



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 03:32 am BST

PDB ID : 3ZRF  
Title : pVHL54-213-EloB-EloC complex\_apo  
Authors : Van Molle, I.; Buckley, D.L.; Crews, C.M.; Ciulli, A.  
Deposited on : 2011-06-16  
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

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

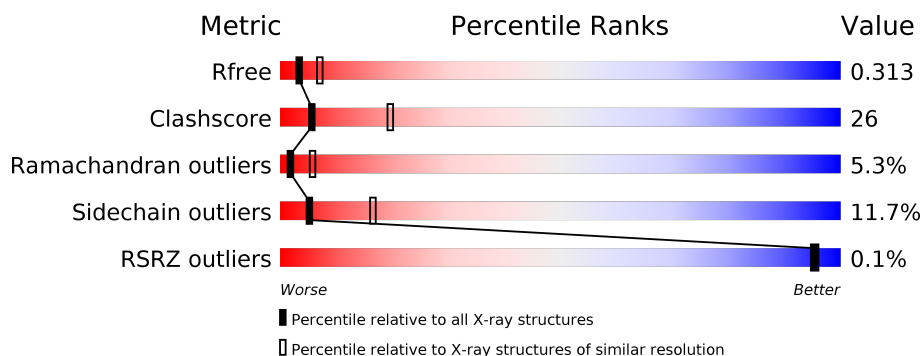
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	118	
1	D	118	
1	G	118	
1	J	118	
2	B	97	
2	E	97	

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Mol	Chain	Length	Quality of chain
2	H	97	
2	K	97	
3	C	163	
3	F	163	
3	I	163	
3	L	163	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10354 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 TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	101	Total	C	N	O	S	0	0	0
			768	490	127	147	4			
1	D	98	Total	C	N	O	S	0	0	0
			719	457	119	139	4			
1	G	105	Total	C	N	O	S	0	0	0
			809	512	136	156	5			
1	J	105	Total	C	N	O	S	0	0	0
			822	520	139	158	5			

- Molecule 2 is a protein called TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	86	Total	C	N	O	S	0	0	0
			666	431	105	124	6			
2	E	87	Total	C	N	O	S	0	0	0
			680	440	107	127	6			
2	H	86	Total	C	N	O	S	0	0	0
			683	442	109	126	6			
2	K	85	Total	C	N	O	S	0	0	0
			678	439	108	125	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	16	MET	-	expression tag	UNP Q15369
E	16	MET	-	expression tag	UNP Q15369
H	16	MET	-	expression tag	UNP Q15369
K	16	MET	-	expression tag	UNP Q15369

- Molecule 3 is a protein called VON HIPPEL-LINDAU DISEASE TUMOR SUPPRESSOR,.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	142	Total	C	N	O	S	0	0	0
			1058	675	188	193	2			
3	F	142	Total	C	N	O	S	0	0	0
			1115	710	198	205	2			
3	I	145	Total	C	N	O	S	0	0	0
			1164	741	211	210	2			
3	L	143	Total	C	N	O	S	0	0	0
			1143	730	207	204	2			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	51	GLY	-	expression tag	UNP P40337
C	52	SER	-	expression tag	UNP P40337
C	53	HIS	-	expression tag	UNP P40337
F	51	GLY	-	expression tag	UNP P40337
F	52	SER	-	expression tag	UNP P40337
F	53	HIS	-	expression tag	UNP P40337
I	51	GLY	-	expression tag	UNP P40337
I	52	SER	-	expression tag	UNP P40337
I	53	HIS	-	expression tag	UNP P40337
L	51	GLY	-	expression tag	UNP P40337
L	52	SER	-	expression tag	UNP P40337
L	53	HIS	-	expression tag	UNP P40337

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	O	0	0
			3	3		
4	C	4	Total	O	0	0
			4	4		
4	D	2	Total	O	0	0
			2	2		
4	E	1	Total	O	0	0
			1	1		
4	F	6	Total	O	0	0
			6	6		
4	G	7	Total	O	0	0
			7	7		
4	H	4	Total	O	0	0
			4	4		
4	I	5	Total	O	0	0
			5	5		

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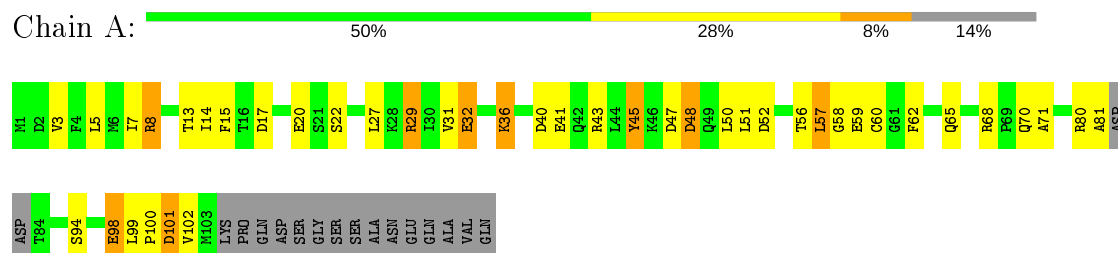
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	J	3	Total	O	0	0
			3	3		
4	K	5	Total	O	0	0
			5	5		
4	L	9	Total	O	0	0
			9	9		

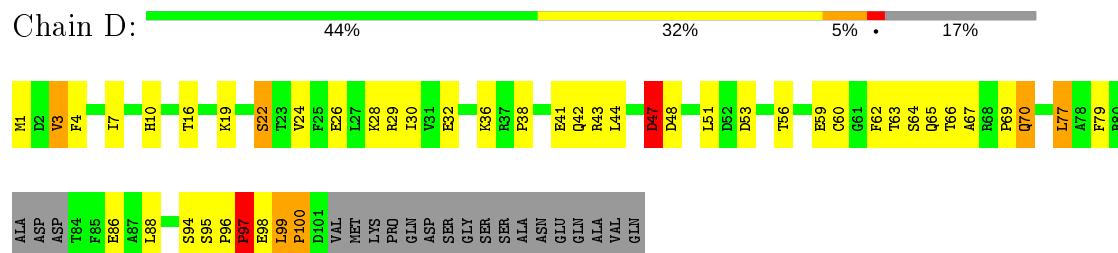
### 3 Residue-property plots [i](#)

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

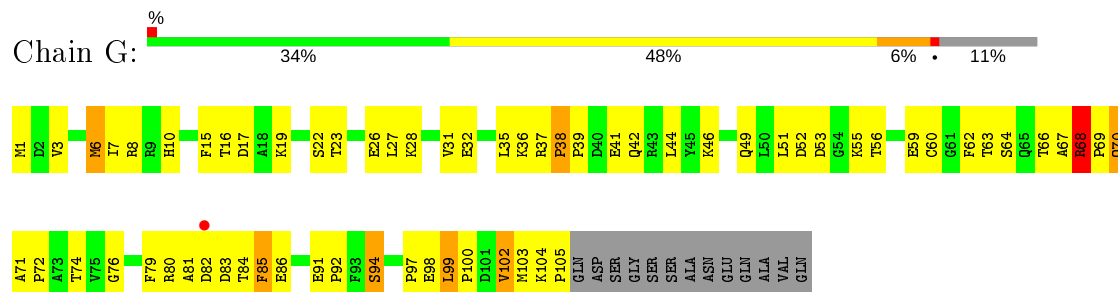
#### • Molecule 1: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 2



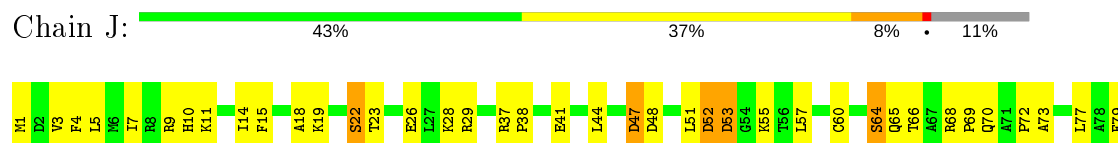
#### • Molecule 1: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 2



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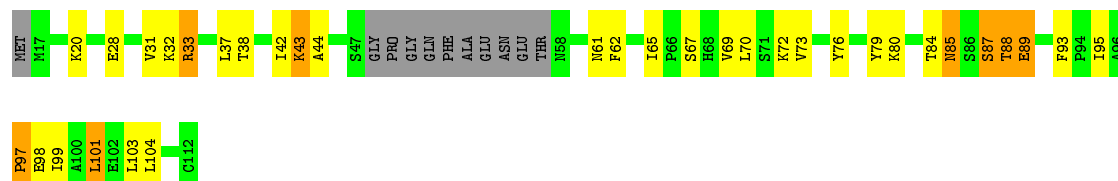


#### • Molecule 1: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 2

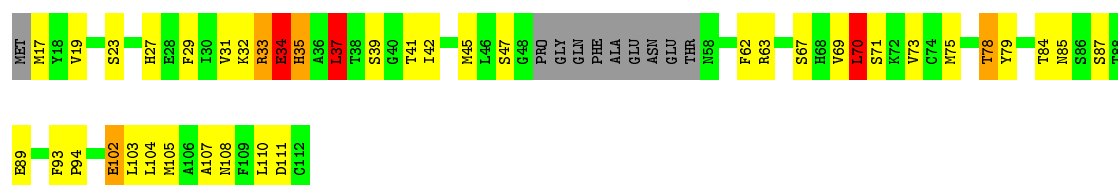




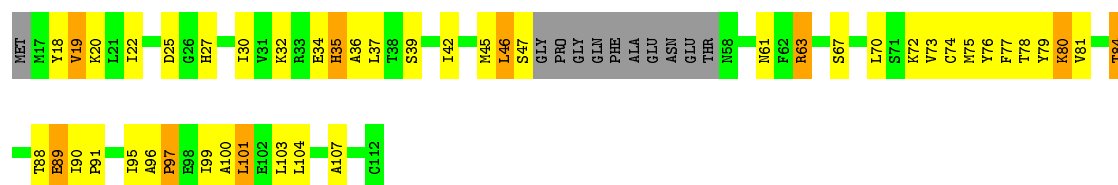
• Molecule 2: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 1



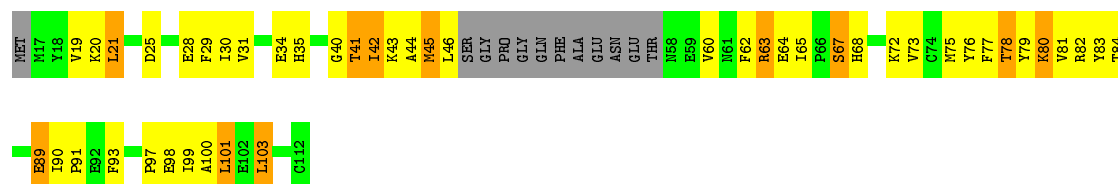
• Molecule 2: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 1



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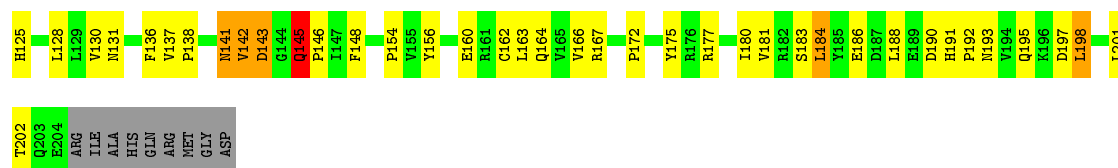
• Molecule 2: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 1



• Molecule 3: VON HIPPEL-LINDAU DISEASE TUMOR SUPPRESSOR,

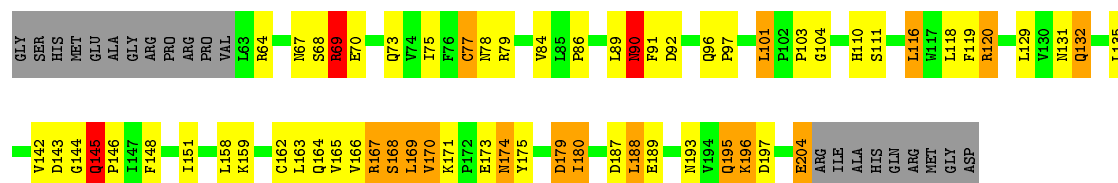






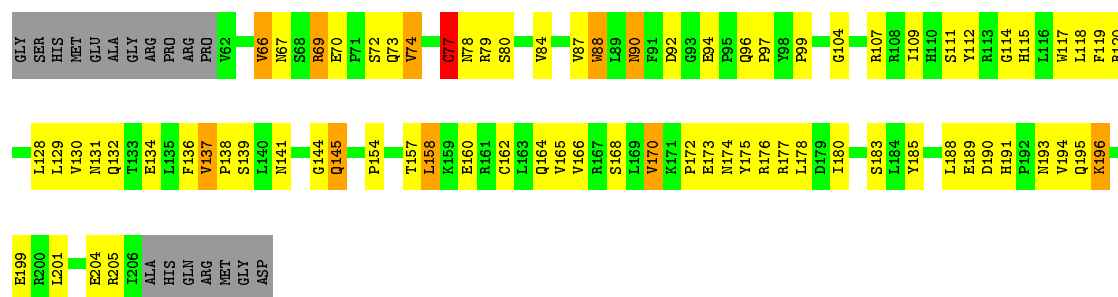
- Molecule 3: VON HIPPEL-LINDAU DISEASE TUMOR SUPPRESSOR,

Chain F: 48% 27% 10% 13%



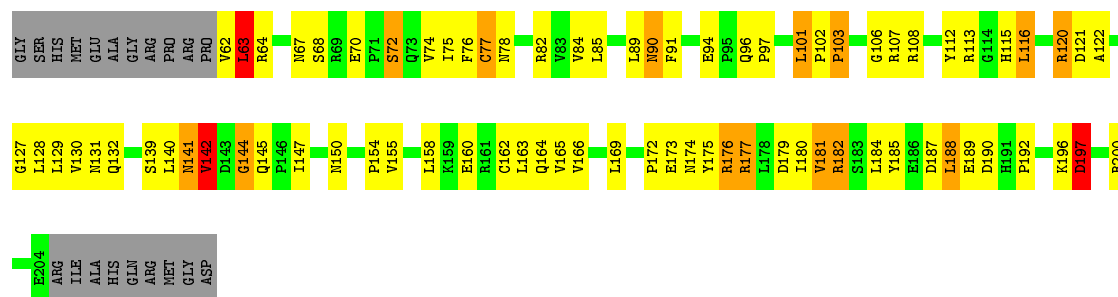
- Molecule 3: VON HIPPEL-LINDAU DISEASE TUMOR SUPPRESSOR,

Chain I: 42% 40% 6% 11%



- Molecule 3: VON HIPPEL-LINDAU DISEASE TUMOR SUPPRESSOR,

Chain L: 40% 37% 9% 12%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.08 Å 93.08 Å 364.58 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.54 – 2.80 46.54 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.54-2.80) 99.6 (46.54-2.80)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.78 (at 2.81 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.223 , 0.320 0.219 , 0.313	Depositor DCC
$R_{free}$ test set	2027 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.0	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 50.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	10354	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.47 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5400e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality

### 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	1.11	0/783	1.17	4/1061 (0.4%)
1	D	0.98	0/733	1.03	1/997 (0.1%)
1	G	0.93	1/826 (0.1%)	1.04	1/1120 (0.1%)
1	J	1.06	0/839	1.15	2/1135 (0.2%)
2	B	1.08	0/680	1.12	2/920 (0.2%)
2	E	1.12	1/694 (0.1%)	1.02	1/936 (0.1%)
2	H	0.98	0/697	0.98	0/940
2	K	1.16	0/692	1.13	3/933 (0.3%)
3	C	0.93	1/1086 (0.1%)	1.02	1/1493 (0.1%)
3	F	1.01	2/1144 (0.2%)	1.07	4/1566 (0.3%)
3	I	1.10	2/1194 (0.2%)	1.08	1/1631 (0.1%)
3	L	1.08	1/1173 (0.1%)	1.17	6/1603 (0.4%)
All	All	1.04	8/10541 (0.1%)	1.09	26/14335 (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	G	0	1
1	J	0	1
3	C	0	1
3	F	0	1
3	L	0	2
All	All	0	6

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	77	CYS	CB-SG	13.66	2.05	1.82
3	F	77	CYS	CB-SG	8.64	1.97	1.82
3	L	77	CYS	CB-SG	7.22	1.94	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	60	CYS	CB-SG	-6.61	1.71	1.82
3	F	189	GLU	CG-CD	5.64	1.60	1.51
2	E	34	GLU	CG-CD	5.45	1.60	1.51
3	C	88	TRP	CB-CG	5.39	1.59	1.50
3	I	88	TRP	CB-CG	5.05	1.59	1.50

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	101	LEU	CA-CB-CG	-7.74	97.49	115.30
1	A	8	ARG	NE-CZ-NH2	-7.50	116.55	120.30
3	F	101	LEU	CA-CB-CG	6.50	130.24	115.30
2	K	101	LEU	CA-CB-CG	-6.20	101.04	115.30
2	K	21	LEU	CA-CB-CG	6.09	129.31	115.30
1	A	57	LEU	CB-CG-CD1	6.05	121.28	111.00
3	L	197	ASP	CB-CG-OD1	5.78	123.50	118.30
1	J	52	ASP	CB-CG-OD1	5.77	123.49	118.30
2	E	70	LEU	CA-CB-CG	5.76	128.54	115.30
3	L	187	ASP	CB-CG-OD1	5.65	123.39	118.30
1	D	47	ASP	CB-CG-OD1	5.63	123.37	118.30
3	L	89	LEU	CB-CG-CD1	-5.62	101.45	111.00
3	I	158	LEU	CB-CG-CD2	-5.59	101.50	111.00
3	F	135	LEU	CB-CG-CD2	-5.39	101.83	111.00
1	A	8	ARG	NE-CZ-NH1	5.38	122.99	120.30
3	F	129	LEU	CB-CG-CD2	5.27	119.95	111.00
2	K	103	LEU	CB-CG-CD1	-5.23	102.11	111.00
1	A	52	ASP	CB-CA-C	-5.20	100.00	110.40
3	L	101	LEU	CA-CB-CG	5.20	127.25	115.30
1	G	68	ARG	NE-CZ-NH1	-5.13	117.74	120.30
2	B	70	LEU	CA-CB-CG	5.11	127.05	115.30
3	L	200	ARG	NE-CZ-NH1	5.06	122.83	120.30
3	F	188	LEU	CA-CB-CG	5.06	126.93	115.30
3	C	190	ASP	CB-CG-OD2	5.05	122.85	118.30
1	J	47	ASP	CB-CG-OD2	-5.01	113.79	118.30
3	L	103	PRO	C-N-CA	-5.01	111.79	122.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	145	GLN	Peptide
3	F	145	GLN	Peptide

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Mol	Chain	Res	Type	Group
1	G	41	GLU	Peptide
1	J	83	ASP	Peptide
3	L	142	VAL	Peptide
3	L	144	GLY	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	768	0	752	31	0
1	D	719	0	676	32	0
1	G	809	0	787	62	0
1	J	822	0	818	51	0
2	B	666	0	646	26	0
2	E	680	0	668	31	0
2	H	683	0	681	46	0
2	K	678	0	679	40	0
3	C	1058	0	975	61	0
3	F	1115	0	1073	43	0
3	I	1164	0	1141	69	0
3	L	1143	0	1123	62	0
4	A	3	0	0	0	0
4	C	4	0	0	3	0
4	D	2	0	0	0	0
4	E	1	0	0	0	0
4	F	6	0	0	0	0
4	G	7	0	0	5	0
4	H	4	0	0	0	0
4	I	5	0	0	3	0
4	J	3	0	0	0	0
4	K	5	0	0	1	0
4	L	9	0	0	1	0
All	All	10354	0	10019	520	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 26.

All (520) 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:I:77:CYS:SG	3:I:77:CYS:CB	2.05	1.45
3:C:68:SER:CB	3:C:69:ARG:HA	1.30	1.36
3:C:68:SER:CB	3:C:69:ARG:CA	2.20	1.20
1:D:98:GLU:CB	1:D:99:LEU:HA	1.74	1.16
3:I:69:ARG:HG2	3:I:69:ARG:HH11	1.07	1.12
3:C:68:SER:HB2	3:C:69:ARG:HA	1.16	1.11
4:G:2003:HOH:O	2:H:27:HIS:HD2	1.32	1.10
3:F:104:GLY:HA3	2:H:63:ARG:HD2	1.29	1.09
3:C:78:ASN:HB2	3:C:101:LEU:HD23	1.18	1.09
2:K:45:MET:O	2:K:46:LEU:HD12	1.54	1.07
3:C:68:SER:HB2	3:C:69:ARG:CA	1.80	1.05
3:C:167:ARG:HB2	4:C:2003:HOH:O	1.54	1.05
3:C:65:SER:HB2	3:C:89:LEU:O	1.57	1.04
3:F:75:ILE:HD13	3:F:146:PRO:HB2	1.39	1.04
3:C:68:SER:HB3	3:C:69:ARG:HA	1.07	1.03
1:G:36:LYS:O	1:G:37:ARG:HG2	1.59	1.02
3:L:177:ARG:HH11	3:L:177:ARG:HG3	1.24	1.01
3:C:78:ASN:HB2	3:C:101:LEU:CD2	1.89	1.01
3:I:175:TYR:O	3:I:185:TYR:HE1	1.44	0.99
3:I:90:ASN:HD22	3:I:94:GLU:HB2	1.30	0.94
3:F:195:GLN:HA	3:F:195:GLN:OE1	1.64	0.93
2:K:77:PHE:O	2:K:81:VAL:HG23	1.69	0.93
1:A:8:ARG:HG2	1:A:13:THR:HG23	1.52	0.92
3:C:78:ASN:CB	3:C:101:LEU:HD23	2.00	0.92
3:C:163:LEU:CD2	3:C:188:LEU:HD23	2.00	0.91
1:G:99:LEU:H	1:G:100:PRO:HD3	1.34	0.90
1:D:99:LEU:CB	1:D:100:PRO:HD3	2.03	0.88
3:I:144:GLY:HA3	3:I:145:GLN:HB2	1.56	0.88
1:G:68:ARG:HH11	1:G:68:ARG:HG2	1.36	0.87
3:C:163:LEU:HD23	3:C:188:LEU:HD23	1.52	0.87
3:F:75:ILE:CD1	3:F:146:PRO:HB2	2.05	0.86
3:L:62:VAL:O	3:L:63:LEU:HB2	1.74	0.86
1:G:68:ARG:NH1	1:G:68:ARG:HG2	1.89	0.85
3:L:176:ARG:NH1	3:L:185:TYR:HB3	1.91	0.85
1:G:94:SER:H	2:H:67:SER:HB2	1.41	0.85
3:I:69:ARG:CG	3:I:69:ARG:HH11	1.90	0.84
3:I:73:GLN:H	3:I:141:ASN:ND2	1.75	0.84
1:A:47:ASP:O	1:A:48:ASP:HB2	1.78	0.83
3:I:144:GLY:HA3	3:I:145:GLN:CB	2.09	0.83
3:I:69:ARG:NH1	3:I:69:ARG:HG2	1.77	0.82
2:B:95:ILE:HD13	2:B:103:LEU:HD23	1.61	0.82
1:G:66:THR:HG22	1:G:66:THR:O	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:68:SER:HB2	3:C:69:ARG:CB	2.10	0.81
3:L:76:PHE:HB3	3:L:101:LEU:HD11	1.62	0.81
3:L:177:ARG:HH11	3:L:177:ARG:CG	1.94	0.81
3:C:73:GLN:H	3:C:141:ASN:ND2	1.79	0.80
3:C:67:ASN:HA	3:C:91:PHE:HE1	1.45	0.80
4:G:2003:HOH:O	2:H:27:HIS:CD2	2.15	0.78
2:K:68:HIS:O	4:K:2003:HOH:O	2.02	0.78
3:C:68:SER:HB3	3:C:69:ARG:CA	2.00	0.78
1:J:104:LYS:HG3	1:J:105:PRO:HB3	1.66	0.78
3:I:73:GLN:H	3:I:141:ASN:HD21	1.30	0.77
3:I:88:TRP:HZ3	3:I:96:GLN:NE2	1.80	0.77
3:F:64:ARG:HD2	3:F:91:PHE:O	1.83	0.77
3:L:177:ARG:NH1	3:L:177:ARG:HG3	2.00	0.77
3:C:78:ASN:ND2	3:C:103:PRO:HA	2.00	0.77
3:L:76:PHE:O	3:L:106:GLY:HA2	1.85	0.77
1:D:98:GLU:CB	1:D:99:LEU:CA	2.61	0.76
3:I:141:ASN:OD1	3:I:145:GLN:O	2.03	0.76
1:D:79:PHE:H	1:D:86:GLU:HG2	1.51	0.76
3:I:175:TYR:O	3:I:185:TYR:CE1	2.35	0.75
1:J:83:ASP:CG	1:J:84:THR:H	1.88	0.75
2:H:34:GLU:OE1	2:H:34:GLU:N	2.19	0.75
1:D:99:LEU:CB	1:D:100:PRO:CD	2.64	0.74
3:F:67:ASN:HA	3:F:91:PHE:CE1	2.22	0.74
3:F:131:ASN:O	3:F:132:GLN:HB2	1.86	0.74
3:C:163:LEU:HD23	3:C:188:LEU:CD2	2.18	0.73
3:F:165:VAL:O	3:F:169:LEU:HD12	1.88	0.73
3:F:67:ASN:HA	3:F:91:PHE:HE1	1.53	0.73
3:F:69:ARG:HH11	3:F:69:ARG:HG3	1.55	0.72
3:C:160:GLU:HA	3:C:163:LEU:HD12	1.69	0.72
3:I:193:ASN:HB3	3:I:196:LYS:HB2	1.72	0.72
1:A:29:ARG:O	1:A:32:GLU:HB3	1.90	0.71
1:G:23:THR:OG1	1:G:26:GLU:HG3	1.90	0.71
1:J:83:ASP:O	1:J:84:THR:HG23	1.90	0.70
1:J:41:GLU:HA	1:J:80:ARG:HG2	1.72	0.70
3:C:73:GLN:N	3:C:141:ASN:ND2	2.38	0.70
3:L:68:SER:HB2	3:L:70:GLU:HG2	1.73	0.70
1:J:9:ARG:HB2	1:J:77:LEU:HB3	1.74	0.70
1:A:43:ARG:HG2	1:A:45:TYR:CE1	2.27	0.69
1:A:47:ASP:O	1:A:48:ASP:CB	2.40	0.69
1:G:66:THR:CG2	1:G:66:THR:O	2.39	0.69
1:J:41:GLU:CG	1:J:80:ARG:HG2	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:42:ILE:O	2:K:45:MET:HB2	1.92	0.69
1:D:51:LEU:HD22	1:D:60:CYS:SG	2.33	0.69
3:C:130:VAL:HG11	3:C:136:PHE:HB2	1.75	0.69
3:C:67:ASN:HA	3:C:91:PHE:CE1	2.28	0.69
3:F:204:GLU:C	3:F:204:GLU:OE1	2.32	0.68
3:L:64:ARG:HD2	3:L:91:PHE:O	1.94	0.67
3:C:163:LEU:HD22	3:C:188:LEU:HD23	1.76	0.67
3:L:70:GLU:HG3	3:L:113:ARG:HB2	1.75	0.67
3:L:131:ASN:O	3:L:132:GLN:HB2	1.93	0.67
2:K:103:LEU:HB3	3:L:162:CYS:SG	2.34	0.67
1:J:19:LYS:O	1:J:57:LEU:HD12	1.95	0.67
3:L:120:ARG:NH1	3:L:197:ASP:OD2	2.27	0.67
2:E:104:LEU:HB2	3:F:162:CYS:HB3	1.77	0.67
1:G:70:GLN:O	4:G:2005:HOH:O	2.11	0.67
2:B:33:ARG:O	2:B:37:LEU:HG	1.95	0.66
1:A:43:ARG:HG3	1:A:50:LEU:HD11	1.77	0.66
3:L:102:PRO:HB2	3:L:103:PRO:HD2	1.75	0.66
2:E:71:SER:O	2:E:75:MET:HG3	1.96	0.66
1:G:32:GLU:OE1	1:G:39:PRO:HD3	1.95	0.66
3:F:73:GLN:OE1	3:F:110:HIS:CD2	2.49	0.66
2:E:34:GLU:H	2:E:34:GLU:CD	1.99	0.66
1:G:27:LEU:O	1:G:31:VAL:HG23	1.96	0.65
3:I:131:ASN:O	3:I:132:GLN:HB2	1.96	0.65
1:D:19:LYS:O	1:D:22:SER:HB3	1.97	0.65
2:H:46:LEU:O	2:H:47:SER:O	2.13	0.65
3:I:88:TRP:HZ3	3:I:96:GLN:HE22	1.43	0.65
2:H:39:SER:HB3	2:H:42:ILE:HB	1.77	0.65
3:I:90:ASN:ND2	3:I:94:GLU:HB2	2.06	0.65
2:E:37:LEU:HD23	2:E:37:LEU:N	2.12	0.65
3:I:88:TRP:CZ3	3:I:96:GLN:NE2	2.63	0.65
2:K:19:VAL:HG22	2:K:31:VAL:O	1.98	0.64
2:H:73:VAL:HG12	2:H:77:PHE:CZ	2.32	0.64
1:D:28:LYS:HE2	1:D:53:ASP:OD1	1.98	0.64
3:I:90:ASN:HD22	3:I:94:GLU:CB	2.08	0.64
1:G:52:ASP:HB2	1:G:55:LYS:CG	2.28	0.63
3:I:189:GLU:O	3:I:191:HIS:N	2.31	0.63
3:L:127:GLY:O	3:L:128:LEU:HD23	1.99	0.63
3:I:172:PRO:HD2	3:I:173:GLU:OE1	1.98	0.63
3:I:78:ASN:O	3:I:104:GLY:HA2	1.99	0.63
2:H:22:ILE:HA	2:H:27:HIS:O	1.99	0.63
1:G:28:LYS:HG2	1:G:42:GLN:NE2	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:62:PHE:HB3	2:K:65:ILE:HG13	1.80	0.63
3:C:130:VAL:CG1	3:C:136:PHE:HB2	2.29	0.62
3:L:90:ASN:HB2	3:L:94:GLU:O	1.99	0.62
1:G:56:THR:OG1	1:G:59:GLU:HG3	2.00	0.62
1:J:103:MET:O	1:J:104:LYS:HB2	1.98	0.62
3:C:137:VAL:O	3:C:137:VAL:HG12	2.00	0.62
2:E:34:GLU:CD	2:E:34:GLU:N	2.53	0.62
2:H:76:TYR:CD1	2:H:76:TYR:C	2.73	0.61
1:J:19:LYS:HB2	1:J:22:SER:HB3	1.81	0.61
2:K:20:LYS:HE2	2:K:30:ILE:HD11	1.81	0.61
3:F:67:ASN:CA	3:F:91:PHE:CE1	2.83	0.61
1:G:8:ARG:NH2	1:G:91:GLU:O	2.34	0.61
3:L:181:VAL:O	3:L:182:ARG:C	2.38	0.61
3:C:73:GLN:N	3:C:141:ASN:HD21	1.98	0.60
3:C:164:GLN:HA	4:C:2003:HOH:O	2.02	0.60
3:C:141:ASN:O	3:C:142:VAL:O	2.20	0.60
1:J:26:GLU:O	1:J:29:ARG:HB2	2.02	0.60
1:A:29:ARG:NH1	1:A:32:GLU:OE1	2.34	0.60
2:E:37:LEU:HD23	2:E:37:LEU:H	1.65	0.60
2:B:95:ILE:HD13	2:B:103:LEU:CD2	2.31	0.60
3:L:141:ASN:O	3:L:142:VAL:C	2.41	0.59
1:G:32:GLU:OE1	1:G:38:PRO:HA	2.01	0.59
1:D:28:LYS:NZ	1:D:43:ARG:HA	2.16	0.59
2:B:87:SER:O	2:B:88:THR:C	2.40	0.59
1:G:97:PRO:O	1:G:98:GLU:HB2	2.03	0.59
2:H:73:VAL:CG1	2:H:77:PHE:CZ	2.86	0.59
1:J:1:MET:O	1:J:19:LYS:HA	2.02	0.59
2:H:88:THR:O	2:H:89:GLU:C	2.41	0.59
1:J:28:LYS:HE2	1:J:53:ASP:OD1	2.02	0.59
3:L:140:LEU:O	3:L:141:ASN:O	2.21	0.58
1:D:42:GLN:HE21	1:D:77:LEU:HD13	1.69	0.58
3:I:69:ARG:HG3	4:I:2003:HOH:O	2.03	0.58
3:C:84:VAL:O	3:C:100:THR:HG22	2.03	0.58
3:C:78:ASN:O	3:C:103:PRO:O	2.21	0.58
3:I:144:GLY:CA	3:I:145:GLN:CB	2.82	0.58
1:J:41:GLU:HG2	1:J:80:ARG:CG	2.34	0.58
3:I:112:TYR:O	3:I:138:PRO:HB2	2.03	0.58
1:J:3:VAL:HG22	1:J:18:ALA:O	2.04	0.58
3:L:160:GLU:O	3:L:164:GLN:HG3	2.03	0.58
1:J:80:ARG:HA	1:J:85:PHE:HA	1.86	0.57
2:K:44:ALA:C	2:K:46:LEU:H	2.07	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:36:ALA:HB1	2:H:42:ILE:HG21	1.85	0.57
3:I:69:ARG:CG	4:I:2003:HOH:O	2.50	0.57
2:H:18:TYR:O	2:H:19:VAL:HG12	2.04	0.57
3:L:184:LEU:O	3:L:188:LEU:HB2	2.03	0.57
3:F:67:ASN:CA	3:F:91:PHE:HE1	2.17	0.57
1:A:68:ARG:O	1:A:71:ALA:N	2.37	0.57
2:B:104:LEU:HB2	3:C:162:CYS:HB3	1.87	0.57
1:J:37:ARG:HH12	1:J:41:GLU:HG2	1.69	0.57
2:E:33:ARG:O	2:E:37:LEU:HD23	2.05	0.57
3:F:90:ASN:HB3	3:F:92:ASP:H	1.69	0.57
3:I:157:THR:OG1	3:I:160:GLU:HB2	2.04	0.57
3:I:164:GLN:O	3:I:168:SER:HB3	2.04	0.57
2:B:87:SER:O	2:B:89:GLU:N	2.37	0.56
1:D:29:ARG:O	1:D:32:GLU:HB3	2.04	0.56
3:I:90:ASN:HB3	3:I:92:ASP:H	1.70	0.56
1:J:41:GLU:CG	1:J:80:ARG:CG	2.83	0.56
2:K:19:VAL:O	2:K:30:ILE:HA	2.04	0.56
3:F:163:LEU:HD22	3:F:188:LEU:HD23	1.86	0.56
1:J:83:ASP:CG	1:J:84:THR:N	2.57	0.56
1:G:79:PHE:O	1:G:85:PHE:CD1	2.59	0.56
1:J:37:ARG:NH1	1:J:41:GLU:HG2	2.21	0.56
1:D:44:LEU:HD23	1:D:77:LEU:HB2	1.86	0.56
3:C:78:ASN:HD21	3:C:103:PRO:HA	1.67	0.56
2:E:110:LEU:O	2:E:111:ASP:HB3	2.06	0.56
2:K:25:ASP:N	2:K:25:ASP:OD1	2.33	0.56
3:I:166:VAL:HG11	3:I:188:LEU:HD11	1.87	0.55
1:J:94:SER:O	2:K:68:HIS:HB3	2.07	0.55
1:A:22:SER:OG	1:A:57:LEU:HD12	2.06	0.55
3:C:145:GLN:CB	3:C:146:PRO:HD3	2.36	0.55
3:F:120:ARG:NH1	3:F:197:ASP:OD2	2.39	0.55
3:C:105:THR:HG22	2:K:64:GLU:OE1	2.07	0.55
1:A:56:THR:OG1	1:A:59:GLU:HB2	2.06	0.55
1:J:66:THR:HG22	1:J:66:THR:O	2.05	0.55
3:F:174:ASN:HD22	3:F:174:ASN:N	2.05	0.55
1:G:22:SER:HB2	1:G:26:GLU:OE1	2.07	0.55
1:A:32:GLU:O	1:A:36:LYS:HA	2.06	0.55
2:E:23:SER:HA	2:E:70:LEU:HD23	1.88	0.55
1:D:70:GLN:HG3	2:E:79:TYR:CD1	2.40	0.55
1:G:8:ARG:NH2	4:G:2001:HOH:O	2.38	0.55
1:J:4:PHE:CE2	1:J:69:PRO:HG3	2.41	0.55
2:K:35:HIS:HD2	2:K:78:THR:HG22	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:10:HIS:O	1:G:91:GLU:HB2	2.07	0.55
3:I:73:GLN:HB2	3:I:141:ASN:HD21	1.71	0.55
1:G:99:LEU:N	1:G:100:PRO:HD3	2.13	0.54
1:G:52:ASP:HB2	1:G:55:LYS:HG2	1.88	0.54
1:G:52:ASP:HB2	1:G:55:LYS:HG3	1.89	0.54
3:L:70:GLU:O	3:L:112:TYR:HA	2.07	0.54
1:A:65:GLN:O	1:A:68:ARG:HD2	2.06	0.54
3:I:129:LEU:HG	3:I:154:PRO:HB3	1.87	0.54
1:J:41:GLU:HG3	1:J:80:ARG:HG2	1.87	0.54
2:H:104:LEU:HB2	3:I:162:CYS:HB3	1.90	0.54
1:J:51:LEU:HD22	1:J:60:CYS:SG	2.48	0.54
1:G:28:LYS:HD3	1:G:42:GLN:HB3	1.89	0.54
1:G:92:PRO:HA	4:G:2002:HOH:O	2.07	0.54
3:F:86:PRO:HB3	3:F:119:PHE:HE1	1.70	0.54
3:F:89:LEU:HD12	3:F:116:LEU:HD23	1.89	0.54
1:D:70:GLN:HG3	2:E:79:TYR:HD1	1.74	0.53
1:J:11:LYS:HG3	1:J:91:GLU:HG3	1.91	0.53
2:E:39:SER:OG	2:E:110:LEU:O	2.26	0.53
1:G:3:VAL:HG22	1:G:67:ALA:HB3	1.90	0.53
1:G:7:ILE:HD13	1:G:31:VAL:HG22	1.91	0.53
2:B:42:ILE:HG12	2:B:62:PHE:HZ	1.73	0.53
1:A:15:PHE:HB2	2:B:31:VAL:HG22	1.90	0.53
3:C:67:ASN:C	3:C:67:ASN:HD22	2.12	0.53
2:B:84:THR:O	2:B:85:ASN:HB2	2.09	0.53
1:G:72:PRO:HD3	2:H:75:MET:HG2	1.90	0.53
1:D:70:GLN:H	1:D:70:GLN:NE2	2.06	0.53
1:G:98:GLU:HB3	1:G:99:LEU:CB	2.38	0.53
2:B:89:GLU:HG3	3:C:79:ARG:HB3	1.90	0.52
3:I:160:GLU:O	3:I:164:GLN:HG3	2.09	0.52
2:H:80:LYS:O	2:H:84:THR:HB	2.09	0.52
3:I:66:VAL:HG23	3:I:114:GLY:O	2.09	0.52
3:L:129:LEU:HD11	3:L:154:PRO:HB3	1.92	0.52
3:F:86:PRO:HB3	3:F:119:PHE:CE1	2.44	0.52
3:F:84:VAL:HG21	3:F:151:ILE:HG21	1.91	0.52
2:E:27:HIS:ND1	2:E:67:SER:OG	2.43	0.52
3:F:68:SER:O	3:F:68:SER:OG	2.25	0.52
3:L:130:VAL:HG13	3:L:130:VAL:O	2.09	0.52
2:B:98:GLU:H	2:B:98:GLU:CD	2.14	0.51
3:F:78:ASN:HB2	3:F:101:LEU:HD13	1.91	0.51
1:G:68:ARG:CG	1:G:68:ARG:HH11	2.06	0.51
3:I:129:LEU:HD13	3:I:132:GLN:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:40:GLY:O	2:K:43:LYS:HB3	2.11	0.51
3:C:142:VAL:O	3:C:143:ASP:C	2.48	0.51
3:C:78:ASN:ND2	3:C:103:PRO:CA	2.73	0.51
3:I:74:VAL:HG12	3:I:109:ILE:HB	1.92	0.51
2:H:76:TYR:CD2	3:I:158:LEU:HB2	2.46	0.51
2:E:102:GLU:HA	2:E:105:MET:HE2	1.93	0.51
3:L:112:TYR:HB2	3:L:115:HIS:CE1	2.46	0.51
3:L:192:PRO:HA	4:L:2009:HOH:O	2.09	0.51
3:C:181:VAL:O	3:C:184:LEU:HB2	2.11	0.51
2:E:35:HIS:HD2	2:E:78:THR:HG22	1.74	0.51
1:G:46:LYS:HD2	1:G:62:PHE:CZ	2.45	0.51
1:J:104:LYS:HG3	1:J:105:PRO:CB	2.38	0.51
2:E:33:ARG:O	2:E:37:LEU:HG	2.11	0.51
3:I:70:GLU:O	3:I:112:TYR:HA	2.11	0.51
3:C:65:SER:OG	3:C:115:HIS:HA	2.11	0.50
3:I:73:GLN:N	3:I:141:ASN:HD21	2.03	0.50
1:G:28:LYS:HE2	1:G:42:GLN:O	2.11	0.50
3:L:140:LEU:HD23	3:L:141:ASN:O	2.11	0.50
1:D:42:GLN:HE21	1:D:77:LEU:CD1	2.24	0.50
3:L:72:SER:OG	3:L:139:SER:O	2.29	0.50
1:G:94:SER:H	2:H:67:SER:CB	2.18	0.50
2:H:35:HIS:CE1	2:H:81:VAL:HG11	2.46	0.50
1:J:103:MET:O	1:J:104:LYS:CB	2.60	0.50
2:E:37:LEU:N	2:E:37:LEU:CD2	2.75	0.50
3:I:130:VAL:O	3:I:130:VAL:HG13	2.11	0.50
3:C:75:ILE:HG22	3:C:146:PRO:HB3	1.94	0.50
2:E:108:ASN:OD1	3:F:159:LYS:HE3	2.11	0.50
1:J:65:GLN:O	1:J:68:ARG:HD2	2.11	0.50
2:K:72:LYS:O	2:K:73:VAL:C	2.48	0.50
2:B:37:LEU:O	2:B:38:THR:C	2.50	0.49
1:D:28:LYS:HZ1	1:D:43:ARG:HA	1.77	0.49
1:D:69:PRO:HD2	1:D:70:GLN:HE22	1.75	0.49
1:G:28:LYS:HA	1:G:42:GLN:HE22	1.77	0.49
1:J:15:PHE:HE1	2:K:29:PHE:HD1	1.59	0.49
1:G:97:PRO:O	1:G:98:GLU:CB	2.60	0.49
3:L:84:VAL:HG12	3:L:85:LEU:N	2.28	0.49
2:E:33:ARG:O	2:E:37:LEU:CD2	2.60	0.49
2:B:76:TYR:C	2:B:76:TYR:CD1	2.85	0.49
2:K:45:MET:O	2:K:46:LEU:CD1	2.44	0.49
1:G:68:ARG:HD3	1:G:71:ALA:HB3	1.95	0.49
1:J:47:ASP:O	1:J:48:ASP:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:100:PRO:O	1:J:102:VAL:HG22	2.12	0.48
3:C:102:PRO:HG2	3:C:105:THR:HG21	1.94	0.48
2:H:103:LEU:HG	3:I:158:LEU:HD11	1.93	0.48
1:A:100:PRO:O	1:A:101:ASP:CB	2.61	0.48
1:G:16:THR:OG1	1:G:17:ASP:N	2.45	0.48
1:J:41:GLU:HG2	1:J:80:ARG:HG3	1.94	0.48
3:L:141:ASN:O	3:L:142:VAL:O	2.30	0.48
1:J:9:ARG:HG3	1:J:77:LEU:O	2.14	0.48
3:C:172:PRO:HA	3:C:175:TYR:CB	2.44	0.48
1:D:3:VAL:HG21	1:D:62:PHE:O	2.14	0.48
2:H:96:ALA:HA	2:H:97:PRO:HD2	1.71	0.48
2:H:104:LEU:O	2:H:107:ALA:HB3	2.14	0.48
1:A:45:TYR:HD2	1:A:48:ASP:O	1.97	0.48
2:B:79:TYR:CZ	2:B:93:PHE:HB2	2.49	0.48
1:J:70:GLN:O	1:J:70:GLN:HG2	2.11	0.48
1:G:99:LEU:H	1:G:100:PRO:CD	2.16	0.48
3:F:118:LEU:HD12	3:F:118:LEU:C	2.33	0.47
2:K:89:GLU:HG2	2:K:89:GLU:O	2.14	0.47
3:L:102:PRO:CB	3:L:103:PRO:HD2	2.42	0.47
3:L:115:HIS:O	3:L:116:LEU:HD12	2.14	0.47
3:L:140:LEU:C	3:L:141:ASN:O	2.52	0.47
1:J:23:THR:OG1	1:J:26:GLU:HG3	2.14	0.47
1:J:72:PRO:HD3	2:K:75:MET:HG2	1.96	0.47
3:L:176:ARG:HH12	3:L:185:TYR:HB3	1.70	0.47
1:A:51:LEU:HD22	1:A:60:CYS:SG	2.55	0.47
3:L:160:GLU:HA	3:L:163:LEU:HD12	1.96	0.47
1:D:26:GLU:O	1:D:29:ARG:HB2	2.14	0.47
3:C:78:ASN:CB	3:C:101:LEU:CD2	2.75	0.47
1:D:3:VAL:HG22	1:D:67:ALA:HB3	1.95	0.47
3:I:84:VAL:HG22	3:I:128:LEU:HD13	1.97	0.47
2:H:95:ILE:HB	3:I:165:VAL:HG21	1.96	0.47
3:I:172:PRO:CD	3:I:173:GLU:OE1	2.62	0.47
2:H:34:GLU:O	2:H:37:LEU:HB2	2.15	0.47
2:H:61:ASN:O	2:H:63:ARG:NH1	2.47	0.47
1:G:69:PRO:HB3	2:H:78:THR:HG22	1.97	0.47
3:I:137:VAL:HA	3:I:138:PRO:HD2	1.75	0.47
3:L:101:LEU:HD21	3:L:107:ARG:HG2	1.96	0.47
2:B:42:ILE:O	2:B:43:LYS:C	2.51	0.47
2:K:79:TYR:CE2	2:K:93:PHE:HB2	2.50	0.47
2:K:25:ASP:OD2	2:K:67:SER:HB3	2.15	0.47
2:E:69:VAL:O	2:E:73:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:164:GLN:O	3:F:168:SER:HB3	2.16	0.46
3:I:157:THR:OG1	3:I:160:GLU:N	2.40	0.46
2:K:20:LYS:NZ	2:K:28:GLU:CD	2.69	0.46
1:J:44:LEU:HD21	1:J:77:LEU:HD13	1.96	0.46
2:E:89:GLU:HG3	3:F:79:ARG:O	2.14	0.46
3:F:179:ASP:O	3:F:180:ILE:HG23	2.16	0.46
3:L:70:GLU:CG	3:L:113:ARG:HB2	2.43	0.46
3:L:78:ASN:C	3:L:78:ASN:OD1	2.52	0.46
1:G:79:PHE:H	1:G:86:GLU:HG2	1.81	0.46
3:L:131:ASN:O	3:L:132:GLN:CB	2.60	0.46
2:H:18:TYR:C	2:H:19:VAL:CG1	2.84	0.46
1:G:100:PRO:HD2	1:G:103:MET:HG3	1.98	0.46
2:H:73:VAL:HG12	2:H:77:PHE:CE2	2.50	0.46
2:H:88:THR:O	2:H:89:GLU:O	2.33	0.46
1:J:5:LEU:HA	1:J:73:ALA:O	2.15	0.46
1:A:94:SER:H	2:B:67:SER:HB2	1.80	0.46
2:B:38:THR:HG21	2:B:80:LYS:HD3	1.98	0.46
3:C:154:PRO:HD2	3:C:156:TYR:CZ	2.50	0.46
1:D:56:THR:OG1	1:D:59:GLU:HB2	2.16	0.46
3:L:67:ASN:HB2	3:L:91:PHE:CE1	2.50	0.46
3:L:179:ASP:O	3:L:180:ILE:HG23	2.16	0.45
2:B:101:LEU:HA	2:B:101:LEU:HD23	1.64	0.45
1:G:98:GLU:CA	1:G:99:LEU:CB	2.94	0.45
1:D:4:PHE:CE2	1:D:69:PRO:HG3	2.51	0.45
3:L:172:PRO:HA	3:L:175:TYR:CE1	2.51	0.45
3:L:176:ARG:HA	3:L:176:ARG:HD2	1.64	0.45
3:F:193:ASN:HB3	3:F:196:LYS:HB2	1.98	0.45
1:G:98:GLU:HA	1:G:99:LEU:CB	2.46	0.45
3:C:192:PRO:HB3	4:C:2002:HOH:O	2.16	0.45
1:G:32:GLU:OE1	1:G:39:PRO:CD	2.63	0.45
2:K:82:ARG:HG3	2:K:82:ARG:O	2.16	0.45
3:L:176:ARG:CZ	3:L:189:GLU:OE2	2.65	0.45
3:C:74:VAL:HG11	3:C:136:PHE:HE2	1.82	0.45
1:J:79:PHE:O	1:J:86:GLU:HG2	2.16	0.45
1:A:101:ASP:O	1:A:102:VAL:HG13	2.17	0.45
3:C:193:ASN:OD1	3:C:195:GLN:CB	2.65	0.45
3:C:197:ASP:O	3:C:201:LEU:N	2.28	0.45
1:D:96:PRO:HA	1:D:97:PRO:HD2	1.68	0.45
3:F:69:ARG:NH1	3:F:69:ARG:HG3	2.23	0.45
2:K:34:GLU:N	2:K:34:GLU:OE1	2.37	0.45
1:D:70:GLN:H	1:D:70:GLN:CD	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:34:GLU:HA	2:H:37:LEU:HG	1.99	0.45
2:K:76:TYR:OH	2:K:80:LYS:HG3	2.16	0.45
1:A:5:LEU:HD13	1:A:27:LEU:HD11	1.99	0.45
3:C:102:PRO:CB	3:C:103:PRO:HD2	2.46	0.44
2:E:102:GLU:HA	2:E:105:MET:CE	2.47	0.44
2:E:69:VAL:HG21	2:E:102:GLU:HB3	1.99	0.44
3:L:112:TYR:O	3:L:113:ARG:C	2.54	0.44
1:D:47:ASP:O	1:D:48:ASP:CB	2.63	0.44
1:G:28:LYS:NZ	1:G:53:ASP:OD1	2.51	0.44
1:G:81:ALA:O	1:G:83:ASP:N	2.50	0.44
3:I:99:PRO:HB2	3:I:107:ARG:HH12	1.81	0.44
1:J:1:MET:HE1	1:J:64:SER:HB3	1.98	0.44
2:K:45:MET:C	2:K:46:LEU:HD12	2.33	0.44
3:L:174:ASN:HD22	3:L:174:ASN:N	2.16	0.44
1:D:38:PRO:HB2	1:D:41:GLU:CG	2.47	0.44
3:I:96:GLN:HA	3:I:97:PRO:HD2	1.80	0.44
1:J:11:LYS:CG	1:J:91:GLU:HG3	2.46	0.44
2:E:41:THR:O	2:E:45:MET:HG3	2.17	0.44
3:L:96:GLN:HA	3:L:97:PRO:HD3	1.87	0.44
1:D:24:VAL:HB	1:D:53:ASP:HA	1.99	0.44
1:G:46:LYS:HB2	1:G:51:LEU:HD11	2.00	0.44
2:H:76:TYR:CE1	2:H:80:LYS:HB2	2.53	0.44
3:C:78:ASN:OD1	3:C:80:SER:HB3	2.18	0.44
1:G:102:VAL:O	3:I:170:VAL:HB	2.18	0.44
2:B:69:VAL:O	2:B:73:VAL:HG23	2.17	0.44
3:C:112:TYR:O	3:C:113:ARG:C	2.56	0.44
3:I:117:TRP:HB2	3:I:136:PHE:HB3	2.00	0.44
1:J:37:ARG:NH1	1:J:41:GLU:CG	2.80	0.44
1:A:22:SER:OG	1:A:57:LEU:CD1	2.66	0.44
2:K:79:TYR:CZ	2:K:93:PHE:HB2	2.53	0.44
3:L:82:ARG:HD2	3:L:121:ASP:OD2	2.17	0.44
1:A:7:ILE:HB	1:A:14:ILE:HB	2.00	0.43
3:C:115:HIS:O	3:C:138:PRO:HD2	2.17	0.43
3:C:86:PRO:HA	3:C:119:PHE:CD2	2.52	0.43
1:D:32:GLU:O	1:D:36:LYS:HA	2.18	0.43
1:D:66:THR:HG22	1:D:66:THR:O	2.18	0.43
1:G:6:MET:CE	1:G:74:THR:OG1	2.67	0.43
3:L:129:LEU:CD1	3:L:154:PRO:HA	2.48	0.43
2:E:102:GLU:O	2:E:103:LEU:C	2.56	0.43
2:E:42:ILE:HG12	2:E:62:PHE:HZ	1.83	0.43
2:B:20:LYS:HD3	2:B:28:GLU:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:143:ASP:O	3:F:145:GLN:N	2.44	0.43
1:J:44:LEU:CD2	1:J:77:LEU:HD13	2.48	0.43
2:K:103:LEU:HD22	3:L:158:LEU:HD11	2.00	0.43
3:C:120:ARG:C	3:C:128:LEU:HD12	2.39	0.43
1:D:69:PRO:HD2	1:D:70:GLN:NE2	2.34	0.43
2:H:101:LEU:HD21	3:I:178:LEU:HD22	2.00	0.43
2:H:18:TYR:O	2:H:19:VAL:CG1	2.66	0.43
2:H:61:ASN:HB3	2:H:63:ARG:HH22	1.83	0.43
2:K:100:ALA:HB1	3:L:166:VAL:HG23	2.00	0.43
1:A:68:ARG:O	1:A:71:ALA:C	2.57	0.43
3:F:170:VAL:HG22	3:F:175:TYR:CD1	2.53	0.43
1:G:37:ARG:HA	1:G:38:PRO:HD2	1.70	0.43
1:G:3:VAL:HG22	1:G:67:ALA:CB	2.48	0.43
3:I:112:TYR:HB2	3:I:115:HIS:CE1	2.53	0.43
3:I:173:GLU:CD	3:I:173:GLU:H	2.19	0.43
3:L:141:ASN:C	3:L:142:VAL:O	2.57	0.43
2:K:44:ALA:O	2:K:46:LEU:N	2.50	0.43
3:L:165:VAL:O	3:L:169:LEU:HD12	2.19	0.43
2:B:65:ILE:HG23	2:B:69:VAL:CG1	2.48	0.43
1:J:52:ASP:CB	1:J:55:LYS:HG2	2.49	0.43
2:K:84:THR:HG22	3:L:155:VAL:HB	2.00	0.43
3:I:114:GLY:HA2	3:I:137:VAL:HG12	2.00	0.43
1:J:15:PHE:HE1	2:K:29:PHE:CD1	2.37	0.43
3:F:118:LEU:HD12	3:F:119:PHE:N	2.34	0.42
3:I:172:PRO:HA	3:I:175:TYR:CE1	2.53	0.42
1:J:1:MET:HB3	1:J:1:MET:HE2	1.85	0.42
3:F:96:GLN:HA	3:F:97:PRO:HD2	1.64	0.42
3:I:90:ASN:C	3:I:92:ASP:N	2.72	0.42
1:J:91:GLU:HA	1:J:92:PRO:HD3	1.84	0.42
2:K:83:TYR:HB3	2:K:90:ILE:HG12	2.01	0.42
1:A:7:ILE:HD11	1:A:27:LEU:HD22	2.02	0.42
2:E:63:ARG:CD	2:E:63:ARG:N	2.82	0.42
3:F:142:VAL:O	3:F:143:ASP:C	2.57	0.42
1:A:70:GLN:HG2	1:A:71:ALA:N	2.28	0.42
2:B:95:ILE:CD1	2:B:103:LEU:HD23	2.40	0.42
3:F:166:VAL:O	3:F:167:ARG:C	2.57	0.42
1:G:15:PHE:CE2	2:H:74:CYS:HB2	2.55	0.42
1:G:80:ARG:O	1:G:85:PHE:CE1	2.72	0.42
2:H:18:TYR:CE1	2:H:32:LYS:HG3	2.54	0.42
3:C:72:SER:N	3:C:111:SER:O	2.53	0.42
3:I:170:VAL:O	3:I:175:TYR:HE1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:84:VAL:CG1	3:L:85:LEU:N	2.82	0.42
2:K:101:LEU:HD23	2:K:101:LEU:HA	1.89	0.42
3:L:70:GLU:HB2	3:L:113:ARG:HB2	2.00	0.42
2:H:72:LYS:O	2:H:73:VAL:C	2.58	0.42
1:A:58:GLY:HA2	1:A:62:PHE:O	2.20	0.42
3:C:183:SER:OG	3:C:184:LEU:N	2.51	0.42
2:E:107:ALA:HB2	3:F:158:LEU:HG	2.02	0.42
1:G:44:LEU:HA	1:G:76:GLY:O	2.20	0.42
1:G:70:GLN:HG2	2:H:79:TYR:CD1	2.55	0.42
2:H:90:ILE:HA	2:H:91:PRO:HD3	1.85	0.42
3:L:75:ILE:HD13	3:L:108:ARG:HG3	2.02	0.42
1:A:31:VAL:O	1:A:32:GLU:C	2.58	0.41
2:B:31:VAL:CG1	2:B:32:LYS:N	2.82	0.41
2:H:20:LYS:HE2	2:H:30:ILE:HD11	2.02	0.41
2:H:96:ALA:O	2:H:97:PRO:C	2.59	0.41
3:I:176:ARG:HD3	3:I:176:ARG:HA	1.89	0.41
3:F:204:GLU:CA	3:F:204:GLU:OE1	2.69	0.41
1:G:36:LYS:C	1:G:37:ARG:HG2	2.34	0.41
3:L:85:LEU:HB2	3:L:122:ALA:HB2	2.02	0.41
2:B:20:LYS:HB2	2:B:20:LYS:HE3	1.88	0.41
2:E:19:VAL:HG13	2:E:33:ARG:HG3	2.00	0.41
3:F:75:ILE:CD1	3:F:146:PRO:CB	2.89	0.41
2:H:76:TYR:O	2:H:79:TYR:HB3	2.20	0.41
3:I:87:VAL:HB	3:I:118:LEU:HD12	2.02	0.41
3:I:180:ILE:O	3:I:185:TYR:CE2	2.73	0.41
2:K:90:ILE:HA	2:K:91:PRO:HD3	1.89	0.41
1:A:98:GLU:HA	1:A:98:GLU:OE1	2.20	0.41
3:C:121:ASP:O	3:C:125:HIS:N	2.49	0.41
1:G:91:GLU:HA	1:G:92:PRO:HD2	1.83	0.41
2:K:20:LYS:NZ	2:K:28:GLU:OE1	2.46	0.41
3:C:130:VAL:O	3:C:131:ASN:C	2.59	0.41
3:F:68:SER:O	3:F:70:GLU:N	2.52	0.41
1:G:63:THR:O	1:G:64:SER:C	2.58	0.41
3:C:74:VAL:HG12	3:C:75:ILE:N	2.36	0.41
2:E:29:PHE:CD2	2:E:70:LEU:HG	2.56	0.41
3:I:84:VAL:HG22	3:I:128:LEU:CD1	2.51	0.41
1:A:3:VAL:O	1:A:17:ASP:HA	2.20	0.41
2:B:67:SER:C	2:B:69:VAL:H	2.24	0.41
2:E:93:PHE:HA	2:E:94:PRO:HD3	1.78	0.41
2:H:25:ASP:OD1	2:H:67:SER:OG	2.36	0.41
3:I:134:GLU:HG2	3:I:201:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:38:PRO:HD2	1:J:41:GLU:HB2	2.02	0.41
1:D:63:THR:O	1:D:65:GLN:N	2.54	0.41
2:H:107:ALA:HB2	3:I:158:LEU:HG	2.03	0.41
1:A:99:LEU:HA	1:A:100:PRO:HD3	1.72	0.41
1:J:7:ILE:HB	1:J:14:ILE:HB	2.01	0.41
3:L:74:VAL:HA	3:L:147:ILE:O	2.21	0.41
3:C:198:LEU:HA	3:C:198:LEU:HD23	1.64	0.41
1:G:104:LYS:HA	1:G:105:PRO:HD3	1.92	0.41
1:G:35:LEU:HD23	1:G:35:LEU:HA	1.74	0.41
1:G:56:THR:HG1	1:G:59:GLU:HG3	1.86	0.41
2:H:100:ALA:O	2:H:101:LEU:C	2.58	0.41
1:J:104:LYS:CG	1:J:105:PRO:HB3	2.44	0.41
1:J:9:ARG:O	1:J:10:HIS:HB2	2.20	0.41
3:I:119:PHE:N	3:I:119:PHE:CD1	2.88	0.41
3:I:69:ARG:HG2	4:I:2003:HOH:O	2.16	0.40
2:K:21:LEU:HD22	2:K:62:PHE:HE2	1.86	0.40
3:L:68:SER:CB	3:L:70:GLU:HG2	2.47	0.40
3:L:142:VAL:C	3:L:144:GLY:N	2.69	0.40
1:A:41:GLU:HG3	1:A:81:ALA:C	2.42	0.40
1:A:70:GLN:HB3	2:B:79:TYR:HD2	1.86	0.40
3:I:195:GLN:O	3:I:199:GLU:N	2.51	0.40
2:K:41:THR:HG22	2:K:42:ILE:N	2.36	0.40
2:K:63:ARG:HB2	2:K:63:ARG:HH11	1.86	0.40
3:L:70:GLU:HG3	3:L:113:ARG:HD3	2.04	0.40
3:F:167:ARG:NH2	3:F:187:ASP:O	2.52	0.40
3:I:128:LEU:HD23	3:I:128:LEU:HA	1.92	0.40
3:I:119:PHE:CE1	3:I:130:VAL:HG21	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	97/118 (82%)	84 (87%)	9 (9%)	4 (4%)	3	9
1	D	94/118 (80%)	77 (82%)	10 (11%)	7 (7%)	1	2
1	G	103/118 (87%)	81 (79%)	17 (16%)	5 (5%)	2	7
1	J	103/118 (87%)	88 (85%)	11 (11%)	4 (4%)	3	10
2	B	82/97 (84%)	64 (78%)	12 (15%)	6 (7%)	1	2
2	E	83/97 (86%)	74 (89%)	5 (6%)	4 (5%)	2	7
2	H	82/97 (84%)	65 (79%)	15 (18%)	2 (2%)	6	20
2	K	81/97 (84%)	68 (84%)	7 (9%)	6 (7%)	1	2
3	C	140/163 (86%)	108 (77%)	23 (16%)	9 (6%)	1	3
3	F	140/163 (86%)	113 (81%)	18 (13%)	9 (6%)	1	3
3	I	143/163 (88%)	116 (81%)	21 (15%)	6 (4%)	3	9
3	L	141/163 (86%)	123 (87%)	12 (8%)	6 (4%)	2	8
All	All	1289/1512 (85%)	1061 (82%)	160 (12%)	68 (5%)	2	6

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	ASP
3	C	90	ASN
3	C	142	VAL
1	D	10	HIS
1	D	47	ASP
1	D	94	SER
1	D	97	PRO
1	D	99	LEU
1	D	100	PRO
3	F	144	GLY
3	F	145	GLN
1	G	82	ASP
1	G	99	LEU
3	I	145	GLN
3	I	190	ASP
3	I	205	ARG
1	J	102	VAL
2	K	41	THR
2	K	45	MET
3	L	63	LEU
3	L	90	ASN
3	L	141	ASN

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Mol	Chain	Res	Type
3	L	182	ARG
3	L	190	ASP
1	A	20	GLU
1	A	48	ASP
1	A	80	ARG
2	B	85	ASN
2	B	88	THR
2	B	97	PRO
3	C	145	GLN
3	F	69	ARG
3	F	90	ASN
1	G	84	THR
2	H	89	GLU
2	K	42	ILE
3	L	142	VAL
2	B	89	GLU
3	C	68	SER
3	C	143	ASP
1	D	64	SER
2	E	37	LEU
2	E	87	SER
3	I	90	ASN
3	I	204	GLU
1	J	104	LYS
2	B	44	ALA
2	E	47	SER
3	F	132	GLN
3	F	179	ASP
1	G	94	SER
3	I	67	ASN
1	J	101	ASP
2	B	43	LYS
3	C	177	ARG
2	E	85	ASN
3	F	167	ARG
3	F	173	GLU
1	G	38	PRO
1	J	84	THR
2	K	89	GLU
3	C	83	VAL
2	K	98	GLU
2	K	97	PRO

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Mol	Chain	Res	Type
2	H	97	PRO
3	C	103	PRO
3	C	191	HIS
3	F	103	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	82/103 (80%)	76 (93%)	6 (7%)	14	38
1	D	73/103 (71%)	62 (85%)	11 (15%)	3	9
1	G	87/103 (84%)	79 (91%)	8 (9%)	9	27
1	J	91/103 (88%)	85 (93%)	6 (7%)	16	44
2	B	72/86 (84%)	66 (92%)	6 (8%)	11	32
2	E	74/86 (86%)	63 (85%)	11 (15%)	3	9
2	H	76/86 (88%)	66 (87%)	10 (13%)	4	12
2	K	76/86 (88%)	70 (92%)	6 (8%)	12	34
3	C	107/149 (72%)	87 (81%)	20 (19%)	1	5
3	F	122/149 (82%)	106 (87%)	16 (13%)	4	12
3	I	129/149 (87%)	112 (87%)	17 (13%)	4	12
3	L	126/149 (85%)	112 (89%)	14 (11%)	6	19
All	All	1115/1352 (82%)	984 (88%)	131 (12%)	5	16

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ARG
1	A	32	GLU
1	A	36	LYS
1	A	40	ASP
1	A	45	TYR
1	A	98	GLU

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Mol	Chain	Res	Type
2	B	33	ARG
2	B	61	ASN
2	B	72	LYS
2	B	87	SER
2	B	97	PRO
2	B	99	ILE
3	C	65	SER
3	C	67	ASN
3	C	72	SER
3	C	75	ILE
3	C	77	CYS
3	C	80	SER
3	C	89	LEU
3	C	96	GLN
3	C	101	LEU
3	C	105	THR
3	C	116	LEU
3	C	120	ARG
3	C	141	ASN
3	C	148	PHE
3	C	166	VAL
3	C	180	ILE
3	C	184	LEU
3	C	186	GLU
3	C	198	LEU
3	C	202	THR
1	D	1	MET
1	D	3	VAL
1	D	7	ILE
1	D	16	THR
1	D	22	SER
1	D	30	ILE
1	D	70	GLN
1	D	77	LEU
1	D	88	LEU
1	D	95	SER
1	D	97	PRO
2	E	17	MET
2	E	31	VAL
2	E	32	LYS
2	E	33	ARG
2	E	34	GLU

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Mol	Chain	Res	Type
2	E	35	HIS
2	E	37	LEU
2	E	70	LEU
2	E	78	THR
2	E	84	THR
2	E	102	GLU
3	F	69	ARG
3	F	77	CYS
3	F	90	ASN
3	F	111	SER
3	F	116	LEU
3	F	120	ARG
3	F	148	PHE
3	F	168	SER
3	F	169	LEU
3	F	170	VAL
3	F	171	LYS
3	F	174	ASN
3	F	180	ILE
3	F	195	GLN
3	F	196	LYS
3	F	204	GLU
1	G	1	MET
1	G	6	MET
1	G	19	LYS
1	G	49	GLN
1	G	68	ARG
1	G	70	GLN
1	G	85	PHE
1	G	102	VAL
2	H	19	VAL
2	H	35	HIS
2	H	45	MET
2	H	46	LEU
2	H	63	ARG
2	H	70	LEU
2	H	80	LYS
2	H	84	THR
2	H	99	ILE
2	H	101	LEU
3	I	66	VAL
3	I	69	ARG

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Mol	Chain	Res	Type
3	I	72	SER
3	I	74	VAL
3	I	77	CYS
3	I	79	ARG
3	I	80	SER
3	I	111	SER
3	I	120	ARG
3	I	137	VAL
3	I	139	SER
3	I	170	VAL
3	I	174	ASN
3	I	177	ARG
3	I	183	SER
3	I	194	VAL
3	I	196	LYS
1	J	22	SER
1	J	53	ASP
1	J	64	SER
1	J	80	ARG
1	J	84	THR
1	J	95	SER
2	K	60	VAL
2	K	63	ARG
2	K	67	SER
2	K	78	THR
2	K	80	LYS
2	K	99	ILE
3	L	63	LEU
3	L	72	SER
3	L	77	CYS
3	L	116	LEU
3	L	120	ARG
3	L	145	GLN
3	L	150	ASN
3	L	173	GLU
3	L	176	ARG
3	L	177	ARG
3	L	181	VAL
3	L	188	LEU
3	L	196	LYS
3	L	197	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such



sidechains are listed below:

Mol	Chain	Res	Type
3	C	67	ASN
3	C	141	ASN
1	D	10	HIS
1	D	42	GLN
1	D	70	GLN
2	E	35	HIS
3	F	73	GLN
3	F	90	ASN
3	F	110	HIS
3	F	174	ASN
1	G	42	GLN
2	H	27	HIS
3	I	90	ASN
3	I	96	GLN
3	I	141	ASN
3	I	191	HIS
1	J	42	GLN
1	J	49	GLN
3	L	96	GLN
3	L	174	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

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	101/118 (85%)	-0.49	0 100 100	18, 30, 50, 64	0
1	D	98/118 (83%)	-0.39	0 100 100	26, 42, 56, 63	0
1	G	105/118 (88%)	-0.26	1 (0%) 82 77	24, 45, 61, 76	0
1	J	105/118 (88%)	-0.49	0 100 100	17, 31, 51, 68	0
2	B	86/97 (88%)	-0.46	0 100 100	19, 30, 46, 51	0
2	E	87/97 (89%)	-0.28	0 100 100	21, 36, 49, 53	0
2	H	86/97 (88%)	-0.15	0 100 100	23, 38, 58, 61	0
2	K	85/97 (87%)	-0.39	0 100 100	18, 31, 51, 56	0
3	C	142/163 (87%)	-0.32	0 100 100	17, 41, 63, 65	0
3	F	142/163 (87%)	-0.35	0 100 100	20, 37, 59, 69	0
3	I	145/163 (88%)	-0.33	0 100 100	18, 34, 56, 61	0
3	L	143/163 (87%)	-0.39	0 100 100	14, 28, 50, 56	0
All	All	1325/1512 (87%)	-0.36	1 (0%) 95 95	14, 35, 58, 76	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	82	ASP	2.5

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.