.00
4	F	9	GLY	C-N-CD	6.24	141.49	128.40
4	H	24	GLU	OE1-CD-OE2	-6.23	115.82	123.30
4	H	42	LEU	CB-CA-C	-6.08	98.64	110.20
4	F	23	LEU	CB-CG-CD2	-6.00	100.80	111.00
4	H	10	PRO	N-CA-C	5.92	127.48	112.10
4	F	22	LEU	N-CA-C	5.76	126.55	111.00
3	D	270	SER	C-N-CD	-5.47	108.57	120.60
4	H	12	ARG	CB-CA-C	-5.43	99.55	110.40
4	F	43	GLY	N-CA-C	-5.42	99.55	113.10
4	H	14	PRO	CA-N-CD	-5.29	104.09	111.50
1	B	899	LEU	CA-CB-CG	5.28	127.44	115.30
1	B	724	ILE	N-CA-C	5.26	125.21	111.00
4	F	14	PRO	C-N-CA	5.12	134.50	121.70
4	H	57	VAL	CG1-CB-CG2	-5.02	102.86	110.90

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	F	11	GLN	Peptide
4	F	21	GLU	Peptide
4	H	1	MET	Peptide
4	H	10	PRO	Mainchain
4	H	14	PRO	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	8865	0	8824	173	0
1	B	8703	0	8508	140	0
2	C	2635	0	2533	99	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	2635	0	2533	70	0
3	D	1791	0	1747	48	0
3	G	1791	0	1745	58	0
4	F	632	0	609	58	0
4	H	632	0	609	50	0
All	All	27684	0	27108	671	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 12.

All (671) 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)
3:G:84:PHE:CE1	3:G:130:GLN:NE2	1.71	1.55
3:G:84:PHE:CD1	3:G:130:GLN:NE2	1.84	1.45
4:F:26:LEU:HD13	4:F:65:GLN:NE2	1.53	1.23
2:E:1170:PHE:O	4:F:8:GLN:O	1.60	1.17
4:H:1:MET:HB2	4:H:2:GLU:HG3	1.17	1.11
4:F:20:LEU:HD13	4:F:54:TRP:CZ3	1.88	1.08
2:E:1272:GLU:HB3	2:E:1279:ILE:HD11	1.34	1.06
4:F:20:LEU:HD13	4:F:54:TRP:HZ3	1.24	1.03
4:H:1:MET:CB	4:H:2:GLU:HG3	1.90	1.02
3:G:84:PHE:O	3:G:130:GLN:HG3	1.60	1.01
3:G:85:PHE:HE1	3:G:97:PHE:HZ	1.04	0.97
3:G:85:PHE:CE1	3:G:97:PHE:HZ	1.83	0.96
4:H:12:ARG:HH11	4:H:12:ARG:H	1.04	0.96
4:F:20:LEU:CD1	4:F:54:TRP:HZ3	1.79	0.96
2:C:1281:ASP:HB3	2:C:1284:THR:HG22	1.47	0.94
3:D:172:ASN:ND2	3:D:271:PRO:HD3	1.82	0.94
4:F:26:LEU:CD1	4:F:65:GLN:NE2	2.30	0.94
3:G:84:PHE:HE1	3:G:130:GLN:NE2	1.46	0.93
4:H:13:GLU:HB3	4:H:14:PRO:CD	1.99	0.92
4:F:20:LEU:CD1	4:F:54:TRP:CZ3	2.53	0.91
2:E:1204:ASP:HB3	2:E:1207:THR:HG22	1.51	0.90
2:E:1073:ARG:HD3	2:E:1306:THR:CG2	2.02	0.90
3:G:84:PHE:HD1	3:G:130:GLN:NE2	1.69	0.88
3:G:85:PHE:HE1	3:G:97:PHE:CZ	1.92	0.87
4:F:12:ARG:N	4:F:12:ARG:HD3	1.91	0.86
1:A:10:GLN:HB3	1:A:1037:ILE:HB	1.57	0.86
1:B:361:ASP:HB3	1:B:724:ILE:HG22	1.56	0.85
1:B:724:ILE:HD13	1:B:735:VAL:HG22	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:12:ARG:HH11	4:H:12:ARG:N	1.75	0.84
4:F:26:LEU:HD13	4:F:65:GLN:HE22	1.39	0.84
4:F:61:ILE:O	4:F:65:GLN:HB2	1.79	0.83
2:C:1207:THR:HB	2:C:1209:ASN:HD22	1.45	0.81
3:G:84:PHE:O	3:G:130:GLN:CG	2.28	0.80
2:C:1281:ASP:HB3	2:C:1284:THR:CG2	2.11	0.80
3:D:273:SER:O	3:D:275:TYR:N	2.15	0.80
2:E:1059:SER:HB3	2:E:1060:PHE:HB2	1.64	0.79
2:E:1073:ARG:HE	2:E:1338:ASN:HD21	1.30	0.79
4:H:1:MET:HB2	4:H:2:GLU:CG	2.08	0.79
4:F:26:LEU:CD1	4:F:65:GLN:HE21	1.99	0.76
4:F:32:ARG:HG2	4:F:32:ARG:HH11	1.49	0.76
1:B:167:VAL:HG13	1:B:180:PHE:HB3	1.65	0.76
1:A:413:LEU:HB2	1:A:424:THR:HB	1.69	0.75
3:D:272:LEU:O	3:D:274:VAL:N	2.18	0.75
1:B:177:THR:HG21	1:B:206:PRO:HG2	1.69	0.75
2:C:1059:SER:HB3	2:C:1060:PHE:HB2	1.67	0.75
4:F:15:TYR:C	4:F:17:GLU:H	1.91	0.75
4:F:20:LEU:HD13	4:F:54:TRP:CH2	2.22	0.74
4:H:15:TYR:O	4:H:17:GLU:N	2.19	0.74
2:C:1281:ASP:CB	2:C:1284:THR:HG22	2.16	0.74
4:F:12:ARG:HD3	4:F:12:ARG:H	1.50	0.74
4:H:15:TYR:O	4:H:18:TRP:N	2.19	0.74
1:B:407:ILE:HD13	1:B:694:ALA:HB1	1.70	0.74
4:F:15:TYR:O	4:F:17:GLU:N	2.21	0.74
1:A:257:THR:OG1	1:A:276:MET:SD	2.46	0.74
3:D:291:LEU:HD13	3:D:298:PRO:HA	1.69	0.74
1:A:244:LYS:HD3	1:A:296:THR:HG23	1.69	0.73
1:A:177:THR:HG21	1:A:206:PRO:HG2	1.69	0.73
1:A:407:ILE:HD13	1:A:694:ALA:HB1	1.71	0.73
3:D:131:MET:HG2	3:D:196:ALA:HB3	1.70	0.73
3:D:139:VAL:HG13	3:D:241:VAL:HG13	1.71	0.73
3:G:131:MET:HG2	3:G:196:ALA:HB3	1.70	0.72
1:B:413:LEU:HB2	1:B:424:THR:HB	1.69	0.72
2:C:1181:TYR:HE2	2:C:1183:GLU:HB2	1.54	0.72
4:F:40:HIS:O	4:F:43:GLY:N	2.19	0.72
2:C:1132:ASN:HB2	4:H:10:PRO:HB2	1.71	0.72
3:G:139:VAL:HG13	3:G:241:VAL:HG13	1.71	0.72
2:C:1298:ARG:NH2	2:C:1330:PHE:HB3	2.04	0.72
4:F:58:GLU:O	4:F:62:ARG:HG3	1.90	0.71
4:F:15:TYR:C	4:F:17:GLU:N	2.42	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:291:LEU:HD13	3:G:298:PRO:HA	1.70	0.71
3:G:97:PHE:HD1	3:G:97:PHE:H	1.38	0.70
4:H:53:THR:HG23	4:H:56:GLY:H	1.57	0.70
3:D:131:MET:HG2	3:D:196:ALA:CB	2.22	0.70
1:A:603:LEU:HD23	1:A:611:LEU:HD21	1.72	0.69
4:H:61:ILE:O	4:H:65:GLN:HB2	1.91	0.69
1:B:835:MET:HB2	1:B:845:GLN:HG3	1.74	0.69
4:H:10:PRO:O	4:H:11:GLN:O	2.09	0.69
4:H:9:GLY:O	4:H:11:GLN:N	2.24	0.68
3:D:172:ASN:HD21	3:D:271:PRO:HD3	1.56	0.68
4:H:13:GLU:HB3	4:H:14:PRO:HD3	1.75	0.68
3:G:131:MET:HG2	3:G:196:ALA:CB	2.23	0.68
2:C:1279:ILE:HD11	2:C:1291:VAL:HG23	1.74	0.68
2:C:1105:GLU:OE1	2:C:1361:THR:HG23	1.94	0.67
4:H:1:MET:CA	4:H:2:GLU:HG3	2.25	0.67
1:B:724:ILE:CD1	1:B:735:VAL:HG22	2.25	0.67
2:E:1207:THR:HG23	2:E:1209:ASN:H	1.60	0.67
1:B:168:LYS:HG3	1:B:219:VAL:O	1.93	0.66
4:H:9:GLY:O	4:H:11:GLN:HG2	1.95	0.66
1:A:39:LEU:HD13	1:A:64:MET:CE	2.25	0.66
2:C:1192:VAL:HG23	2:C:1205:ILE:HG22	1.77	0.66
2:E:1357:LEU:HD12	2:E:1366:LEU:HD11	1.77	0.66
2:C:1087:ARG:HH12	2:C:1372:GLN:NE2	1.94	0.66
2:E:1073:ARG:HD3	2:E:1306:THR:HG23	1.76	0.66
2:C:1075:LEU:HD23	2:C:1076:ILE:HG13	1.77	0.66
1:A:39:LEU:HD13	1:A:64:MET:HE2	1.78	0.66
3:D:288:ASN:HA	3:D:291:LEU:HD12	1.78	0.65
1:A:936:LYS:HG3	1:A:943:GLU:HG3	1.76	0.65
1:A:658:VAL:HG11	1:A:707:ILE:HD12	1.78	0.65
2:E:1272:GLU:CB	2:E:1279:ILE:HD11	2.20	0.65
4:H:12:ARG:NH1	4:H:12:ARG:H	1.85	0.65
3:D:273:SER:O	3:D:274:VAL:C	2.31	0.65
2:E:1075:LEU:HD23	2:E:1076:ILE:HG13	1.77	0.64
1:B:143:ILE:HG12	1:B:154:ALA:HB2	1.79	0.64
4:F:44:GLN:O	4:F:47:TYR:N	2.30	0.64
3:D:146:PRO:HD3	3:D:206:VAL:HG12	1.79	0.64
1:A:329:GLY:HA3	1:A:384:GLU:HB3	1.80	0.64
4:H:11:GLN:HB3	4:H:12:ARG:HH12	1.62	0.64
1:B:582:LEU:HA	1:B:626:ARG:HH22	1.63	0.64
2:E:1223:TYR:HE2	2:E:1241:GLY:HA3	1.63	0.64
3:G:288:ASN:HA	3:G:291:LEU:HD12	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:GLY:HA3	1:B:384:GLU:HB3	1.80	0.63
1:B:596:PHE:HB3	1:B:661:SER:HB2	1.80	0.63
1:A:143:ILE:HG12	1:A:154:ALA:HB2	1.81	0.63
1:A:596:PHE:HB3	1:A:661:SER:HB2	1.81	0.63
4:F:31:VAL:O	4:F:31:VAL:HG12	1.97	0.63
2:C:1279:ILE:CD1	2:C:1291:VAL:HG23	2.28	0.63
4:F:22:LEU:HD12	4:F:22:LEU:O	1.99	0.63
3:D:272:LEU:HD22	4:F:60:ILE:HG21	1.81	0.63
3:D:242:PHE:HE2	3:D:256:ILE:HG12	1.63	0.63
1:B:985:THR:HG22	1:B:988:GLU:HG3	1.81	0.62
1:A:459:PHE:HB3	1:A:471:ILE:HD12	1.81	0.62
1:B:459:PHE:HB3	1:B:471:ILE:HD12	1.81	0.62
3:G:242:PHE:HE2	3:G:256:ILE:HG12	1.63	0.62
1:A:235:GLU:HB2	1:A:254:LYS:HG2	1.80	0.62
1:A:582:LEU:HA	1:A:626:ARG:HH22	1.64	0.62
1:A:282:MET:HB2	1:A:305:LEU:HD21	1.82	0.62
2:E:1272:GLU:HB3	2:E:1279:ILE:CD1	2.22	0.62
4:F:11:GLN:HG3	4:F:12:ARG:CD	2.29	0.62
1:A:998:PHE:CE1	1:A:1074:ARG:HD3	2.35	0.61
1:A:835:MET:HB2	1:A:845:GLN:HG3	1.82	0.61
4:H:54:TRP:O	4:H:57:VAL:HB	1.99	0.61
1:A:84:TYR:HE2	1:A:135:LEU:HB3	1.63	0.61
3:D:172:ASN:HD22	3:D:271:PRO:HD3	1.62	0.61
4:F:18:TRP:CZ3	4:F:22:LEU:HD23	2.34	0.61
1:A:934:ALA:CB	1:A:945:ILE:HD11	2.30	0.61
3:D:166:PRO:HB2	3:D:171:GLU:HG2	1.81	0.61
1:A:36:ASN:HD22	1:A:37:THR:HG22	1.65	0.61
4:H:10:PRO:C	4:H:11:GLN:O	2.37	0.61
1:A:1113:GLN:HB3	1:A:1121:LYS:HD2	1.82	0.61
1:B:282:MET:HB2	1:B:305:LEU:HD21	1.82	0.61
1:B:731:GLN:HA	1:B:796:GLN:HE21	1.66	0.61
1:A:114:ARG:HD2	1:A:1079:GLU:OE2	2.01	0.61
2:C:1073:ARG:NH1	2:C:1073:ARG:HB3	2.16	0.61
2:C:1187:HIS:CG	2:C:1188:SER:N	2.68	0.60
2:C:1201:HIS:CD2	2:C:1210:LYS:HD2	2.36	0.60
1:B:864:LYS:HB2	1:B:899:LEU:HD12	1.83	0.60
4:F:11:GLN:CG	4:F:12:ARG:HD3	2.32	0.60
1:A:731:GLN:HA	1:A:796:GLN:HE21	1.66	0.60
1:A:934:ALA:HB2	1:A:945:ILE:HD11	1.84	0.60
3:D:258:ARG:HD3	3:D:263:VAL:HB	1.84	0.60
1:B:32:LEU:HD23	1:B:39:LEU:HD11	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:32:ARG:CG	4:F:32:ARG:HH11	2.13	0.59
3:G:146:PRO:HD3	3:G:206:VAL:HG12	1.84	0.59
2:C:1099:CYS:HB3	2:C:1369:ILE:HD11	1.83	0.59
3:D:272:LEU:N	3:D:272:LEU:HD23	2.16	0.59
1:B:934:ALA:CB	1:B:945:ILE:HD11	2.31	0.59
2:C:1281:ASP:HB2	2:C:1288:LEU:HD11	1.82	0.59
1:B:658:VAL:HG23	1:B:671:VAL:HG22	1.84	0.59
1:B:207:TRP:HB3	1:B:242:GLY:HA2	1.84	0.59
1:A:327:ARG:HH12	2:C:1060:PHE:H	1.50	0.59
2:C:1267:HIS:ND1	2:C:1268:PRO:HD2	2.17	0.59
2:E:1073:ARG:HD3	2:E:1306:THR:HG22	1.82	0.59
3:G:250:GLN:HE21	3:G:265:GLN:HB2	1.68	0.59
1:B:724:ILE:HD13	1:B:735:VAL:CG2	2.31	0.59
1:B:934:ALA:HB2	1:B:945:ILE:HD11	1.84	0.59
2:C:1059:SER:CB	2:C:1060:PHE:HB2	2.32	0.59
1:A:415:SER:H	1:A:423:ASP:CG	2.06	0.59
1:B:235:GLU:HB3	1:B:254:LYS:HD2	1.85	0.59
2:C:1152:THR:O	2:C:1161:SER:HA	2.02	0.58
2:E:1059:SER:CB	2:E:1060:PHE:HB2	2.31	0.58
2:E:1187:HIS:CG	2:E:1188:SER:N	2.71	0.58
2:E:1136:SER:HB3	2:E:1155:THR:HB	1.84	0.58
1:A:593:MET:HG2	1:A:602:LEU:HD12	1.84	0.58
1:B:114:ARG:HD2	1:B:1079:GLU:OE2	2.03	0.58
3:D:274:VAL:HG21	4:F:39:LEU:O	2.03	0.58
3:G:258:ARG:HD3	3:G:263:VAL:HB	1.84	0.58
1:A:658:VAL:HG23	1:A:671:VAL:HG22	1.84	0.58
4:F:16:ASN:N	4:F:16:ASN:HD22	2.01	0.58
2:C:1136:SER:HB3	2:C:1155:THR:HG22	1.86	0.58
3:D:250:GLN:HE21	3:D:265:GLN:HB2	1.68	0.58
1:B:143:ILE:HG21	1:B:152:LEU:HD23	1.86	0.58
1:B:764:SER:HB2	1:B:803:HIS:NE2	2.18	0.58
3:D:273:SER:C	3:D:275:TYR:N	2.56	0.57
1:A:764:SER:HB2	1:A:803:HIS:NE2	2.17	0.57
4:H:11:GLN:HA	4:H:12:ARG:NH1	2.18	0.57
2:C:1131:TYR:OH	4:H:5:PRO:HG2	2.04	0.57
1:A:40:GLU:HB3	1:A:42:TYR:HE1	1.70	0.57
1:B:795:ASP:HB2	1:B:802:LEU:HD21	1.86	0.57
2:C:1350:VAL:HG21	2:C:1354:ILE:CG2	2.34	0.57
2:E:1378:LEU:HD11	4:F:46:ILE:HD13	1.86	0.57
1:A:423:ASP:O	1:A:437:MET:HE3	2.04	0.57
2:C:1352:ARG:HD3	2:C:1372:GLN:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:46:ILE:HD11	4:H:63:ILE:HD12	1.86	0.57
1:A:1078:THR:HG23	1:A:1080:ARG:HG3	1.87	0.57
1:B:10:GLN:HB3	1:B:1037:ILE:HB	1.87	0.57
4:H:11:GLN:HB3	4:H:12:ARG:NH1	2.20	0.57
1:A:795:ASP:HB2	1:A:802:LEU:HD21	1.87	0.56
1:A:617:ASN:HB2	1:A:622:LEU:H	1.70	0.56
2:C:1294:LEU:HD11	2:C:1308:MET:HE2	1.86	0.56
3:D:213:GLN:HB3	3:D:216:SER:HB3	1.88	0.56
3:G:213:GLN:HB3	3:G:216:SER:HB3	1.87	0.56
3:G:113:ARG:HG3	3:G:118:VAL:HB	1.87	0.56
2:C:1161:SER:HB2	2:C:1176:PHE:HB2	1.88	0.56
2:C:1066:VAL:HG22	2:C:1067:ASP:H	1.70	0.56
2:C:1100:ALA:O	2:C:1109:MET:N	2.39	0.56
4:H:13:GLU:HB3	4:H:14:PRO:HD2	1.86	0.56
2:E:1355:PHE:CE1	2:E:1371:ASN:HB2	2.41	0.55
2:C:1149:LEU:HD12	2:C:1205:ILE:HD12	1.88	0.55
1:A:40:GLU:HB3	1:A:42:TYR:CE1	2.42	0.55
1:A:917:LYS:NZ	1:A:962:ASP:OD2	2.36	0.55
1:B:1078:THR:HG23	1:B:1080:ARG:HG3	1.89	0.55
3:D:88:SER:HB2	3:D:134:ILE:HG22	1.87	0.55
1:A:43:VAL:HG23	1:A:52:VAL:HG21	1.88	0.55
2:C:1073:ARG:CZ	2:C:1073:ARG:HB3	2.35	0.55
1:A:361:ASP:HA	1:A:1006:VAL:HG11	1.88	0.55
1:A:248:ILE:HD13	1:A:300:LEU:HB2	1.89	0.55
1:A:879:LYS:HG2	1:A:892:GLU:HG3	1.89	0.55
1:B:617:ASN:HB2	1:B:622:LEU:H	1.71	0.55
1:A:607:GLY:HA2	1:A:635:PRO:HB3	1.89	0.54
1:A:969:GLU:HG2	1:A:973:ASN:HB2	1.88	0.54
2:C:1135:ASN:HB2	2:C:1157:SER:HB2	1.89	0.54
4:F:15:TYR:O	4:F:18:TRP:N	2.40	0.54
1:A:167:VAL:HG23	1:A:180:PHE:HB3	1.88	0.54
1:A:458:PHE:HE1	1:A:473:SER:HA	1.72	0.54
1:A:512:VAL:HB	1:A:515:ALA:HB3	1.87	0.54
1:A:969:GLU:HG3	1:A:971:ALA:H	1.71	0.54
1:B:284:LEU:HB2	1:B:301:ARG:HB2	1.90	0.54
1:B:969:GLU:HG3	1:B:971:ALA:H	1.72	0.54
1:A:743:GLN:HG2	1:A:749:THR:HG22	1.88	0.54
1:B:387:LEU:HG	1:B:717:LEU:HD11	1.89	0.54
2:C:1279:ILE:HD11	2:C:1291:VAL:CG2	2.37	0.54
1:B:928:ARG:HH11	1:B:928:ARG:HG3	1.73	0.54
1:B:969:GLU:HG2	1:B:973:ASN:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1284:THR:HG23	2:C:1286:HIS:H	1.73	0.54
4:F:16:ASN:ND2	4:F:16:ASN:H	2.05	0.54
1:B:40:GLU:HB3	1:B:42:TYR:HE1	1.72	0.54
2:C:1284:THR:HG23	2:C:1286:HIS:HB2	1.90	0.54
2:E:1165:GLY:HA3	2:E:1173:LYS:HE2	1.89	0.54
2:E:1357:LEU:HA	2:E:1367:ALA:O	2.08	0.54
1:A:143:ILE:HG21	1:A:152:LEU:HD23	1.89	0.54
1:B:427:LEU:HD21	1:B:699:LEU:HD22	1.90	0.54
1:B:81:THR:HG21	1:B:85:ASN:HD22	1.72	0.54
1:B:369:ARG:HG3	1:B:370:GLN:H	1.72	0.54
2:C:1221:ASN:HD21	2:C:1254:LYS:HG3	1.73	0.54
4:F:11:GLN:CG	4:F:12:ARG:CD	2.86	0.54
1:B:40:GLU:HB3	1:B:42:TYR:CE1	2.43	0.53
1:B:607:GLY:HA2	1:B:635:PRO:HB3	1.89	0.53
2:C:1180:HIS:HD1	2:C:1181:TYR:N	2.07	0.53
2:E:1068:GLY:HA3	2:E:1070:CYS:H	1.72	0.53
2:C:1046:ALA:HB2	2:C:1066:VAL:N	2.24	0.53
2:E:1150:LEU:HD23	2:E:1164:TRP:HB2	1.90	0.53
1:A:250:PRO:HD2	1:A:253:ILE:HD11	1.90	0.53
1:A:63:VAL:HG11	1:A:122:GLY:HA3	1.90	0.53
1:A:724:ILE:HG23	1:A:735:VAL:HG22	1.91	0.53
1:A:387:LEU:HG	1:A:717:LEU:HD11	1.91	0.53
1:A:58:TYR:HD1	1:A:1073:TRP:CD1	2.26	0.53
1:B:63:VAL:HG11	1:B:122:GLY:HA3	1.89	0.53
1:B:458:PHE:HE1	1:B:473:SER:HA	1.73	0.53
1:A:928:ARG:HH11	1:A:928:ARG:HG3	1.74	0.53
2:C:1113:CYS:O	2:C:1137:ALA:HA	2.08	0.53
2:C:1200:ALA:HB3	2:C:1214:LEU:HB2	1.92	0.52
3:D:85:PHE:CE1	3:D:97:PHE:HZ	2.27	0.52
1:A:284:LEU:HB2	1:A:301:ARG:HB2	1.90	0.52
2:C:1131:TYR:CZ	4:H:5:PRO:HG2	2.44	0.52
3:G:273:SER:O	4:H:40:HIS:HD2	1.93	0.52
1:A:427:LEU:HD21	1:A:699:LEU:HD22	1.90	0.52
1:B:998:PHE:CZ	1:B:1074:ARG:HD3	2.44	0.52
2:C:1167:LYS:HG3	2:C:1168:SER:H	1.73	0.52
1:A:837:TYR:HB2	1:A:840:GLU:HG2	1.92	0.52
1:B:248:ILE:HD13	1:B:300:LEU:HB2	1.91	0.52
1:B:43:VAL:HG23	1:B:52:VAL:HG21	1.91	0.52
1:A:9:ALA:HB3	1:A:1037:ILE:HG22	1.91	0.52
1:A:985:THR:HG22	1:A:988:GLU:OE2	2.09	0.52
1:B:378:CYS:SG	1:B:724:ILE:HB	2.49	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:837:TYR:HB2	1:B:840:GLU:HG2	1.92	0.52
2:E:1184:PHE:HB3	2:E:1189:GLN:HG2	1.91	0.52
1:A:133:LEU:HD13	1:A:135:LEU:HD21	1.91	0.51
2:E:1329:PRO:HD2	4:F:74:ILE:HD11	1.91	0.51
3:G:275:TYR:HE2	4:H:40:HIS:ND1	2.08	0.51
1:A:490:TRP:CD1	1:A:519:LEU:HD21	2.45	0.51
2:C:1298:ARG:HB2	2:C:1311:ALA:HB3	1.92	0.51
2:C:1181:TYR:CE2	2:C:1183:GLU:HB2	2.39	0.51
3:D:241:VAL:HG11	3:D:287:THR:HG23	1.93	0.51
4:F:32:ARG:CG	4:F:32:ARG:NH1	2.73	0.51
1:B:724:ILE:HG23	1:B:724:ILE:O	2.10	0.51
2:C:1048:ILE:O	2:C:1053:ARG:NH1	2.43	0.51
2:E:1274:ILE:HG13	2:E:1279:ILE:HD13	1.93	0.51
2:E:1298:ARG:HB2	2:E:1311:ALA:HB3	1.92	0.51
1:A:742:VAL:HG22	1:A:785:GLU:HG2	1.92	0.51
1:B:335:LYS:HB3	1:B:348:VAL:HB	1.91	0.51
2:C:1353:ASN:ND2	2:C:1375:MET:SD	2.84	0.51
1:A:105:HIS:HA	1:A:152:LEU:HD12	1.93	0.51
2:C:1350:VAL:HG21	2:C:1354:ILE:HG22	1.91	0.51
4:F:32:ARG:NH1	4:F:32:ARG:HG2	2.24	0.51
2:C:1149:LEU:HD13	2:C:1163:LEU:HD11	1.93	0.51
3:G:275:TYR:CE2	4:H:40:HIS:ND1	2.79	0.51
2:E:1328:SER:O	2:E:1353:ASN:ND2	2.44	0.50
1:A:494:GLN:HE21	1:A:496:LYS:HD3	1.76	0.50
1:A:400:ALA:HB3	1:A:701:ILE:HB	1.93	0.50
4:F:16:ASN:ND2	4:F:16:ASN:N	2.60	0.50
3:G:241:VAL:HG11	3:G:287:THR:HG23	1.94	0.50
1:A:378:CYS:SG	1:A:721:PRO:HB2	2.51	0.50
2:E:1238:LEU:HD13	2:E:1273:VAL:HG21	1.94	0.50
1:B:58:TYR:HD1	1:B:1073:TRP:CD1	2.29	0.50
1:B:252:ILE:HD13	1:B:252:ILE:H	1.76	0.50
4:H:12:ARG:HB2	4:H:13:GLU:CA	2.41	0.50
1:A:594:THR:HG21	1:A:649:VAL:HG21	1.94	0.50
1:B:400:ALA:HB3	1:B:701:ILE:HB	1.93	0.50
2:C:1308:MET:O	2:C:1336:THR:HA	2.11	0.50
3:D:113:ARG:NH1	3:D:120:PRO:O	2.44	0.50
2:E:1245:ASP:HB2	2:E:1252:ILE:HD11	1.93	0.50
3:G:166:PRO:HB2	3:G:171:GLU:HG2	1.94	0.50
1:A:321:VAL:HG13	1:A:350:MET:CE	2.42	0.50
1:B:164:VAL:HG11	1:B:167:VAL:HG22	1.94	0.50
1:B:270:ARG:HG2	1:B:284:LEU:HD23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:889:ARG:HG2	1:B:904:ASN:ND2	2.27	0.50
2:C:1281:ASP:CG	2:C:1284:THR:HG22	2.32	0.50
1:A:999:HIS:O	1:A:1074:ARG:NH1	2.45	0.49
1:A:413:LEU:HD23	1:A:468:LEU:HD22	1.94	0.49
1:B:966:LEU:HB2	1:B:976:VAL:HG22	1.93	0.49
3:G:85:PHE:CD2	3:G:129:THR:HG21	2.47	0.49
1:A:405:PRO:HA	1:A:697:SER:HA	1.93	0.49
1:B:218:MET:HB2	1:B:232:ILE:HG22	1.94	0.49
1:B:594:THR:HG21	1:B:649:VAL:HG21	1.94	0.49
1:B:879:LYS:HG2	1:B:892:GLU:HG3	1.94	0.49
3:G:241:VAL:HG23	3:G:264:LEU:HD13	1.94	0.49
1:A:998:PHE:CZ	1:A:1074:ARG:HD3	2.47	0.49
3:D:241:VAL:HG23	3:D:264:LEU:HD13	1.94	0.49
3:D:273:SER:C	3:D:275:TYR:H	2.15	0.49
1:A:78:PHE:HD1	1:A:88:ILE:HD13	1.78	0.49
1:B:84:TYR:HE2	1:B:135:LEU:HB3	1.77	0.49
2:C:1047:PRO:HG2	2:C:1053:ARG:HA	1.94	0.49
1:A:288:GLU:HB2	1:A:298:LYS:HB2	1.94	0.49
1:A:471:ILE:HG23	1:A:476:VAL:HG22	1.95	0.49
3:G:242:PHE:CE2	3:G:256:ILE:HG12	2.47	0.49
1:A:1005:ASN:HD21	1:A:1033:VAL:HG22	1.78	0.49
1:A:328:LEU:HD13	1:A:381:ALA:HB3	1.95	0.49
2:C:1233:THR:O	2:C:1234:ASP:HB2	2.12	0.49
2:E:1155:THR:HG22	2:E:1156:TRP:HD1	1.77	0.49
2:E:1250:GLN:HE21	2:E:1251:ALA:H	1.61	0.49
3:D:166:PRO:HB3	3:D:170:LEU:HD23	1.94	0.49
2:E:1109:MET:HB3	2:E:1119:LEU:CD2	2.43	0.49
4:F:50:TYR:HB3	4:F:56:GLY:HA3	1.95	0.49
2:C:1298:ARG:HH22	2:C:1330:PHE:HB3	1.76	0.49
1:A:830:ILE:HG23	1:A:850:VAL:HG22	1.95	0.48
3:G:97:PHE:CD1	3:G:97:PHE:N	2.77	0.48
1:A:320:GLY:O	1:A:335:LYS:HA	2.12	0.48
2:E:1202:ILE:HG22	2:E:1211:LEU:HB2	1.94	0.48
3:G:88:SER:HB2	3:G:134:ILE:HG22	1.94	0.48
1:A:958:GLU:HB3	1:A:966:LEU:HD23	1.95	0.48
1:B:413:LEU:HD23	1:B:468:LEU:HD22	1.94	0.48
1:B:946:ALA:HB3	1:B:992:LEU:HD13	1.94	0.48
4:H:15:TYR:CE2	4:H:19:THR:OG1	2.65	0.48
1:B:1005:ASN:HD21	1:B:1033:VAL:HG22	1.78	0.48
1:B:830:ILE:HG23	1:B:850:VAL:HG22	1.95	0.48
1:A:270:ARG:HG2	1:A:284:LEU:HD23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:946:ALA:HB3	1:A:992:LEU:HD13	1.95	0.48
1:B:405:PRO:HA	1:B:697:SER:HA	1.95	0.48
2:E:1198:ASP:HA	2:E:1226:ASN:HD22	1.79	0.48
1:A:258:ILE:HG21	1:A:273:LEU:HB3	1.95	0.48
1:B:394:ILE:HG23	1:B:705:ASP:HB2	1.95	0.48
1:B:78:PHE:HD1	1:B:88:ILE:HD13	1.79	0.48
3:D:256:ILE:O	3:D:258:ARG:NH1	2.47	0.48
4:F:46:ILE:CD1	4:F:63:ILE:HD13	2.44	0.48
1:B:22:HIS:O	1:B:75:ASP:HB2	2.14	0.48
2:E:1054:LEU:HD12	2:E:1057:ARG:HD2	1.95	0.48
3:G:256:ILE:O	3:G:258:ARG:NH1	2.47	0.48
1:B:258:ILE:HG21	1:B:273:LEU:HB3	1.96	0.48
3:D:290:LEU:HD23	3:D:293:LYS:HD2	1.96	0.48
1:A:516:LEU:O	1:A:531:HIS:HA	2.14	0.47
1:A:775:THR:HA	1:A:776:ALA:HA	1.54	0.47
1:A:966:LEU:HB2	1:A:976:VAL:HG22	1.95	0.47
1:B:958:GLU:HB3	1:B:966:LEU:HD23	1.94	0.47
2:E:1073:ARG:HE	2:E:1338:ASN:ND2	2.07	0.47
1:B:1058:LEU:HD23	1:B:1062:ILE:HD11	1.96	0.47
1:B:288:GLU:HB2	1:B:298:LYS:HB2	1.95	0.47
1:B:375:LEU:HD23	1:B:390:ILE:HD13	1.96	0.47
2:C:1204:ASP:HB3	2:C:1207:THR:OG1	2.14	0.47
2:C:1074:HIS:HA	2:C:1345:ILE:HD13	1.96	0.47
1:A:375:LEU:HD23	1:A:390:ILE:HD13	1.96	0.47
1:A:1002:GLU:HB3	1:A:1032:THR:HG21	1.97	0.47
2:C:1236:LEU:HD13	2:C:1243:LEU:HD11	1.95	0.47
2:E:1049:ASN:OD1	2:E:1051:THR:HG22	2.15	0.47
2:E:1096:PHE:HA	2:E:1111:GLY:O	2.14	0.47
3:G:290:LEU:HD23	3:G:293:LYS:HD2	1.97	0.47
4:H:34:PHE:HB2	4:H:39:LEU:HD11	1.96	0.47
1:A:218:MET:HB2	1:A:232:ILE:HG22	1.95	0.47
2:C:1153:SER:HA	2:C:1160:LEU:O	2.15	0.47
4:F:18:TRP:CZ3	4:F:22:LEU:CD2	2.97	0.47
1:B:985:THR:HG22	1:B:988:GLU:CG	2.44	0.47
2:C:1273:VAL:HB	2:C:1282:LEU:HD13	1.97	0.47
3:G:275:TYR:CE2	4:H:40:HIS:CG	3.02	0.47
1:A:394:ILE:HG23	1:A:705:ASP:HB2	1.96	0.47
3:D:208:THR:O	3:D:217:HIS:HB2	2.15	0.47
1:A:910:MET:HB3	1:A:926:LEU:HB2	1.97	0.47
3:G:85:PHE:CE1	3:G:97:PHE:CZ	2.76	0.47
4:H:13:GLU:CB	4:H:14:PRO:CD	2.84	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:691:LEU:HD21	1:A:704:ILE:HB	1.96	0.47
1:A:889:ARG:HG2	1:A:904:ASN:ND2	2.30	0.47
1:B:328:LEU:HD13	1:B:381:ALA:HB3	1.97	0.47
1:B:637:VAL:HB	1:B:652:CYS:HB2	1.97	0.47
2:C:1137:ALA:O	2:C:1139:THR:HG23	2.16	0.46
2:C:1379:ASN:ND2	2:C:1379:ASN:H	2.13	0.46
4:F:18:TRP:CH2	4:F:22:LEU:CD2	2.99	0.46
2:E:1088:GLU:CD	4:F:62:ARG:HH22	2.19	0.46
3:G:85:PHE:HD2	3:G:86:GLY:H	1.63	0.46
1:A:1058:LEU:HD23	1:A:1062:ILE:HD11	1.96	0.46
1:B:998:PHE:CE1	1:B:1074:ARG:HD3	2.50	0.46
1:B:830:ILE:HG12	1:B:850:VAL:HG13	1.97	0.46
1:B:873:MET:HB3	1:B:880:LEU:HD11	1.96	0.46
2:C:1054:LEU:HD12	2:C:1057:ARG:HD2	1.97	0.46
2:C:1294:LEU:HD11	2:C:1308:MET:CE	2.45	0.46
2:C:1298:ARG:HH22	2:C:1330:PHE:CB	2.28	0.46
3:D:275:TYR:CD2	4:F:40:HIS:CE1	3.03	0.46
1:A:362:MET:HB2	1:A:1006:VAL:HG21	1.96	0.46
1:A:1057:ARG:HH12	1:A:1110:ALA:HB3	1.80	0.46
2:C:1156:TRP:CG	4:H:29:GLU:HG2	2.50	0.46
1:B:1057:ARG:HH12	1:B:1110:ALA:HB3	1.81	0.46
3:D:242:PHE:CE2	3:D:256:ILE:HG12	2.47	0.46
2:E:1187:HIS:HE1	2:E:1190:ASP:H	1.63	0.46
4:F:18:TRP:CH2	4:F:22:LEU:HD22	2.50	0.46
2:C:1187:HIS:HE1	2:C:1190:ASP:H	1.62	0.46
2:C:1298:ARG:NH2	2:C:1330:PHE:CB	2.77	0.46
3:D:85:PHE:CE1	3:D:97:PHE:CZ	3.04	0.46
1:A:316:TYR:CZ	1:A:318:ASP:HA	2.51	0.46
1:B:547:GLY:HA2	1:B:548:ASP:HA	1.72	0.46
2:C:1068:GLY:HA3	2:C:1069:GLY:HA3	1.42	0.46
3:G:189:HIS:CD2	3:G:191:ASP:HB3	2.51	0.46
1:B:316:TYR:CZ	1:B:318:ASP:HA	2.50	0.46
2:C:1049:ASN:OD1	2:C:1051:THR:HG22	2.15	0.46
1:B:836:VAL:HG22	2:E:1051:THR:HG21	1.96	0.46
4:F:8:GLN:HB3	4:F:8:GLN:HE21	1.59	0.46
1:A:478:LEU:HD23	1:A:526:LEU:HG	1.98	0.46
1:B:361:ASP:H	1:B:378:CYS:HB2	1.81	0.46
1:B:471:ILE:HG23	1:B:476:VAL:HG22	1.96	0.46
2:E:1342:TYR:CD1	2:E:1342:TYR:N	2.84	0.46
1:A:637:VAL:HB	1:A:652:CYS:HB2	1.98	0.46
1:B:820:LYS:HD3	1:B:825:PRO:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1279:ILE:HG22	2:E:1289:HIS:O	2.16	0.46
4:H:46:ILE:CD1	4:H:60:ILE:HG13	2.46	0.46
2:E:1149:LEU:HD13	2:E:1163:LEU:HD21	1.98	0.45
4:F:12:ARG:N	4:F:12:ARG:CD	2.72	0.45
1:A:141:LYS:HE2	1:A:154:ALA:HB3	1.98	0.45
1:A:820:LYS:HD3	1:A:825:PRO:HA	1.97	0.45
2:C:1082:PRO:HA	2:C:1386:LEU:O	2.17	0.45
2:C:1359:THR:HB	2:C:1366:LEU:HD12	1.98	0.45
2:E:1073:ARG:CD	2:E:1306:THR:HG22	2.45	0.45
1:A:39:LEU:HD13	1:A:64:MET:HE1	1.96	0.45
1:B:1002:GLU:HB3	1:B:1032:THR:HG21	1.96	0.45
3:D:148:HIS:ND1	3:D:212:HIS:HA	2.31	0.45
3:D:97:PHE:HD1	3:D:97:PHE:H	1.63	0.45
2:E:1180:HIS:HD2	2:E:1197:GLY:H	1.63	0.45
3:G:208:THR:O	3:G:217:HIS:HB2	2.17	0.45
1:A:830:ILE:HG12	1:A:850:VAL:HG13	1.98	0.45
3:G:126:PHE:HB3	3:G:129:THR:CG2	2.47	0.45
4:H:44:GLN:O	4:H:47:TYR:N	2.49	0.45
1:A:504:ASN:HD21	1:A:507:GLN:HB2	1.81	0.45
1:A:857:LYS:HG2	1:A:858:LEU:H	1.82	0.45
2:C:1088:GLU:CD	4:H:62:ARG:HH22	2.20	0.45
3:D:271:PRO:O	4:F:27:LYS:NZ	2.45	0.45
1:A:416:ASP:HB3	1:A:419:ARG:HD3	1.99	0.45
1:A:731:GLN:O	1:A:796:GLN:HB2	2.17	0.45
1:B:691:LEU:HD21	1:B:704:ILE:HB	1.99	0.45
2:C:1087:ARG:HH12	2:C:1372:GLN:HE21	1.64	0.45
2:C:1342:TYR:H	2:C:1342:TYR:HD1	1.64	0.45
1:B:64:MET:HG3	1:B:77:LEU:HD11	1.98	0.45
2:C:1250:GLN:HE21	2:C:1251:ALA:H	1.64	0.45
4:F:40:HIS:C	4:F:42:LEU:N	2.69	0.45
1:A:123:ILE:HD12	1:A:169:PHE:CD1	2.52	0.45
1:B:84:TYR:OH	1:B:115:PRO:HB3	2.17	0.45
1:B:775:THR:HA	1:B:776:ALA:HA	1.53	0.45
2:C:1066:VAL:HG13	2:C:1067:ASP:N	2.31	0.45
2:E:1102:SER:HB3	2:E:1107:PHE:O	2.17	0.45
1:A:561:TRP:CD1	1:A:587:ILE:HD11	2.52	0.45
2:C:1096:PHE:HA	2:C:1111:GLY:O	2.16	0.45
2:E:1099:CYS:HB3	2:E:1369:ILE:HD11	1.98	0.45
1:A:15:VAL:HG13	1:A:33:ILE:HG23	1.99	0.44
1:B:123:ILE:HD12	1:B:169:PHE:CD1	2.53	0.44
1:A:36:ASN:HD21	1:A:60:LYS:HG2	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:PHE:HB2	1:A:623:LEU:HD22	1.99	0.44
3:G:206:VAL:HG22	3:G:222:TRP:HB2	2.00	0.44
4:H:12:ARG:HD3	4:H:12:ARG:N	2.32	0.44
1:A:500:VAL:HG21	1:A:540:CYS:HA	1.99	0.44
1:B:561:TRP:CD1	1:B:587:ILE:HD11	2.53	0.44
1:B:81:THR:HG23	1:B:83:LYS:H	1.82	0.44
3:G:273:SER:O	4:H:40:HIS:CD2	2.70	0.44
2:E:1118:LYS:HE2	2:E:1130:SER:HB2	1.99	0.44
3:G:246:GLY:HA3	3:G:268:HIS:HB2	1.99	0.44
1:B:504:ASN:HD21	1:B:507:GLN:HB2	1.83	0.44
2:E:1159:PRO:HA	2:E:1177:THR:HA	1.99	0.44
3:G:204:ASN:O	3:G:226:THR:HG21	2.18	0.44
4:H:11:GLN:CA	4:H:12:ARG:NH1	2.81	0.44
1:B:81:THR:HG21	1:B:85:ASN:ND2	2.32	0.44
3:D:113:ARG:HG2	3:D:118:VAL:HB	1.98	0.44
3:D:85:PHE:CD1	3:D:97:PHE:HZ	2.35	0.44
2:E:1221:ASN:HB3	2:E:1257:LYS:HD2	2.00	0.44
4:F:42:LEU:O	4:F:46:ILE:HG12	2.17	0.44
4:H:20:LEU:O	4:H:24:GLU:OE1	2.35	0.44
1:B:183:GLN:NE2	1:B:188:ARG:HE	2.14	0.44
1:B:265:ASP:HA	1:B:266:PRO:HD2	1.81	0.44
1:B:15:VAL:HG13	1:B:33:ILE:HG23	1.98	0.44
3:G:105:LEU:HD11	3:G:222:TRP:CE2	2.53	0.44
1:A:105:HIS:CA	1:A:152:LEU:HD12	2.47	0.44
2:C:1102:SER:HB3	2:C:1107:PHE:O	2.18	0.44
3:G:84:PHE:CD1	3:G:84:PHE:O	2.71	0.44
4:H:23:LEU:O	4:H:27:LYS:HG3	2.17	0.44
3:D:204:ASN:O	3:D:226:THR:HG21	2.18	0.44
3:G:173:ILE:HG22	3:G:278:PHE:CZ	2.53	0.44
1:A:168:LYS:HG3	1:A:219:VAL:O	2.16	0.43
1:B:6:VAL:HG22	1:B:1040:VAL:HG22	2.00	0.43
1:B:174:GLN:HG3	1:B:175:ALA:H	1.82	0.43
1:B:404:LEU:O	1:B:407:ILE:HD11	2.18	0.43
2:C:1077:PHE:CD2	2:C:1307:VAL:HG21	2.53	0.43
2:C:1337:PHE:HD1	2:C:1344:PRO:HA	1.83	0.43
4:H:46:ILE:HD13	4:H:60:ILE:HB	1.99	0.43
1:A:936:LYS:HG3	1:A:943:GLU:CG	2.46	0.43
1:B:334:VAL:HG13	1:B:347:VAL:HG23	2.00	0.43
1:B:864:LYS:CB	1:B:899:LEU:HD12	2.48	0.43
2:E:1118:LYS:HB3	2:E:1120:TYR:CE2	2.53	0.43
2:E:1149:LEU:HD13	2:E:1163:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:148:HIS:ND1	3:G:212:HIS:HA	2.33	0.43
3:G:279:PHE:HA	3:G:279:PHE:HD1	1.70	0.43
1:A:935:TYR:O	1:A:937:PRO:HD3	2.18	0.43
1:B:614:PHE:HB2	1:B:623:LEU:HD22	1.99	0.43
2:C:1121:ASN:HB3	2:C:1124:SER:OG	2.18	0.43
1:A:174:GLN:H	1:A:174:GLN:CD	2.22	0.43
1:A:292:ASP:HA	1:A:293:GLY:HA2	1.72	0.43
1:B:816:LEU:HB3	1:B:831:VAL:HG22	2.00	0.43
3:D:105:LEU:HD11	3:D:222:TRP:CE2	2.53	0.43
2:E:1342:TYR:HD1	2:E:1342:TYR:N	2.15	0.43
1:A:780:THR:HA	1:A:781:SER:HA	1.95	0.43
1:A:884:ILE:HD13	1:A:889:ARG:HD2	2.01	0.43
2:C:1149:LEU:CD1	2:C:1205:ILE:HD12	2.47	0.43
2:C:1355:PHE:CE1	2:C:1371:ASN:HB2	2.53	0.43
1:A:541:LEU:HB3	1:A:558:ILE:HD12	2.00	0.43
1:A:64:MET:HG3	1:A:77:LEU:HD11	2.01	0.43
1:B:928:ARG:HD2	1:B:947:ARG:HH12	1.83	0.43
1:A:334:VAL:HG13	1:A:347:VAL:HG23	2.01	0.43
1:A:396:ILE:HD12	1:A:673:LEU:HD11	2.01	0.43
1:A:578:HIS:HE1	1:A:580:GLU:HG2	1.83	0.43
1:A:58:TYR:CD1	1:A:1073:TRP:CD1	3.05	0.43
1:B:114:ARG:HA	1:B:115:PRO:HD3	1.88	0.43
1:B:506:SER:HA	1:B:521:ILE:HB	2.01	0.43
1:B:568:ILE:HD12	1:B:578:HIS:HB3	2.00	0.43
2:E:1081:ARG:O	2:E:1388:GLU:N	2.48	0.43
4:H:16:ASN:OD1	4:H:16:ASN:N	2.47	0.43
1:A:1080:ARG:H	1:A:1080:ARG:HG2	1.48	0.43
1:B:578:HIS:HE1	1:B:580:GLU:HG2	1.83	0.43
2:C:1069:GLY:O	2:C:1073:ARG:HG2	2.18	0.43
4:F:16:ASN:O	4:F:17:GLU:HG3	2.19	0.43
1:A:404:LEU:HD11	1:A:434:ARG:HH12	1.83	0.43
1:B:541:LEU:HB3	1:B:558:ILE:HD12	2.00	0.43
1:B:327:ARG:HH12	2:E:1060:PHE:H	1.66	0.43
4:F:16:ASN:HD22	4:F:16:ASN:H	1.60	0.43
4:F:41:ASN:O	4:F:45:HIS:HD2	2.02	0.43
1:A:84:TYR:OH	1:A:115:PRO:HB3	2.18	0.42
2:C:1366:LEU:HB3	2:C:1387:TYR:HB2	2.01	0.42
3:G:139:VAL:HB	3:G:200:VAL:HG13	2.01	0.42
3:G:97:PHE:N	3:G:97:PHE:HD1	2.12	0.42
2:C:1156:TRP:CD2	4:H:29:GLU:HG2	2.54	0.42
1:A:321:VAL:HG13	1:A:350:MET:HE3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:816:LEU:HB3	1:A:831:VAL:HG22	2.01	0.42
1:A:881:LEU:HD21	1:A:921:ILE:HG21	2.02	0.42
2:C:1342:TYR:CD1	2:C:1342:TYR:N	2.87	0.42
1:A:362:MET:HG3	1:A:377:THR:HG22	2.01	0.42
1:B:1080:ARG:H	1:B:1080:ARG:HG2	1.48	0.42
1:B:881:LEU:HD21	1:B:921:ILE:HG21	2.02	0.42
1:B:974:LEU:HB2	1:B:998:PHE:HB3	2.02	0.42
1:A:506:SER:HA	1:A:521:ILE:HB	2.00	0.42
1:A:578:HIS:CE1	1:A:580:GLU:HG2	2.55	0.42
1:B:58:TYR:CD1	1:B:1073:TRP:CD1	3.07	0.42
1:B:605:ALA:HB1	1:B:636:THR:HB	2.01	0.42
1:A:836:VAL:HG22	2:C:1051:THR:HG21	2.01	0.42
3:D:206:VAL:HG22	3:D:222:TRP:HB2	2.00	0.42
3:G:156:LEU:HB2	3:G:159:SER:HB3	2.00	0.42
3:G:273:SER:C	3:G:275:TYR:H	2.21	0.42
1:A:739:ARG:HG3	1:A:788:VAL:HB	2.02	0.42
1:B:578:HIS:CE1	1:B:580:GLU:HG2	2.55	0.42
1:B:935:TYR:O	1:B:937:PRO:HD3	2.19	0.42
1:A:1030:PHE:CE1	1:A:1036:MET:CE	3.02	0.42
1:A:605:ALA:HB1	1:A:636:THR:HB	2.00	0.42
2:C:1059:SER:HG	2:C:1060:PHE:HD1	1.66	0.42
2:C:1274:ILE:HD12	2:C:1279:ILE:HG12	2.02	0.42
1:A:407:ILE:HG21	1:A:427:LEU:HD23	2.02	0.42
1:B:316:TYR:CE2	1:B:318:ASP:HA	2.54	0.42
1:B:739:ARG:HG3	1:B:788:VAL:HB	2.02	0.42
2:E:1082:PRO:HA	2:E:1387:TYR:HA	2.01	0.42
2:E:1180:HIS:CD2	2:E:1197:GLY:H	2.38	0.42
4:F:46:ILE:HD12	4:F:63:ILE:HD13	2.02	0.42
1:A:404:LEU:O	1:A:407:ILE:HD11	2.19	0.42
1:A:638:LEU:HD23	1:A:649:VAL:HG11	2.01	0.42
1:B:927:MET:HG3	1:B:953:TRP:CE2	2.55	0.42
3:D:126:PHE:HB3	3:D:129:THR:CG2	2.49	0.42
2:E:1047:PRO:HG2	2:E:1053:ARG:HA	2.02	0.42
1:B:518:TYR:CD1	1:B:529:ILE:HB	2.55	0.42
1:B:731:GLN:O	1:B:796:GLN:HB2	2.19	0.42
1:B:724:ILE:CD1	1:B:735:VAL:CG2	2.93	0.42
2:E:1109:MET:HB2	2:E:1117:LEU:HD11	2.02	0.42
3:G:158:PHE:O	3:G:170:LEU:HD13	2.20	0.42
1:A:411:TRP:HA	1:A:412:PRO:HD3	1.96	0.42
1:A:568:ILE:HD12	1:A:578:HIS:HB3	2.02	0.42
1:B:141:LYS:HE2	1:B:154:ALA:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1223:TYR:HE2	2:C:1241:GLY:HA3	1.85	0.42
2:E:1074:HIS:CD2	2:E:1345:ILE:HG12	2.55	0.42
1:A:1131:LYS:HD2	1:A:1131:LYS:HA	1.94	0.41
3:G:140:VAL:HB	3:G:242:PHE:CE1	2.55	0.41
3:G:131:MET:HG3	3:G:197:LYS:HG3	2.02	0.41
1:A:518:TYR:CD1	1:A:529:ILE:HB	2.55	0.41
3:D:140:VAL:HB	3:D:242:PHE:CE1	2.55	0.41
3:G:275:TYR:CD2	4:H:40:HIS:CG	3.09	0.41
4:H:15:TYR:HB3	4:H:16:ASN:H	1.71	0.41
1:A:476:VAL:HB	1:A:490:TRP:HB3	2.02	0.41
1:A:39:LEU:CD1	1:A:64:MET:CE	2.97	0.41
2:E:1259:ASN:OD1	2:E:1262:ILE:N	2.49	0.41
1:A:182:TYR:CE2	1:A:189:HIS:HB2	2.54	0.41
1:A:317:LEU:HD12	1:A:321:VAL:HG12	2.01	0.41
1:A:415:SER:N	1:A:423:ASP:OD1	2.43	0.41
1:A:727:GLN:HB3	1:A:730:SER:HB2	2.02	0.41
1:A:824:ASP:HA	1:A:825:PRO:HD3	1.90	0.41
2:E:1243:LEU:HB2	2:E:1255:PHE:HE2	1.86	0.41
4:F:23:LEU:HD11	4:F:60:ILE:HG23	2.01	0.41
4:F:64:LEU:HA	4:F:67:LEU:HD12	2.02	0.41
1:A:928:ARG:HD2	1:A:947:ARG:HH12	1.85	0.41
3:D:139:VAL:HB	3:D:200:VAL:HG13	2.02	0.41
2:E:1202:ILE:O	2:E:1210:LYS:HA	2.20	0.41
4:F:59:ALA:O	4:F:63:ILE:HD12	2.21	0.41
1:A:305:LEU:HA	1:A:346:TYR:HD2	1.85	0.41
2:E:1330:PHE:CD1	2:E:1330:PHE:N	2.88	0.41
1:A:125:ASP:OD2	1:A:127:GLU:HB2	2.21	0.41
1:B:578:HIS:HD2	1:B:622:LEU:HD23	1.86	0.41
1:B:884:ILE:HD13	1:B:889:ARG:HD2	2.03	0.41
1:B:910:MET:O	1:B:912:LEU:HG	2.21	0.41
4:H:12:ARG:NH1	4:H:12:ARG:HG2	2.36	0.41
1:A:654:ASP:HA	1:A:675:GLU:HG3	2.03	0.41
1:B:826:ASN:HB2	1:B:828:TYR:CZ	2.56	0.41
2:E:1151:LEU:HD11	2:E:1192:VAL:HG22	2.02	0.41
1:A:985:THR:HA	3:D:219:GLU:OE2	2.21	0.41
1:B:369:ARG:HG3	1:B:370:GLN:N	2.35	0.41
2:E:1376:ASP:C	2:E:1378:LEU:H	2.25	0.41
1:A:6:VAL:HG22	1:A:1040:VAL:HG22	2.02	0.41
1:A:910:MET:O	1:A:912:LEU:HG	2.21	0.41
3:D:131:MET:HG3	3:D:197:LYS:HG3	2.03	0.41
3:D:156:LEU:HB2	3:D:159:SER:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1342:TYR:H	2:E:1342:TYR:HD1	1.69	0.41
1:A:592:LEU:HD22	1:A:594:THR:HB	2.04	0.40
2:C:1088:GLU:HB3	2:C:1094:SER:HA	2.03	0.40
2:C:1191:ARG:HA	2:C:1203:TYR:O	2.21	0.40
4:F:22:LEU:O	4:F:22:LEU:CG	2.69	0.40
3:G:170:LEU:HD12	3:G:173:ILE:CG1	2.50	0.40
1:A:57:MET:SD	1:A:1065:VAL:HB	2.61	0.40
1:B:396:ILE:HD12	1:B:673:LEU:HD11	2.03	0.40
2:C:1267:HIS:CE1	2:C:1268:PRO:HD2	2.55	0.40
2:C:1267:HIS:ND1	2:C:1269:ASN:ND2	2.70	0.40
1:A:328:LEU:HA	1:A:328:LEU:HD23	1.76	0.40
1:A:58:TYR:HB3	1:A:1073:TRP:HB2	2.02	0.40
1:A:677:ASN:HB2	1:A:695:ASN:HA	2.02	0.40
1:B:638:LEU:HD23	1:B:649:VAL:HG11	2.03	0.40
1:B:727:GLN:HB3	1:B:730:SER:HB2	2.02	0.40
2:C:1187:HIS:ND1	2:C:1188:SER:N	2.69	0.40
2:C:1245:ASP:HB2	2:C:1252:ILE:HD11	2.03	0.40
4:F:2:GLU:HB3	4:F:3:GLN:H	1.70	0.40
1:A:101:ILE:H	1:A:101:ILE:HG13	1.64	0.40
1:A:725:CYS:SG	1:A:817:VAL:HA	2.62	0.40
1:B:292:ASP:HA	1:B:293:GLY:HA2	1.73	0.40
3:G:140:VAL:HG21	3:G:233:LEU:HD13	2.03	0.40
4:H:1:MET:HA	4:H:2:GLU:CG	2.51	0.40
1:A:207:TRP:HB3	1:A:242:GLY:HA2	2.04	0.40
1:A:930:VAL:HG13	1:A:954:MET:HE2	2.03	0.40
1:B:407:ILE:HG21	1:B:427:LEU:HD23	2.03	0.40
2:C:1089:ALA:HB2	2:C:1127:GLU:OE1	2.22	0.40
2:E:1269:ASN:O	2:E:1271:LEU:HD13	2.21	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	1127/1140 (99%)	991 (88%)	106 (9%)	30 (3%)	6	40
1	B	1127/1140 (99%)	997 (88%)	104 (9%)	26 (2%)	7	43
2	C	327/361 (91%)	278 (85%)	31 (10%)	18 (6%)	2	22
2	E	327/361 (91%)	279 (85%)	35 (11%)	13 (4%)	3	30
3	D	219/222 (99%)	191 (87%)	17 (8%)	11 (5%)	2	24
3	G	219/222 (99%)	186 (85%)	22 (10%)	11 (5%)	2	24
4	F	72/96 (75%)	50 (69%)	12 (17%)	10 (14%)	0	4
4	H	72/96 (75%)	57 (79%)	8 (11%)	7 (10%)	1	9
All	All	3490/3638 (96%)	3029 (87%)	335 (10%)	126 (4%)	4	33

All (126) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	LEU
1	A	206	PRO
1	A	290	GLN
1	A	576	LEU
1	A	770	LEU
1	A	772	SER
1	A	1110	ALA
1	B	162	LEU
1	B	206	PRO
1	B	290	GLN
1	B	576	LEU
1	B	770	LEU
1	B	772	SER
1	B	1110	ALA
2	C	1060	PHE
2	C	1089	ALA
2	C	1188	SER
2	C	1329	PRO
2	C	1342	TYR
2	C	1378	LEU
2	C	1379	ASN
3	D	94	SER
3	D	214	ALA
3	D	216	SER
3	D	247	SER
3	D	273	SER
3	D	276	ARG

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Mol	Chain	Res	Type
2	E	1060	PHE
2	E	1067	ASP
2	E	1089	ALA
2	E	1188	SER
2	E	1342	TYR
2	E	1375	MET
2	E	1379	ASN
4	F	6	GLU
4	F	7	ASP
4	F	10	PRO
4	F	16	ASN
3	G	94	SER
3	G	214	ALA
3	G	216	SER
3	G	247	SER
4	H	2	GLU
4	H	10	PRO
4	H	11	GLN
4	H	15	TYR
4	H	16	ASN
1	A	214	ALA
1	A	318	ASP
1	A	371	GLY
1	A	618	ILE
1	A	780	THR
1	A	907	ASN
1	B	214	ALA
1	B	318	ASP
1	B	618	ILE
1	B	707	ILE
1	B	780	THR
1	B	907	ASN
2	C	1167	LYS
2	C	1187	HIS
2	C	1189	GLN
2	C	1256	ASP
2	C	1362	LYS
2	C	1374	SER
3	D	274	VAL
2	E	1167	LYS
2	E	1189	GLN
2	E	1256	ASP

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Mol	Chain	Res	Type
2	E	1362	LYS
4	F	2	GLU
4	F	44	GLN
4	F	45	HIS
4	H	13	GLU
1	A	36	ASN
1	A	369	ARG
1	A	534	MET
1	A	1080	ARG
1	B	147	ARG
1	B	319	ASN
1	B	534	MET
1	B	598	SER
1	B	1080	ARG
2	C	1278	GLU
3	D	122	PRO
2	E	1187	HIS
2	E	1380	MET
4	F	15	TYR
3	G	122	PRO
3	G	219	GLU
3	G	273	SER
1	A	234	GLN
1	A	319	ASN
1	A	370	GLN
1	A	562	THR
1	A	598	SER
1	B	562	THR
4	F	41	ASN
1	A	147	ARG
1	B	234	GLN
1	B	266	PRO
2	C	1375	MET
3	D	218	LYS
3	D	219	GLU
4	F	13	GLU
3	G	218	LYS
3	G	222	TRP
3	G	277	GLY
1	A	597	GLU
1	A	698	THR
1	A	707	ILE

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Mol	Chain	Res	Type
1	B	148	ASP
1	B	597	GLU
2	C	1066	VAL
2	C	1137	ALA
3	D	222	TRP
4	H	58	GLU
1	A	233	GLY
1	A	185	PRO
1	A	266	PRO
1	B	185	PRO
1	B	233	GLY
1	A	564	ILE
1	B	564	ILE
2	C	1138	ILE
3	G	274	VAL

### 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	994/999 (100%)	852 (86%)	142 (14%)	4	22
1	B	934/999 (94%)	801 (86%)	133 (14%)	4	22
2	C	291/317 (92%)	239 (82%)	52 (18%)	2	11
2	E	291/317 (92%)	238 (82%)	53 (18%)	2	11
3	D	193/194 (100%)	181 (94%)	12 (6%)	21	59
3	G	193/194 (100%)	179 (93%)	14 (7%)	16	53
4	F	66/83 (80%)	50 (76%)	16 (24%)	1	4
4	H	66/83 (80%)	55 (83%)	11 (17%)	2	14
All	All	3028/3186 (95%)	2595 (86%)	433 (14%)	4	22

All (433) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	37	THR
1	A	49	LEU
1	A	54	GLU
1	A	68	ARG
1	A	73	SER
1	A	74	LYS
1	A	101	ILE
1	A	111	ARG
1	A	130	MET
1	A	146	ASP
1	A	148	ASP
1	A	150	LYS
1	A	152	LEU
1	A	160	GLU
1	A	162	LEU
1	A	173	CYS
1	A	184	ASP
1	A	208	LYS
1	A	209	GLN
1	A	210	GLU
1	A	213	GLU
1	A	218	MET
1	A	219	VAL
1	A	232	ILE
1	A	235	GLU
1	A	255	GLN
1	A	258	ILE
1	A	264	VAL
1	A	284	LEU
1	A	288	GLU
1	A	294	THR
1	A	299	ASP
1	A	300	LEU
1	A	304	LEU
1	A	307	GLU
1	A	317	LEU
1	A	322	VAL
1	A	328	LEU
1	A	340	SER
1	A	345	SER
1	A	354	THR
1	A	355	ASN

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Mol	Chain	Res	Type
1	A	366	ASP
1	A	369	ARG
1	A	378	CYS
1	A	392	ASN
1	A	403	ASP
1	A	407	ILE
1	A	414	ARG
1	A	434	ARG
1	A	435	VAL
1	A	438	LEU
1	A	439	ASN
1	A	442	GLU
1	A	445	GLU
1	A	472	THR
1	A	478	LEU
1	A	488	SER
1	A	516	LEU
1	A	520	GLN
1	A	528	GLN
1	A	541	LEU
1	A	544	THR
1	A	555	LEU
1	A	558	ILE
1	A	560	LEU
1	A	577	LEU
1	A	585	GLU
1	A	590	SER
1	A	598	SER
1	A	602	LEU
1	A	620	THR
1	A	640	THR
1	A	646	THR
1	A	647	THR
1	A	661	SER
1	A	680	CYS
1	A	685	ASP
1	A	691	LEU
1	A	698	THR
1	A	713	ARG
1	A	724	ILE
1	A	725	CYS
1	A	730	SER

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Mol	Chain	Res	Type
1	A	737	SER
1	A	738	SER
1	A	775	THR
1	A	780	THR
1	A	781	SER
1	A	790	ASN
1	A	796	GLN
1	A	797	HIS
1	A	806	GLN
1	A	809	GLN
1	A	817	VAL
1	A	820	LYS
1	A	829	PHE
1	A	830	ILE
1	A	849	VAL
1	A	858	LEU
1	A	864	LYS
1	A	873	MET
1	A	874	VAL
1	A	877	ASN
1	A	883	SER
1	A	895	THR
1	A	901	THR
1	A	902	GLU
1	A	904	ASN
1	A	908	ASN
1	A	909	ILE
1	A	923	VAL
1	A	936	LYS
1	A	938	MET
1	A	947	ARG
1	A	962	ASP
1	A	965	PHE
1	A	966	LEU
1	A	985	THR
1	A	992	LEU
1	A	993	GLN
1	A	1006	VAL
1	A	1007	PHE
1	A	1036	MET
1	A	1039	LEU
1	A	1042	SER

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Mol	Chain	Res	Type
1	A	1045	GLU
1	A	1051	LEU
1	A	1058	LEU
1	A	1063	LYS
1	A	1065	VAL
1	A	1075	SER
1	A	1080	ARG
1	A	1083	GLU
1	A	1094	ILE
1	A	1101	SER
1	A	1102	ARG
1	A	1122	ARG
1	A	1128	ASP
1	A	1137	THR
1	A	1139	ILE
1	B	20	THR
1	B	49	LEU
1	B	54	GLU
1	B	74	LYS
1	B	81	THR
1	B	101	ILE
1	B	130	MET
1	B	146	ASP
1	B	148	ASP
1	B	150	LYS
1	B	152	LEU
1	B	160	GLU
1	B	162	LEU
1	B	173	CYS
1	B	174	GLN
1	B	184	ASP
1	B	207	TRP
1	B	208	LYS
1	B	209	GLN
1	B	210	GLU
1	B	213	GLU
1	B	218	MET
1	B	219	VAL
1	B	232	ILE
1	B	235	GLU
1	B	252	ILE
1	B	255	GLN

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Mol	Chain	Res	Type
1	B	258	ILE
1	B	264	VAL
1	B	265	ASP
1	B	284	LEU
1	B	288	GLU
1	B	294	THR
1	B	299	ASP
1	B	300	LEU
1	B	304	LEU
1	B	307	GLU
1	B	317	LEU
1	B	322	VAL
1	B	340	SER
1	B	345	SER
1	B	354	THR
1	B	355	ASN
1	B	366	ASP
1	B	392	ASN
1	B	403	ASP
1	B	407	ILE
1	B	414	ARG
1	B	423	ASP
1	B	435	VAL
1	B	437	MET
1	B	438	LEU
1	B	439	ASN
1	B	442	GLU
1	B	445	GLU
1	B	472	THR
1	B	488	SER
1	B	516	LEU
1	B	519	LEU
1	B	520	GLN
1	B	528	GLN
1	B	541	LEU
1	B	544	THR
1	B	555	LEU
1	B	558	ILE
1	B	560	LEU
1	B	577	LEU
1	B	589	ARG
1	B	590	SER

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Mol	Chain	Res	Type
1	B	593	MET
1	B	598	SER
1	B	602	LEU
1	B	611	LEU
1	B	620	THR
1	B	640	THR
1	B	646	THR
1	B	647	THR
1	B	661	SER
1	B	680	CYS
1	B	685	ASP
1	B	691	LEU
1	B	698	THR
1	B	707	ILE
1	B	713	ARG
1	B	730	SER
1	B	737	SER
1	B	738	SER
1	B	790	ASN
1	B	796	GLN
1	B	797	HIS
1	B	806	GLN
1	B	809	GLN
1	B	817	VAL
1	B	820	LYS
1	B	829	PHE
1	B	830	ILE
1	B	849	VAL
1	B	858	LEU
1	B	874	VAL
1	B	877	ASN
1	B	883	SER
1	B	895	THR
1	B	902	GLU
1	B	904	ASN
1	B	908	ASN
1	B	909	ILE
1	B	910	MET
1	B	923	VAL
1	B	938	MET
1	B	947	ARG
1	B	962	ASP

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Mol	Chain	Res	Type
1	B	965	PHE
1	B	966	LEU
1	B	984	THR
1	B	985	THR
1	B	992	LEU
1	B	993	GLN
1	B	1006	VAL
1	B	1007	PHE
1	B	1036	MET
1	B	1039	LEU
1	B	1042	SER
1	B	1051	LEU
1	B	1058	LEU
1	B	1063	LYS
1	B	1065	VAL
1	B	1075	SER
1	B	1080	ARG
1	B	1083	GLU
1	B	1094	ILE
1	B	1101	SER
1	B	1128	ASP
1	B	1137	THR
2	C	1048	ILE
2	C	1057	ARG
2	C	1063	TYR
2	C	1066	VAL
2	C	1072	ASP
2	C	1073	ARG
2	C	1074	HIS
2	C	1075	LEU
2	C	1090	ASN
2	C	1102	SER
2	C	1108	LEU
2	C	1109	MET
2	C	1117	LEU
2	C	1119	LEU
2	C	1146	ASP
2	C	1155	THR
2	C	1157	SER
2	C	1168	SER
2	C	1169	VAL
2	C	1172	MET

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Mol	Chain	Res	Type
2	C	1190	ASP
2	C	1207	THR
2	C	1211	LEU
2	C	1229	THR
2	C	1230	PHE
2	C	1231	ASN
2	C	1234	ASP
2	C	1235	ASP
2	C	1256	ASP
2	C	1259	ASN
2	C	1260	MET
2	C	1272	GLU
2	C	1275	ILE
2	C	1278	GLU
2	C	1286	HIS
2	C	1289	HIS
2	C	1294	LEU
2	C	1296	GLN
2	C	1299	VAL
2	C	1313	LEU
2	C	1330	PHE
2	C	1341	ASP
2	C	1342	TYR
2	C	1343	LYS
2	C	1350	VAL
2	C	1352	ARG
2	C	1354	ILE
2	C	1357	LEU
2	C	1362	LYS
2	C	1374	SER
2	C	1379	ASN
2	C	1386	LEU
3	D	84	PHE
3	D	85	PHE
3	D	88	SER
3	D	90	LYS
3	D	111	GLU
3	D	178	SER
3	D	182	GLU
3	D	206	VAL
3	D	212	HIS
3	D	237	SER

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Mol	Chain	Res	Type
3	D	270	SER
3	D	279	PHE
2	E	1055	ASN
2	E	1063	TYR
2	E	1072	ASP
2	E	1074	HIS
2	E	1075	LEU
2	E	1087	ARG
2	E	1090	ASN
2	E	1091	GLU
2	E	1102	SER
2	E	1119	LEU
2	E	1126	GLN
2	E	1145	ARG
2	E	1146	ASP
2	E	1149	LEU
2	E	1150	LEU
2	E	1160	LEU
2	E	1163	LEU
2	E	1168	SER
2	E	1169	VAL
2	E	1171	ASP
2	E	1172	MET
2	E	1177	THR
2	E	1192	VAL
2	E	1211	LEU
2	E	1229	THR
2	E	1234	ASP
2	E	1235	ASP
2	E	1247	ARG
2	E	1256	ASP
2	E	1260	MET
2	E	1275	ILE
2	E	1277	THR
2	E	1284	THR
2	E	1286	HIS
2	E	1289	HIS
2	E	1294	LEU
2	E	1296	GLN
2	E	1299	VAL
2	E	1313	LEU
2	E	1328	SER

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Mol	Chain	Res	Type
2	E	1330	PHE
2	E	1338	ASN
2	E	1341	ASP
2	E	1342	TYR
2	E	1343	LYS
2	E	1352	ARG
2	E	1353	ASN
2	E	1357	LEU
2	E	1362	LYS
2	E	1372	GLN
2	E	1379	ASN
2	E	1382	THR
2	E	1389	VAL
4	F	1	MET
4	F	6	GLU
4	F	8	GLN
4	F	10	PRO
4	F	11	GLN
4	F	12	ARG
4	F	15	TYR
4	F	21	GLU
4	F	23	LEU
4	F	26	LEU
4	F	46	ILE
4	F	48	GLU
4	F	58	GLU
4	F	63	ILE
4	F	65	GLN
4	F	73	ARG
3	G	84	PHE
3	G	85	PHE
3	G	88	SER
3	G	90	LYS
3	G	97	PHE
3	G	113	ARG
3	G	160	VAL
3	G	172	ASN
3	G	178	SER
3	G	198	GLN
3	G	206	VAL
3	G	212	HIS
3	G	237	SER

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Mol	Chain	Res	Type
3	G	279	PHE
4	H	10	PRO
4	H	14	PRO
4	H	15	TYR
4	H	16	ASN
4	H	22	LEU
4	H	28	SER
4	H	36	ARG
4	H	37	ILE
4	H	42	LEU
4	H	65	GLN
4	H	73	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	36	ASN
1	A	189	HIS
1	A	234	GLN
1	A	261	HIS
1	A	374	GLN
1	A	392	ASN
1	A	432	GLN
1	A	494	GLN
1	A	520	GLN
1	A	524	GLN
1	A	578	HIS
1	A	796	GLN
1	A	904	ASN
1	A	908	ASN
1	A	993	GLN
1	A	1005	ASN
1	A	1016	ASN
1	A	1140	HIS
1	B	85	ASN
1	B	183	GLN
1	B	189	HIS
1	B	209	GLN
1	B	234	GLN
1	B	261	HIS
1	B	392	ASN

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Mol	Chain	Res	Type
1	B	432	GLN
1	B	520	GLN
1	B	578	HIS
1	B	796	GLN
1	B	904	ASN
1	B	908	ASN
1	B	993	GLN
1	B	1005	ASN
1	B	1016	ASN
2	C	1090	ASN
2	C	1174	HIS
2	C	1209	ASN
2	C	1250	GLN
2	C	1338	ASN
2	C	1353	ASN
2	C	1372	GLN
2	C	1379	ASN
3	D	124	GLN
3	D	130	GLN
3	D	172	ASN
3	D	250	GLN
2	E	1090	ASN
2	E	1140	HIS
2	E	1180	HIS
2	E	1201	HIS
2	E	1209	ASN
2	E	1239	ASN
2	E	1250	GLN
2	E	1338	ASN
2	E	1353	ASN
4	F	8	GLN
4	F	16	ASN
4	F	33	HIS
4	F	41	ASN
4	F	45	HIS
4	F	65	GLN
4	F	71	HIS
3	G	124	GLN
3	G	250	GLN
4	H	33	HIS
4	H	40	HIS
4	H	41	ASN

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Mol	Chain	Res	Type
4	H	65	GLN

### 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	1133/1140 (99%)	0.03	38 (3%) 46 38	110, 180, 236, 272	0
1	B	1133/1140 (99%)	1.14	274 (24%) 1 1	157, 231, 290, 296	0
2	C	331/361 (91%)	-0.03	3 (0%) 84 77	107, 149, 194, 240	0
2	E	331/361 (91%)	0.03	9 (2%) 55 46	121, 174, 216, 242	0
3	D	221/222 (99%)	-0.16	6 (2%) 55 46	121, 178, 222, 248	0
3	G	221/222 (99%)	-0.27	0 100 100	129, 172, 221, 253	0
4	F	74/96 (77%)	-0.25	0 100 100	125, 161, 196, 206	0
4	H	74/96 (77%)	-0.19	0 100 100	120, 149, 184, 200	0
All	All	3518/3638 (96%)	0.34	330 (9%) 9 9	107, 190, 284, 296	0

All (330) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	470	GLN	19.4
1	B	520	GLN	11.9
1	B	562	THR	10.8
1	B	521	ILE	10.5
1	B	526	LEU	9.9
1	B	454	ASP	9.8
1	B	576	LEU	9.5
1	B	431	GLY	9.4
1	B	546	LEU	9.1
1	B	409	GLY	9.1
1	B	433	THR	8.7
1	B	434	ARG	8.6
1	B	507	GLN	8.5
1	B	490	TRP	8.5
1	B	556	CYS	8.4
1	B	1011	SER	8.4

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Mol	Chain	Res	Type	RSRZ
1	B	415	SER	8.3
1	B	579	LYS	8.3
1	B	522	HIS	8.2
1	B	525	GLU	8.1
1	B	569	LEU	8.0
1	B	432	GLN	7.9
1	B	443	VAL	7.8
1	B	449	MET	7.6
1	B	410	LEU	7.6
1	B	640	THR	7.6
1	B	604	CYS	7.6
1	B	554	PRO	7.5
1	B	578	HIS	7.2
1	B	428	SER	7.1
1	B	446	THR	6.9
1	B	643	SER	6.8
1	B	484	LYS	6.8
1	B	396	ILE	6.8
1	B	476	VAL	6.8
1	B	506	SER	6.7
1	B	577	LEU	6.5
1	B	1119	GLY	6.5
1	B	457	THR	6.5
1	B	452	VAL	6.4
1	B	610	ALA	6.4
1	B	600	HIS	6.3
1	B	651	ALA	6.3
1	B	612	PHE	6.3
1	B	435	VAL	6.3
1	B	478	LEU	6.2
1	B	656	PRO	6.2
1	B	453	ASP	6.2
1	B	553	SER	6.1
2	E	1328	SER	6.1
1	B	455	GLN	5.9
1	B	630	THR	5.8
1	B	563	ASP	5.7
1	B	580	GLU	5.6
1	B	544	THR	5.6
1	B	451	PHE	5.6
1	B	408	LYS	5.5
1	B	527	ARG	5.5

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Mol	Chain	Res	Type	RSRZ
1	B	465	HIS	5.5
1	B	100	ILE	5.5
1	B	568	ILE	5.5
1	B	697	SER	5.4
1	B	628	LYS	5.4
1	B	920	PHE	5.3
1	B	932	LEU	5.1
1	B	1120	MET	5.1
1	B	528	GLN	5.1
2	E	1314	GLN	5.1
1	B	464	ALA	5.0
1	B	466	GLN	5.0
1	B	430	VAL	5.0
1	B	261	HIS	5.0
1	B	661	SER	4.9
1	B	429	PHE	4.9
1	B	467	GLN	4.9
1	B	495	ALA	4.9
1	B	417	PRO	4.9
1	B	587	ILE	4.9
1	B	673	LEU	4.8
1	B	402	ILE	4.8
1	B	473	SER	4.8
1	A	367	LEU	4.8
1	A	872	SER	4.8
1	B	483	PRO	4.8
1	B	620	THR	4.8
1	B	646	THR	4.8
1	B	49	LEU	4.8
1	B	488	SER	4.7
1	B	626	ARG	4.7
1	B	416	ASP	4.7
1	B	652	CYS	4.7
1	B	64	MET	4.7
1	B	555	LEU	4.7
1	B	39	LEU	4.7
1	B	618	ILE	4.7
1	B	523	PRO	4.6
1	B	397	HIS	4.6
1	B	57	MET	4.6
1	B	405	PRO	4.6
1	B	666	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	919	ASP	4.6
1	B	564	ILE	4.6
1	B	468	LEU	4.6
1	B	638	LEU	4.6
1	B	456	GLN	4.6
1	B	477	ARG	4.5
1	B	605	ALA	4.5
1	B	519	LEU	4.5
1	B	621	GLY	4.5
1	A	100	ILE	4.5
1	B	684	SER	4.4
1	B	657	THR	4.4
1	B	496	LYS	4.4
1	B	479	VAL	4.4
1	B	1023	PRO	4.4
1	B	492	GLU	4.3
1	B	447	GLU	4.3
1	B	89	LEU	4.3
1	B	647	THR	4.3
1	B	427	LEU	4.2
1	B	590	SER	4.2
1	B	1115	ASP	4.2
1	B	485	ALA	4.1
1	B	583	GLY	4.1
1	B	614	PHE	4.1
1	B	613	TYR	4.1
1	B	442	GLU	4.0
1	B	617	ASN	4.0
1	B	481	GLN	4.0
1	B	622	LEU	4.0
1	B	574	PHE	4.0
1	B	322	VAL	3.9
1	B	474	ALA	3.9
1	B	599	SER	3.9
1	B	418	ASN	3.9
1	A	1115	ASP	3.9
1	B	582	LEU	3.9
1	B	501	ALA	3.8
1	B	1097	PHE	3.8
1	B	407	ILE	3.8
1	B	536	HIS	3.8
1	B	472	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	502	SER	3.7
3	D	84	PHE	3.7
1	B	1010	GLY	3.6
3	D	304	LEU	3.6
1	B	703	THR	3.6
1	B	864	LYS	3.6
1	B	586	ILE	3.6
1	B	480	SER	3.6
1	B	494	GLN	3.6
1	B	588	PRO	3.5
1	B	547	GLY	3.5
1	B	458	PHE	3.5
1	B	696	ASN	3.5
1	B	505	SER	3.5
1	A	542	ASP	3.4
1	B	1017	LEU	3.4
1	B	503	CYS	3.4
1	B	450	GLY	3.4
1	B	471	ILE	3.4
1	B	444	GLU	3.4
1	B	575	GLU	3.4
1	A	1121	LYS	3.4
1	B	55	VAL	3.3
1	B	880	LEU	3.3
1	B	933	LEU	3.3
1	B	629	VAL	3.3
1	B	489	GLU	3.3
1	B	601	TYR	3.3
1	B	699	LEU	3.3
1	B	504	ASN	3.2
1	B	448	LEU	3.2
1	B	821	LEU	3.2
1	A	566	ALA	3.2
1	B	642	ARG	3.2
1	B	260	CYS	3.2
1	B	436	LEU	3.1
1	A	470	GLN	3.1
1	A	815	SER	3.1
1	B	581	MET	3.1
1	B	639	ARG	3.1
1	B	524	GLN	3.1
1	B	584	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	20	THR	3.1
1	B	469	ILE	3.1
1	B	312	GLU	3.0
1	B	542	ASP	3.0
1	B	644	LEU	3.0
1	B	493	PRO	3.0
1	A	567	ARG	3.0
2	C	1366	LEU	3.0
1	B	799	PHE	3.0
1	B	532	THR	3.0
1	B	865	GLU	3.0
1	A	549	SER	2.9
1	B	606	LEU	2.9
1	B	565	SER	2.9
1	B	611	LEU	2.9
1	B	18	CYS	2.9
1	B	633	THR	2.9
1	B	440	GLY	2.9
1	B	317	LEU	2.9
1	B	552	LEU	2.8
1	B	534	MET	2.8
1	B	921	ILE	2.8
1	B	676	VAL	2.8
2	E	1227	CYS	2.8
1	B	634	GLN	2.7
1	B	168	LYS	2.7
1	B	263	ARG	2.7
1	A	253	ILE	2.7
1	B	561	TRP	2.7
1	B	1007	PHE	2.7
1	B	253	ILE	2.7
1	B	706	GLU	2.7
1	A	1113	GLN	2.7
1	B	122	GLY	2.7
1	B	406	GLY	2.7
1	B	441	GLU	2.7
1	B	627	LYS	2.6
1	B	567	ARG	2.6
1	B	571	LEU	2.6
1	A	725	CYS	2.6
1	B	1016	ASN	2.6
1	B	459	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	1116	ASP	2.6
1	B	594	THR	2.6
1	B	40	GLU	2.6
1	A	261	HIS	2.6
1	B	44	VAL	2.6
1	A	899	LEU	2.6
3	D	93	LEU	2.6
1	A	1005	ASN	2.6
1	B	439	ASN	2.6
1	B	411	TRP	2.6
1	B	1116	ASP	2.5
1	B	774	SER	2.5
1	B	475	SER	2.5
1	B	707	ILE	2.5
1	B	733	PHE	2.5
1	B	863	GLU	2.5
1	A	289	GLU	2.5
1	A	913	TYR	2.5
1	B	313	CYS	2.5
1	B	545	PRO	2.5
1	B	872	SER	2.5
1	A	368	GLU	2.5
1	A	91	TYR	2.5
1	B	333	LEU	2.5
1	B	829	PHE	2.5
1	B	262	ASN	2.4
1	B	648	ASN	2.4
1	B	683	ASN	2.4
1	A	477	ARG	2.4
1	B	667	VAL	2.4
1	A	1114	TYR	2.4
1	B	566	ALA	2.4
1	B	623	LEU	2.4
3	D	85	PHE	2.4
1	B	420	GLU	2.4
1	B	38	ARG	2.4
1	B	403	ASP	2.4
1	B	445	GLU	2.4
1	B	419	ARG	2.4
2	E	1355	PHE	2.4
1	B	705	ASP	2.4
1	B	41	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	959	ILE	2.4
1	B	899	LEU	2.4
1	B	681	PRO	2.3
1	B	543	ILE	2.3
1	B	551	GLY	2.3
1	B	1099	ASP	2.3
1	A	871	TYR	2.3
1	B	491	LYS	2.3
1	B	585	GLU	2.3
1	B	361	ASP	2.3
1	B	425	LEU	2.3
1	B	616	LEU	2.3
1	B	438	LEU	2.3
1	B	95	GLY	2.3
1	B	143	ILE	2.3
1	B	704	ILE	2.2
1	B	592	LEU	2.2
1	A	96	GLU	2.2
1	B	395	GLY	2.2
1	B	541	LEU	2.2
1	B	686	GLY	2.2
1	B	810	ASN	2.2
1	B	858	LEU	2.2
1	A	402	ILE	2.2
1	A	771	PHE	2.2
1	B	144	PRO	2.2
1	A	317	LEU	2.2
2	E	1061	PRO	2.2
1	A	503	CYS	2.2
1	A	1017	LEU	2.2
1	A	770	LEU	2.2
2	E	1282	LEU	2.2
2	E	1329	PRO	2.2
1	B	289	GLU	2.2
1	B	848	ILE	2.2
3	D	156	LEU	2.2
2	C	1227	CYS	2.2
1	B	482	GLU	2.1
1	B	685	ASP	2.1
1	A	49	LEU	2.1
1	B	931	LEU	2.1
1	B	558	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	486	LEU	2.1
1	B	548	ASP	2.1
2	C	1046	ALA	2.1
1	A	591	ILE	2.1
1	B	955	SER	2.1
1	A	1088	PHE	2.1
1	A	955	SER	2.1
1	B	687	TYR	2.1
1	B	1113	GLN	2.1
3	D	139	VAL	2.1
1	B	48	GLY	2.1
1	B	607	GLY	2.1
1	B	550	ASN	2.0
2	E	1366	LEU	2.0
1	B	141	LYS	2.0
1	A	900	ARG	2.0
2	E	1264	GLY	2.0
1	A	64	MET	2.0
1	B	830	ILE	2.0
1	B	873	MET	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.