



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:50 PM GMT

PDB ID : 1VCB  
Title : THE VHL-ELONGINC-ELONGINB STRUCTURE  
Authors : Stebbins, C.E.; Kaelin, W.G.; Pavletich, N.P.  
Deposited on : 1999-03-13  
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

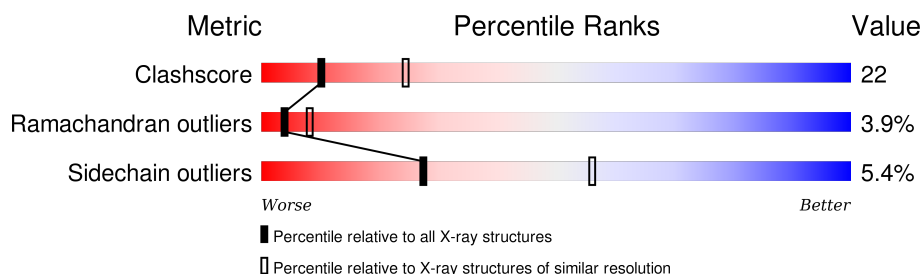
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	118	<div> <div>45%</div> <div>31%</div> <div>7%</div> <div>17%</div> </div>
1	D	118	<div> <div>43%</div> <div>33%</div> <div>7%</div> <div>17%</div> </div>
1	G	118	<div> <div>46%</div> <div>31%</div> <div>6%</div> <div>17%</div> </div>
1	J	118	<div> <div>42%</div> <div>33%</div> <div>8%</div> <div>17%</div> </div>
2	B	112	<div> <div>50%</div> <div>27%</div> <div>•</div> <div>21%</div> </div>
2	E	112	<div> <div>49%</div> <div>28%</div> <div>•</div> <div>21%</div> </div>
2	H	112	<div> <div>48%</div> <div>29%</div> <div>•</div> <div>21%</div> </div>

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Mol	Chain	Length	Quality of chain
2	K	112	
3	C	160	
3	F	160	
3	I	160	
3	L	160	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10858 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 PROTEIN (ELONGIN B).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	98	Total	C	N	O	S	0	0	0
			755	477	128	146	4			
1	D	98	Total	C	N	O	S	0	0	0
			755	477	128	146	4			
1	G	98	Total	C	N	O	S	0	0	0
			755	477	128	146	4			
1	J	98	Total	C	N	O	S	0	0	0
			755	477	128	146	4			

- Molecule 2 is a protein called PROTEIN (ELONGIN C).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	88	Total	C	N	O	S	0	0	0
			692	447	111	128	6			
2	E	88	Total	C	N	O	S	0	0	0
			692	447	111	128	6			
2	H	88	Total	C	N	O	S	0	0	0
			692	447	111	128	6			
2	K	88	Total	C	N	O	S	0	0	0
			692	447	111	128	6			

- Molecule 3 is a protein called PROTEIN (VHL).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	142	Total	C	N	O	S	0	0	0
			1154	734	211	207	2			
3	F	142	Total	C	N	O	S	0	0	0
			1154	734	211	207	2			
3	I	142	Total	C	N	O	S	0	0	0
			1154	734	211	207	2			
3	L	142	Total	C	N	O	S	0	0	0
			1154	734	211	207	2			

- Molecule 4 is water.

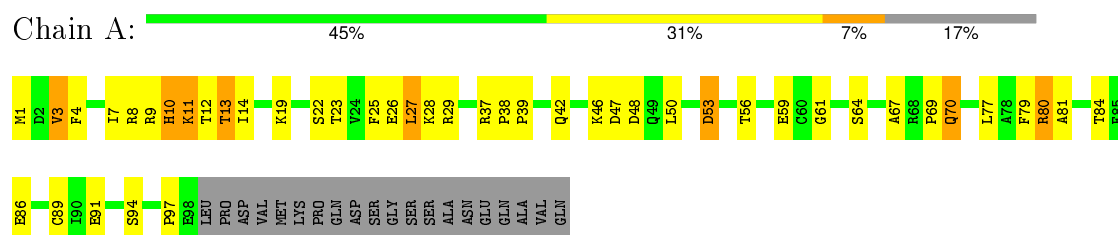
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	32	Total 32	O 32	0	0
4	B	28	Total 28	O 28	0	0
4	C	59	Total 59	O 59	0	0
4	D	27	Total 27	O 27	0	0
4	E	28	Total 28	O 28	0	0
4	F	45	Total 45	O 45	0	0
4	G	22	Total 22	O 22	0	0
4	H	19	Total 19	O 19	0	0
4	I	55	Total 55	O 55	0	0
4	J	41	Total 41	O 41	0	0
4	K	29	Total 29	O 29	0	0
4	L	69	Total 69	O 69	0	0

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

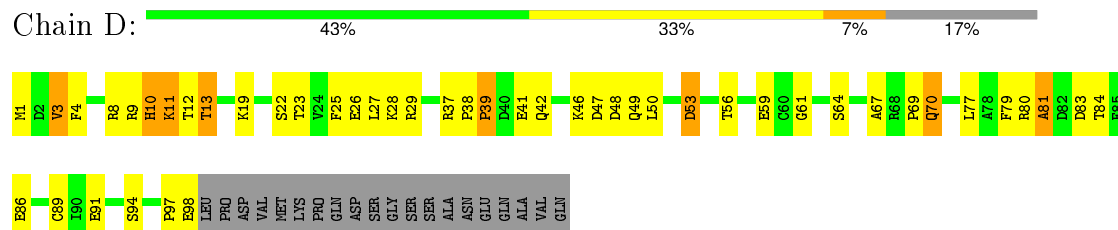
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

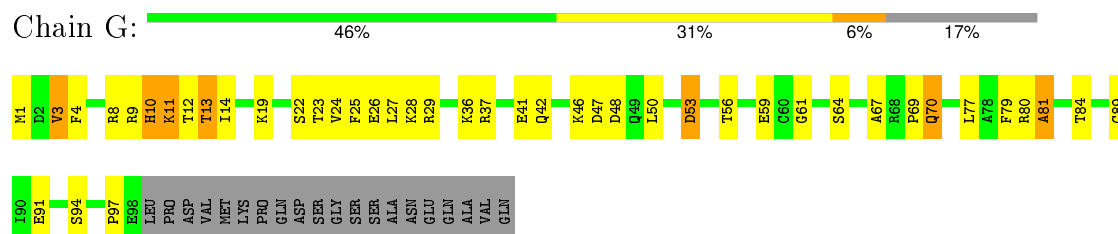
#### • Molecule 1: PROTEIN (ELONGIN B)



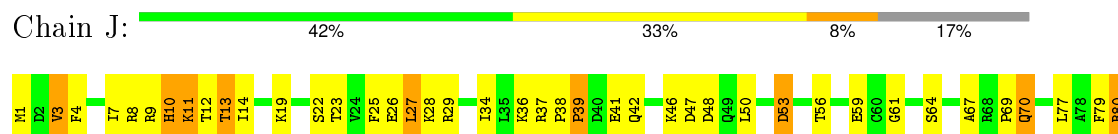
#### • Molecule 1: PROTEIN (ELONGIN B)

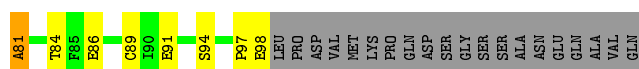


#### • Molecule 1: PROTEIN (ELONGIN B)

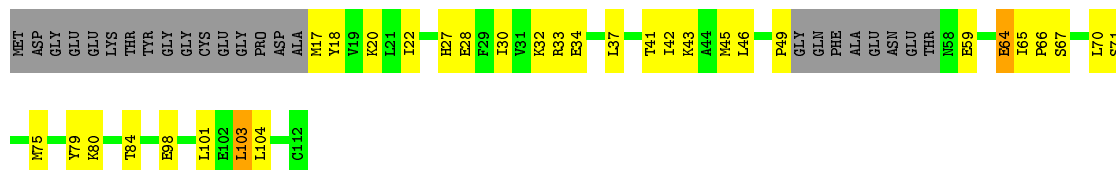
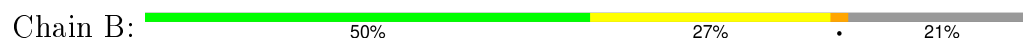


#### • Molecule 1: PROTEIN (ELONGIN B)

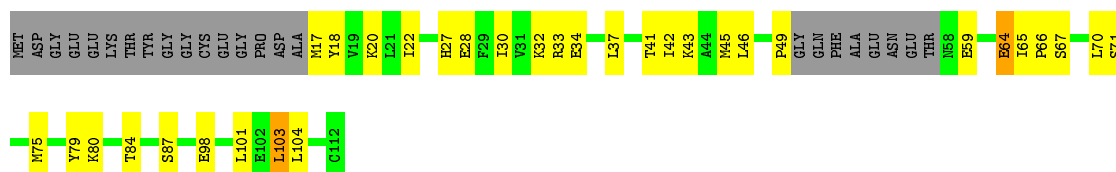




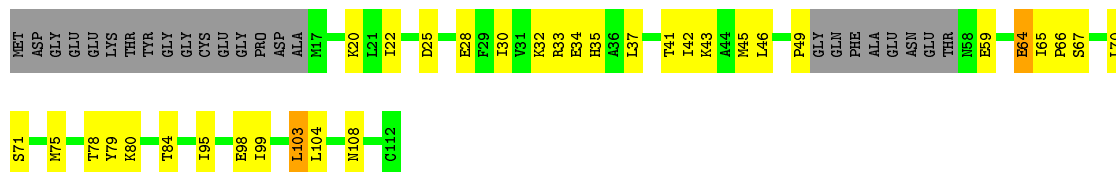
• Molecule 2: PROTEIN (ELONGIN C)



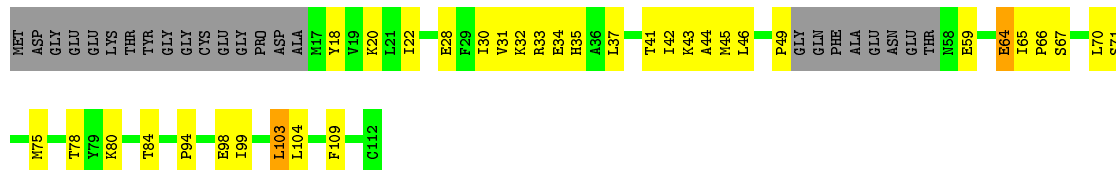
• Molecule 2: PROTEIN (ELONGIN C)



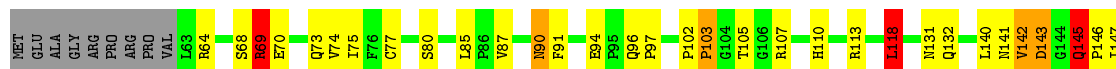
• Molecule 2: PROTEIN (ELONGIN C)



• Molecule 2: PROTEIN (ELONGIN C)



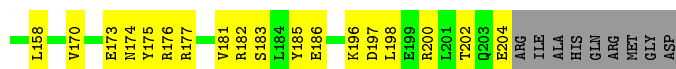
• Molecule 3: PROTEIN (VHL)





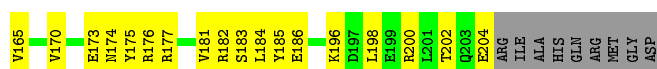
- Molecule 3: PROTEIN (VHL)

Chain F: 56% 29% 11%



- Molecule 3: PROTEIN (VHL)

Chain I: 56% 27% 11%



- Molecule 3: PROTEIN (VHL)

Chain L: 57% 26% 11%





## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.50 Å 93.50 Å 362.30 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70	Depositor
% Data completeness (in resolution range)	84.6 (20.00-2.70)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	7.00	Depositor
Refinement program	CNS 0.3	Depositor
R, $R_{free}$	0.238 , 0.289	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10858	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

## 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	0.66	0/769	0.85	0/1040
1	D	0.60	0/769	0.81	0/1040
1	G	0.62	0/769	0.83	0/1040
1	J	0.66	0/769	0.85	0/1040
2	B	0.68	0/706	0.76	1/952 (0.1%)
2	E	0.64	0/706	0.76	1/952 (0.1%)
2	H	0.63	0/706	0.76	1/952 (0.1%)
2	K	0.66	0/706	0.76	1/952 (0.1%)
3	C	0.64	0/1184	0.90	4/1616 (0.2%)
3	F	0.62	0/1184	0.89	3/1616 (0.2%)
3	I	0.66	1/1184 (0.1%)	0.91	4/1616 (0.2%)
3	L	0.69	1/1184 (0.1%)	0.93	4/1616 (0.2%)
All	All	0.65	2/10636 (0.0%)	0.85	19/14432 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	77	CYS	CB-SG	6.44	1.93	1.82
3	I	77	CYS	CB-SG	5.95	1.92	1.82

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	118	LEU	CA-CB-CG	6.56	130.39	115.30
3	F	118	LEU	CA-CB-CG	6.52	130.31	115.30
3	C	85	LEU	CA-CB-CG	6.36	129.94	115.30
3	I	85	LEU	CA-CB-CG	6.36	129.91	115.30
3	I	145	GLN	N-CA-C	6.34	128.12	111.00
3	I	118	LEU	CA-CB-CG	6.30	129.78	115.30
3	F	145	GLN	N-CA-C	6.29	127.98	111.00
3	L	145	GLN	N-CA-C	6.26	127.91	111.00
3	C	118	LEU	CA-CB-CG	6.25	129.68	115.30
3	C	145	GLN	N-CA-C	6.21	127.78	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	85	LEU	CA-CB-CG	6.21	129.59	115.30
2	E	49	PRO	N-CA-CB	5.91	110.39	103.30
3	F	85	LEU	CA-CB-CG	5.86	128.78	115.30
2	H	49	PRO	N-CA-CB	5.77	110.22	103.30
3	C	153	LEU	CA-CB-CG	5.70	128.41	115.30
2	B	49	PRO	N-CA-CB	5.67	110.11	103.30
2	K	49	PRO	N-CA-CB	5.67	110.10	103.30
3	I	153	LEU	CA-CB-CG	5.14	127.12	115.30
3	L	153	LEU	CA-CB-CG	5.09	127.00	115.30

There are no chirality outliers.

There are no planarity outliers.

## 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	755	0	744	37	0
1	D	755	0	744	33	0
1	G	755	0	744	34	0
1	J	755	0	744	37	0
2	B	692	0	685	23	0
2	E	692	0	685	25	0
2	H	692	0	685	27	0
2	K	692	0	685	36	0
3	C	1154	0	1144	64	1
3	F	1154	0	1144	55	1
3	I	1154	0	1144	58	0
3	L	1154	0	1144	59	0
4	A	32	0	0	1	0
4	B	28	0	0	0	0
4	C	59	0	0	6	0
4	D	27	0	0	2	0
4	E	28	0	0	3	0
4	F	45	0	0	5	0
4	G	22	0	0	0	0
4	H	19	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	55	0	0	7	0
4	J	41	0	0	2	0
4	K	29	0	0	6	0
4	L	69	0	0	11	0
All	All	10858	0	10292	452	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (452) 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:142:VAL:HA	4:I:264:HOH:O	1.59	1.02
3:F:196:LYS:HE3	3:F:200:ARG:HH22	1.21	1.00
3:C:196:LYS:HE3	3:C:200:ARG:HH22	1.25	0.99
3:L:196:LYS:HE3	3:L:200:ARG:HH22	1.25	0.99
3:I:196:LYS:HE3	3:I:200:ARG:HH22	1.24	0.98
1:G:56:THR:OG1	1:G:59:GLU:HG3	1.69	0.93
1:D:56:THR:OG1	1:D:59:GLU:HG3	1.73	0.88
3:I:159:LYS:HE3	4:I:241:HOH:O	1.73	0.88
1:J:56:THR:OG1	1:J:59:GLU:HG3	1.74	0.87
1:A:56:THR:OG1	1:A:59:GLU:HG3	1.75	0.85
3:F:196:LYS:HE3	3:F:200:ARG:NH2	1.94	0.81
1:G:11:LYS:HG3	1:G:91:GLU:HG3	1.63	0.81
1:J:11:LYS:HG3	1:J:91:GLU:HG3	1.63	0.80
1:D:11:LYS:HG3	1:D:91:GLU:HG3	1.64	0.79
1:A:11:LYS:HG3	1:A:91:GLU:HG3	1.64	0.79
3:L:196:LYS:HE3	3:L:200:ARG:NH2	1.97	0.78
3:C:196:LYS:HE3	3:C:200:ARG:NH2	1.97	0.78
3:I:196:LYS:HE3	3:I:200:ARG:NH2	1.97	0.78
3:F:69:ARG:HD3	4:F:237:HOH:O	1.85	0.76
1:J:98:GLU:HG2	4:J:138:HOH:O	1.84	0.75
2:H:99:ILE:HD11	4:H:119:HOH:O	1.87	0.75
2:K:99:ILE:HD11	4:K:113:HOH:O	1.86	0.74
1:J:70:GLN:NE2	1:J:70:GLN:H	1.86	0.73
3:L:143:ASP:N	4:L:240:HOH:O	2.19	0.73
1:G:25:PHE:HB2	1:G:53:ASP:HB3	1.71	0.72
1:J:80:ARG:CB	4:J:130:HOH:O	2.37	0.72
1:G:70:GLN:H	1:G:70:GLN:NE2	1.88	0.71
1:D:94:SER:H	2:E:67:SER:HB2	1.56	0.70
3:C:105:THR:HG21	2:K:64:GLU:OE2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:200:ARG:HG3	4:C:242:HOH:O	1.90	0.70
1:D:25:PHE:HB2	1:D:53:ASP:HB3	1.74	0.69
3:I:144:GLY:HA3	4:I:258:HOH:O	1.93	0.69
3:I:181:VAL:HG12	3:I:183:SER:H	1.59	0.68
1:A:25:PHE:HB2	1:A:53:ASP:HB3	1.75	0.68
1:A:94:SER:H	2:B:67:SER:HB2	1.58	0.68
2:K:64:GLU:HG2	4:K:116:HOH:O	1.93	0.68
1:D:70:GLN:H	1:D:70:GLN:NE2	1.91	0.67
3:I:87:VAL:HB	3:I:118:LEU:HD22	1.77	0.67
3:F:181:VAL:HG12	3:F:183:SER:H	1.60	0.67
2:B:20:LYS:HB3	2:B:59:GLU:HG2	1.77	0.66
3:I:145:GLN:HG2	4:I:264:HOH:O	1.95	0.66
3:C:148:PHE:CZ	2:K:45:MET:HA	2.30	0.66
3:C:87:VAL:HB	3:C:118:LEU:HD22	1.78	0.66
3:C:181:VAL:HG12	3:C:183:SER:H	1.61	0.65
3:F:145:GLN:HG3	4:F:229:HOH:O	1.96	0.65
1:G:23:THR:OG1	1:G:26:GLU:HG3	1.95	0.65
3:C:68:SER:HB2	4:C:249:HOH:O	1.96	0.65
1:J:25:PHE:HB2	1:J:53:ASP:HB3	1.77	0.65
3:F:196:LYS:O	3:F:200:ARG:HG2	1.97	0.65
3:L:63:LEU:N	4:L:228:HOH:O	2.28	0.65
3:C:182:ARG:HG3	3:C:182:ARG:HH11	1.62	0.65
3:I:73:GLN:H	3:I:141:ASN:ND2	1.95	0.64
3:L:73:GLN:H	3:L:141:ASN:ND2	1.95	0.64
1:A:23:THR:OG1	1:A:26:GLU:HG3	1.97	0.64
1:A:70:GLN:NE2	1:A:70:GLN:H	1.95	0.64
3:L:87:VAL:HB	3:L:118:LEU:HD22	1.80	0.64
3:L:181:VAL:HG12	3:L:183:SER:H	1.63	0.64
3:F:73:GLN:H	3:F:141:ASN:ND2	1.96	0.64
2:K:20:LYS:HB3	2:K:59:GLU:HG2	1.80	0.63
3:L:120:ARG:HD2	4:L:262:HOH:O	1.96	0.63
2:H:22:ILE:HG12	2:H:28:GLU:HG2	1.81	0.63
3:I:75:ILE:HD13	3:I:148:PHE:CE1	2.33	0.63
3:C:191:HIS:HB2	4:C:247:HOH:O	1.99	0.63
3:F:182:ARG:HG3	3:F:182:ARG:HH11	1.64	0.62
3:F:87:VAL:HB	3:F:118:LEU:HD22	1.81	0.62
1:J:28:LYS:HE3	1:J:42:GLN:O	1.99	0.62
3:I:196:LYS:O	3:I:200:ARG:HG2	2.00	0.62
3:C:75:ILE:HD13	3:C:148:PHE:CE1	2.35	0.62
3:C:73:GLN:H	3:C:141:ASN:ND2	1.97	0.62
3:C:196:LYS:O	3:C:200:ARG:HG2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:103:LEU:HD22	3:C:158:LEU:HD21	1.81	0.62
2:H:37:LEU:HD22	2:H:43:LYS:HG3	1.82	0.61
3:L:176:ARG:NH1	3:L:185:TYR:HB3	2.16	0.61
3:L:75:ILE:HD13	3:L:148:PHE:CE1	2.35	0.61
2:K:99:ILE:CD1	4:K:113:HOH:O	2.47	0.61
3:C:176:ARG:NH1	3:C:185:TYR:HB3	2.15	0.61
1:D:28:LYS:HE3	1:D:42:GLN:O	2.01	0.61
1:G:94:SER:H	2:H:67:SER:HB2	1.66	0.61
2:E:20:LYS:HB3	2:E:59:GLU:HG2	1.83	0.61
3:L:182:ARG:HH11	3:L:182:ARG:HG3	1.66	0.61
1:A:3:VAL:HG22	1:A:67:ALA:HB3	1.83	0.61
1:J:19:LYS:O	1:J:22:SER:HB3	2.01	0.61
3:I:182:ARG:HH11	3:I:182:ARG:HG3	1.65	0.60
1:G:4:PHE:H	1:G:67:ALA:HB1	1.65	0.60
2:K:22:ILE:HG12	2:K:28:GLU:HG2	1.83	0.60
3:F:176:ARG:NH1	3:F:185:TYR:HB3	2.16	0.60
3:C:105:THR:CG2	2:K:64:GLU:OE2	2.49	0.60
3:F:75:ILE:HD13	3:F:148:PHE:CE1	2.37	0.60
3:I:176:ARG:NH1	3:I:185:TYR:HB3	2.17	0.60
1:D:23:THR:OG1	1:D:26:GLU:HG3	2.01	0.60
2:E:22:ILE:HG12	2:E:28:GLU:HG2	1.83	0.60
2:H:98:GLU:CD	2:H:98:GLU:H	2.04	0.60
1:D:3:VAL:HG22	1:D:67:ALA:HB3	1.84	0.60
1:D:19:LYS:O	1:D:22:SER:HB3	2.02	0.59
1:G:28:LYS:HE3	1:G:42:GLN:O	2.02	0.59
1:D:98:GLU:HB2	4:E:125:HOH:O	2.00	0.59
1:A:1:MET:HE3	4:A:123:HOH:O	2.02	0.59
1:A:19:LYS:O	1:A:22:SER:HB3	2.02	0.59
1:D:83:ASP:CB	4:D:127:HOH:O	2.50	0.59
1:J:23:THR:OG1	1:J:26:GLU:HG3	2.03	0.59
2:K:98:GLU:CD	2:K:98:GLU:H	2.05	0.59
1:J:4:PHE:H	1:J:67:ALA:HB1	1.68	0.59
2:H:99:ILE:CD1	4:H:119:HOH:O	2.49	0.59
4:K:134:HOH:O	3:L:159:LYS:HD3	2.03	0.59
2:E:37:LEU:HD22	2:E:43:LYS:HG3	1.85	0.59
1:A:28:LYS:HE3	1:A:42:GLN:O	2.02	0.58
3:L:203:GLN:CB	4:L:248:HOH:O	2.50	0.58
3:F:143:ASP:N	4:F:229:HOH:O	2.22	0.58
3:F:70:GLU:OE1	3:F:113:ARG:NH1	2.36	0.58
3:L:196:LYS:O	3:L:200:ARG:HG2	2.04	0.58
3:C:146:PRO:HG2	2:K:44:ALA:HB2	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:70:GLU:OE1	3:I:113:ARG:NH1	2.37	0.58
3:L:145:GLN:CG	4:L:240:HOH:O	2.50	0.58
2:H:32:LYS:HB3	2:H:34:GLU:OE2	2.04	0.58
2:B:98:GLU:CD	2:B:98:GLU:H	2.07	0.58
2:K:37:LEU:HD22	2:K:43:LYS:HG3	1.86	0.58
3:C:201:LEU:HD22	4:C:258:HOH:O	2.04	0.58
3:F:90:ASN:HB2	3:F:94:GLU:O	2.04	0.57
3:F:142:VAL:O	3:F:143:ASP:HB3	2.04	0.57
3:C:142:VAL:O	3:C:143:ASP:HB3	2.05	0.57
2:B:32:LYS:HB3	2:B:34:GLU:OE2	2.05	0.57
3:I:63:LEU:HD23	3:I:198:LEU:HD22	1.86	0.57
2:B:37:LEU:HD22	2:B:43:LYS:HG3	1.87	0.57
3:L:131:ASN:O	3:L:132:GLN:HB2	2.05	0.57
1:G:3:VAL:HG22	1:G:67:ALA:HB3	1.85	0.57
3:C:75:ILE:HD12	2:K:41:THR:HG23	1.87	0.57
3:I:181:VAL:HG23	4:I:266:HOH:O	2.05	0.56
3:F:68:SER:HB2	4:F:232:HOH:O	2.05	0.56
3:L:90:ASN:HB2	3:L:94:GLU:O	2.06	0.56
2:E:32:LYS:HB3	2:E:34:GLU:OE2	2.05	0.56
2:E:98:GLU:H	2:E:98:GLU:CD	2.09	0.56
2:K:32:LYS:HB3	2:K:34:GLU:OE2	2.06	0.56
2:B:22:ILE:HG12	2:B:28:GLU:HG2	1.87	0.56
2:E:80:LYS:HE2	2:E:84:THR:HG21	1.87	0.56
3:I:131:ASN:O	3:I:132:GLN:HB2	2.06	0.55
1:G:69:PRO:HD2	1:G:70:GLN:HE22	1.71	0.55
3:C:90:ASN:HB2	3:C:94:GLU:O	2.07	0.55
1:G:19:LYS:O	1:G:22:SER:HB3	2.06	0.55
3:F:182:ARG:HA	3:F:185:TYR:CD2	2.41	0.55
3:F:148:PHE:CZ	2:H:45:MET:HA	2.42	0.55
2:H:20:LYS:HB3	2:H:59:GLU:HG2	1.89	0.55
2:B:103:LEU:CD2	3:C:158:LEU:HD21	2.36	0.55
1:D:4:PHE:H	1:D:67:ALA:HB1	1.72	0.55
3:I:142:VAL:O	3:I:143:ASP:HB3	2.06	0.55
1:G:70:GLN:HG3	2:H:79:TYR:CD1	2.42	0.55
3:C:182:ARG:HA	3:C:185:TYR:CD2	2.42	0.55
1:A:4:PHE:H	1:A:67:ALA:HB1	1.72	0.55
1:A:8:ARG:HG2	1:A:13:THR:HB	1.89	0.55
1:G:10:HIS:O	1:G:12:THR:N	2.40	0.55
3:F:182:ARG:HD2	3:F:185:TYR:HD2	1.72	0.55
3:F:131:ASN:O	3:F:132:GLN:HB2	2.07	0.55
2:H:80:LYS:C	2:H:80:LYS:HD3	2.27	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:69:PRO:HD2	1:G:70:GLN:NE2	2.22	0.55
3:I:182:ARG:HA	3:I:185:TYR:CD2	2.41	0.54
1:A:69:PRO:HD2	1:A:70:GLN:NE2	2.22	0.54
2:H:80:LYS:HE2	2:H:84:THR:HG21	1.89	0.54
2:E:64:GLU:HG2	4:E:124:HOH:O	2.06	0.54
1:G:8:ARG:HG2	1:G:13:THR:HB	1.90	0.54
1:D:69:PRO:HD2	1:D:70:GLN:NE2	2.22	0.54
1:G:26:GLU:O	1:G:29:ARG:HB2	2.06	0.54
3:I:69:ARG:HD2	3:I:69:ARG:H	1.72	0.54
2:H:64:GLU:HB2	4:H:118:HOH:O	2.08	0.54
1:G:11:LYS:CG	1:G:91:GLU:HG3	2.36	0.54
3:L:182:ARG:HA	3:L:185:TYR:CD2	2.42	0.54
3:C:182:ARG:HD2	3:C:185:TYR:HD2	1.73	0.54
1:J:94:SER:H	2:K:67:SER:HB2	1.73	0.54
1:J:69:PRO:HD2	1:J:70:GLN:HE22	1.73	0.54
1:J:69:PRO:HD2	1:J:70:GLN:NE2	2.23	0.54
3:L:142:VAL:O	3:L:143:ASP:HB3	2.07	0.54
1:D:69:PRO:HD2	1:D:70:GLN:HE22	1.73	0.54
3:F:75:ILE:HG23	3:F:148:PHE:HA	1.90	0.54
3:C:110:HIS:HD2	4:C:233:HOH:O	1.91	0.53
3:L:120:ARG:CD	4:L:262:HOH:O	2.53	0.53
2:K:80:LYS:HD3	2:K:80:LYS:C	2.29	0.53
3:L:182:ARG:HD2	3:L:185:TYR:HD2	1.73	0.53
3:I:90:ASN:HB2	3:I:94:GLU:O	2.08	0.53
3:L:170:VAL:HG13	3:L:175:TYR:CE1	2.44	0.53
2:K:80:LYS:HE2	2:K:84:THR:HG21	1.90	0.53
3:C:131:ASN:O	3:C:132:GLN:HB2	2.09	0.53
1:D:11:LYS:CG	1:D:91:GLU:HG3	2.37	0.53
1:D:47:ASP:O	1:D:48:ASP:HB2	2.08	0.53
1:J:47:ASP:O	1:J:48:ASP:HB2	2.09	0.53
3:L:145:GLN:HG2	4:L:240:HOH:O	2.09	0.53
1:A:69:PRO:HD2	1:A:70:GLN:HE22	1.74	0.53
1:D:26:GLU:O	1:D:29:ARG:HB2	2.09	0.53
3:L:90:ASN:HB3	3:L:94:GLU:H	1.73	0.53
1:A:26:GLU:O	1:A:29:ARG:HB2	2.09	0.53
2:B:41:THR:O	2:B:45:MET:HG3	2.09	0.53
1:A:47:ASP:O	1:A:48:ASP:HB2	2.08	0.52
2:K:64:GLU:CB	4:K:114:HOH:O	2.57	0.52
1:D:70:GLN:HG3	2:E:79:TYR:CD1	2.44	0.52
1:J:9:ARG:HB2	1:J:77:LEU:HB3	1.91	0.52
1:J:14:ILE:HG12	2:K:30:ILE:HB	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:103:LEU:HD22	3:F:158:LEU:HD21	1.92	0.52
3:F:69:ARG:H	3:F:69:ARG:HD2	1.74	0.52
3:F:142:VAL:O	3:F:143:ASP:CB	2.58	0.52
3:C:142:VAL:O	3:C:143:ASP:CB	2.58	0.52
1:G:9:ARG:HB2	1:G:77:LEU:HB3	1.91	0.52
3:I:182:ARG:HD2	3:I:185:TYR:HD2	1.74	0.52
3:L:74:VAL:HG12	3:L:75:ILE:N	2.24	0.52
2:E:103:LEU:CD2	3:F:158:LEU:HD21	2.39	0.52
3:I:170:VAL:HG13	3:I:175:TYR:CE1	2.45	0.52
1:D:49:GLN:NE2	4:D:134:HOH:O	2.43	0.52
2:K:64:GLU:HB2	4:K:114:HOH:O	2.08	0.51
2:B:80:LYS:HE2	2:B:84:THR:HG21	1.92	0.51
3:I:75:ILE:HG23	3:I:148:PHE:HA	1.93	0.51
3:I:90:ASN:HB3	3:I:94:GLU:H	1.75	0.51
2:E:80:LYS:C	2:E:80:LYS:HD3	2.31	0.51
3:F:102:PRO:HD2	3:F:105:THR:OG1	2.10	0.51
3:C:69:ARG:H	3:C:69:ARG:HD2	1.75	0.51
2:H:30:ILE:HD12	2:H:30:ILE:N	2.25	0.51
3:C:74:VAL:HG12	3:C:75:ILE:N	2.24	0.51
3:L:69:ARG:HD2	3:L:69:ARG:H	1.76	0.51
3:I:73:GLN:N	3:I:141:ASN:ND2	2.59	0.51
3:C:182:ARG:O	3:C:185:TYR:HB2	2.11	0.50
1:G:47:ASP:O	1:G:48:ASP:HB2	2.12	0.50
2:H:42:ILE:O	2:H:46:LEU:HG	2.10	0.50
1:D:8:ARG:HG2	1:D:13:THR:HB	1.93	0.50
3:I:142:VAL:O	3:I:143:ASP:CB	2.59	0.50
2:E:64:GLU:HB2	4:E:114:HOH:O	2.10	0.50
3:F:182:ARG:O	3:F:185:TYR:HB2	2.10	0.50
1:A:70:GLN:HG3	2:B:79:TYR:CD1	2.46	0.50
2:E:30:ILE:N	2:E:30:ILE:HD12	2.25	0.50
1:D:70:GLN:H	1:D:70:GLN:CD	2.15	0.50
2:B:80:LYS:HD3	2:B:80:LYS:C	2.31	0.50
2:E:41:THR:O	2:E:45:MET:HG3	2.11	0.50
3:I:69:ARG:H	3:I:69:ARG:CD	2.25	0.50
3:F:74:VAL:HG12	3:F:75:ILE:N	2.25	0.50
3:I:102:PRO:HD2	3:I:105:THR:OG1	2.11	0.50
3:L:182:ARG:O	3:L:185:TYR:HB2	2.11	0.50
3:L:73:GLN:N	3:L:141:ASN:ND2	2.60	0.50
1:J:46:LYS:NZ	1:J:61:GLY:HA3	2.27	0.50
2:K:35:HIS:HD2	2:K:78:THR:HG22	1.77	0.49
1:J:10:HIS:O	1:J:12:THR:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:182:ARG:HA	3:I:185:TYR:HD2	1.76	0.49
3:F:129:LEU:HG	3:F:154:PRO:HB3	1.94	0.49
3:C:73:GLN:N	3:C:141:ASN:ND2	2.60	0.49
1:D:10:HIS:O	1:D:12:THR:N	2.45	0.49
3:L:143:ASP:O	3:L:143:ASP:CG	2.51	0.49
3:C:70:GLU:HG3	4:C:249:HOH:O	2.11	0.49
1:J:26:GLU:O	1:J:29:ARG:HB2	2.12	0.49
3:L:70:GLU:OE1	3:L:113:ARG:NH1	2.42	0.49
3:F:182:ARG:HA	3:F:185:TYR:HD2	1.78	0.49
1:J:3:VAL:HG22	1:J:67:ALA:HB3	1.93	0.49
3:F:73:GLN:N	3:F:141:ASN:ND2	2.61	0.49
3:F:69:ARG:CD	3:F:69:ARG:H	2.26	0.49
1:G:14:ILE:HG12	2:H:30:ILE:HB	1.95	0.49
3:C:148:PHE:CE1	2:K:45:MET:HA	2.47	0.48
2:B:33:ARG:O	2:B:37:LEU:HG	2.14	0.48
3:I:182:ARG:O	3:I:185:TYR:HB2	2.12	0.48
2:B:30:ILE:HD12	2:B:30:ILE:N	2.27	0.48
3:L:145:GLN:HG3	4:L:240:HOH:O	2.10	0.48
3:I:74:VAL:HG12	3:I:75:ILE:N	2.28	0.48
3:C:73:GLN:O	3:C:141:ASN:ND2	2.47	0.48
1:J:8:ARG:HG2	1:J:13:THR:HB	1.96	0.48
3:F:73:GLN:O	3:F:141:ASN:ND2	2.47	0.48
2:E:42:ILE:O	2:E:46:LEU:HG	2.13	0.48
3:F:143:ASP:O	3:F:143:ASP:CG	2.52	0.48
3:C:69:ARG:H	3:C:69:ARG:CD	2.27	0.48
2:H:35:HIS:HD2	2:H:78:THR:HG22	1.78	0.48
3:F:90:ASN:HB3	3:F:94:GLU:H	1.78	0.48
3:C:182:ARG:HA	3:C:185:TYR:HD2	1.78	0.48
3:F:202:THR:C	3:F:204:GLU:H	2.17	0.48
3:L:142:VAL:O	3:L:143:ASP:CB	2.61	0.48
3:F:75:ILE:HG22	3:F:147:ILE:O	2.14	0.48
1:A:9:ARG:HB2	1:A:77:LEU:HB3	1.96	0.48
1:J:34:ILE:HD11	2:K:18:TYR:CZ	2.49	0.48
1:A:10:HIS:O	1:A:12:THR:N	2.47	0.48
3:I:145:GLN:CB	3:I:146:PRO:CD	2.91	0.47
1:G:4:PHE:H	1:G:67:ALA:CB	2.27	0.47
2:K:31:VAL:HG12	2:K:32:LYS:N	2.29	0.47
3:I:69:ARG:N	3:I:69:ARG:HD2	2.29	0.47
3:L:69:ARG:CD	3:L:69:ARG:H	2.27	0.47
3:F:69:ARG:HD2	3:F:69:ARG:N	2.29	0.47
1:G:10:HIS:CE1	1:G:89:CYS:HB3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:30:ILE:N	2:K:30:ILE:HD12	2.29	0.47
1:J:10:HIS:CE1	1:J:89:CYS:HB3	2.49	0.47
1:D:46:LYS:NZ	1:D:61:GLY:HA3	2.30	0.47
1:D:9:ARG:HB2	1:D:77:LEU:HB3	1.96	0.47
1:A:70:GLN:CD	1:A:70:GLN:H	2.18	0.47
1:A:46:LYS:NZ	1:A:61:GLY:HA3	2.30	0.47
1:A:11:LYS:HA	2:B:27:HIS:CD2	2.50	0.47
3:I:118:LEU:C	3:I:118:LEU:HD23	2.35	0.47
3:L:182:ARG:HA	3:L:185:TYR:HD2	1.78	0.47
1:G:46:LYS:NZ	1:G:61:GLY:HA3	2.28	0.47
3:C:196:LYS:CE	3:C:200:ARG:HH22	2.13	0.47
3:C:145:GLN:CB	3:C:146:PRO:CD	2.93	0.47
3:C:143:ASP:CG	3:C:143:ASP:O	2.53	0.47
3:C:107:ARG:HA	2:K:109:PHE:CD1	2.50	0.47
3:F:145:GLN:CB	3:F:146:PRO:CD	2.93	0.47
1:G:4:PHE:N	1:G:67:ALA:HB1	2.30	0.47
3:C:145:GLN:HB2	3:C:146:PRO:CD	2.45	0.47
3:C:90:ASN:HB3	3:C:94:GLU:H	1.80	0.47
3:L:73:GLN:O	3:L:141:ASN:ND2	2.48	0.47
3:C:75:ILE:HG23	3:C:148:PHE:HA	1.98	0.46
3:C:148:PHE:HZ	2:K:45:MET:HG2	1.80	0.46
3:F:64:ARG:HD2	3:F:91:PHE:O	2.15	0.46
3:C:170:VAL:HG13	3:C:175:TYR:CE1	2.50	0.46
3:L:144:GLY:HA3	4:L:218:HOH:O	2.16	0.46
1:G:37:ARG:HG3	1:G:79:PHE:CZ	2.51	0.46
2:B:71:SER:O	2:B:75:MET:HG3	2.15	0.46
3:I:73:GLN:O	3:I:141:ASN:ND2	2.48	0.46
3:L:75:ILE:HG23	3:L:148:PHE:HA	1.98	0.46
1:A:11:LYS:CG	1:A:91:GLU:HG3	2.38	0.46
3:C:102:PRO:HD2	3:C:105:THR:OG1	2.15	0.46
2:E:87:SER:HA	3:F:132:GLN:NE2	2.30	0.46
2:K:42:ILE:O	2:K:46:LEU:HG	2.15	0.46
3:C:70:GLU:OE1	3:C:113:ARG:NH1	2.44	0.46
3:C:69:ARG:N	3:C:69:ARG:HD2	2.31	0.46
3:L:170:VAL:HG13	3:L:175:TYR:HE1	1.81	0.46
3:L:69:ARG:HD2	3:L:69:ARG:N	2.30	0.46
3:I:145:GLN:HB2	3:I:146:PRO:CD	2.44	0.46
1:J:4:PHE:N	1:J:67:ALA:HB1	2.30	0.46
2:K:41:THR:O	2:K:45:MET:HG3	2.16	0.46
3:F:118:LEU:C	3:F:118:LEU:HD23	2.37	0.46
1:G:70:GLN:H	1:G:70:GLN:CD	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:118:LEU:HD23	3:C:118:LEU:C	2.37	0.45
3:L:118:LEU:C	3:L:118:LEU:HD23	2.36	0.45
3:F:170:VAL:HG13	3:F:175:TYR:CE1	2.51	0.45
3:F:145:GLN:HB2	3:F:146:PRO:CD	2.46	0.45
2:E:33:ARG:O	2:E:37:LEU:HG	2.17	0.45
2:B:42:ILE:O	2:B:46:LEU:HG	2.16	0.45
1:J:70:GLN:H	1:J:70:GLN:CD	2.13	0.45
1:A:10:HIS:CE1	1:A:89:CYS:HB3	2.51	0.45
3:C:173:GLU:C	3:C:174:ASN:HD22	2.20	0.45
3:I:143:ASP:O	3:I:143:ASP:CG	2.55	0.45
2:K:103:LEU:HD22	3:L:158:LEU:HD21	1.99	0.45
2:E:65:ILE:HA	2:E:66:PRO:HD3	1.78	0.45
3:L:145:GLN:CB	3:L:146:PRO:CD	2.94	0.45
3:C:182:ARG:HG3	3:C:182:ARG:NH1	2.29	0.45
3:C:64:ARG:HD2	3:C:91:PHE:O	2.17	0.45
3:F:120:ARG:NH1	3:F:197:ASP:OD2	2.49	0.45
3:L:181:VAL:HG12	3:L:182:ARG:N	2.32	0.44
1:A:1:MET:HB3	1:A:64:SER:OG	2.17	0.44
1:D:9:ARG:NH1	1:D:86:GLU:OE2	2.50	0.44
2:B:65:ILE:HA	2:B:66:PRO:HD3	1.78	0.44
3:C:202:THR:C	3:C:204:GLU:H	2.21	0.44
3:L:145:GLN:HB2	3:L:146:PRO:CD	2.46	0.44
2:H:33:ARG:O	2:H:37:LEU:HG	2.16	0.44
3:I:68:SER:C	3:I:70:GLU:H	2.21	0.44
3:L:202:THR:C	3:L:204:GLU:H	2.21	0.44
2:H:108:ASN:ND2	3:I:184:LEU:HD21	2.32	0.44
3:I:202:THR:C	3:I:204:GLU:H	2.21	0.44
1:A:9:ARG:NH1	1:A:86:GLU:OE2	2.50	0.44
1:D:38:PRO:HA	1:D:39:PRO:HD3	1.94	0.44
1:J:1:MET:HB3	1:J:64:SER:OG	2.17	0.44
2:H:41:THR:O	2:H:45:MET:HG3	2.17	0.44
1:J:9:ARG:NH1	1:J:86:GLU:OE2	2.51	0.44
3:I:64:ARG:HD2	3:I:91:PHE:O	2.17	0.44
3:I:181:VAL:HG12	3:I:182:ARG:N	2.32	0.44
1:D:1:MET:HB3	1:D:64:SER:OG	2.17	0.44
1:A:22:SER:O	1:A:56:THR:HA	2.18	0.44
2:H:25:ASP:OD2	2:H:67:SER:OG	2.36	0.44
3:C:148:PHE:CZ	2:K:45:MET:HG2	2.53	0.43
1:J:4:PHE:H	1:J:67:ALA:CB	2.30	0.43
2:B:64:GLU:OE1	2:B:64:GLU:HA	2.18	0.43
1:D:11:LYS:HA	2:E:27:HIS:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:101:LEU:HD23	2:E:101:LEU:HA	1.85	0.43
2:K:33:ARG:O	2:K:37:LEU:HG	2.18	0.43
2:B:101:LEU:HD23	2:B:101:LEU:HA	1.84	0.43
3:F:198:LEU:HD23	3:F:198:LEU:HA	1.90	0.43
3:I:173:GLU:C	3:I:174:ASN:HD22	2.21	0.43
3:L:177:ARG:HH11	3:L:177:ARG:HG2	1.84	0.43
2:H:71:SER:O	2:H:75:MET:HG3	2.19	0.43
3:I:182:ARG:NH1	3:I:182:ARG:HG3	2.32	0.43
1:D:10:HIS:CE1	1:D:89:CYS:HB3	2.53	0.43
1:G:1:MET:HB3	1:G:64:SER:OG	2.19	0.43
3:L:68:SER:C	3:L:70:GLU:H	2.22	0.43
1:A:14:ILE:HG12	2:B:30:ILE:HB	2.00	0.43
2:K:71:SER:O	2:K:75:MET:HG3	2.19	0.43
2:K:65:ILE:HA	2:K:66:PRO:HD3	1.77	0.43
1:J:38:PRO:HA	1:J:39:PRO:HD3	1.93	0.43
1:J:70:GLN:HB3	2:K:94:PRO:HD2	2.01	0.43
1:J:37:ARG:HG3	1:J:79:PHE:CZ	2.54	0.43
3:C:181:VAL:HG12	3:C:182:ARG:N	2.34	0.43
3:L:102:PRO:HD2	3:L:105:THR:OG1	2.19	0.43
3:F:177:ARG:HG2	3:F:177:ARG:HH11	1.83	0.43
3:F:182:ARG:NH1	3:F:182:ARG:HG3	2.31	0.42
3:I:143:ASP:N	4:I:233:HOH:O	2.52	0.42
1:A:37:ARG:HG3	1:A:79:PHE:CZ	2.54	0.42
3:L:173:GLU:C	3:L:174:ASN:HD22	2.22	0.42
3:L:64:ARG:HD2	3:L:91:PHE:O	2.19	0.42
1:J:11:LYS:CG	1:J:91:GLU:HG3	2.39	0.42
3:F:68:SER:C	3:F:70:GLU:H	2.22	0.42
2:B:17:MET:HG3	2:B:18:TYR:CD1	2.54	0.42
2:H:65:ILE:HA	2:H:66:PRO:HD3	1.75	0.42
3:I:129:LEU:HG	3:I:154:PRO:HB3	2.00	0.42
3:L:85:LEU:HD13	3:L:87:VAL:CG2	2.50	0.42
1:D:37:ARG:HG3	1:D:79:PHE:CZ	2.54	0.42
3:I:144:GLY:O	3:I:146:PRO:HD2	2.19	0.42
3:C:74:VAL:CG1	3:C:75:ILE:N	2.82	0.42
3:C:68:SER:C	3:C:70:GLU:H	2.23	0.42
3:L:182:ARG:NH1	3:L:182:ARG:HG3	2.32	0.42
3:L:159:LYS:HE3	4:L:265:HOH:O	2.19	0.42
3:F:86:PRO:HG2	3:F:98:TYR:HB2	2.01	0.42
1:J:7:ILE:HD11	1:J:27:LEU:HD22	2.01	0.42
3:F:173:GLU:C	3:F:174:ASN:HD22	2.24	0.42
1:G:56:THR:HG1	1:G:59:GLU:HG3	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:75:ILE:HG22	3:L:147:ILE:O	2.20	0.42
3:I:170:VAL:HG13	3:I:175:TYR:HE1	1.85	0.42
1:G:36:LYS:O	1:G:37:ARG:HG2	2.20	0.42
3:C:80:SER:O	3:C:103:PRO:O	2.37	0.42
3:L:142:VAL:HA	4:L:240:HOH:O	2.19	0.41
2:K:64:GLU:HA	2:K:64:GLU:OE1	2.20	0.41
3:C:166:VAL:O	3:C:170:VAL:HG12	2.20	0.41
1:D:41:GLU:HG2	1:D:81:ALA:HB2	2.01	0.41
3:I:85:LEU:HD13	3:I:87:VAL:CG2	2.50	0.41
1:A:70:GLN:HG3	2:B:79:TYR:HD1	1.82	0.41
1:J:36:LYS:O	1:J:37:ARG:HG2	2.20	0.41
3:C:107:ARG:HA	2:K:109:PHE:CE1	2.55	0.41
3:F:130:VAL:O	3:F:130:VAL:HG13	2.20	0.41
3:L:196:LYS:CE	3:L:200:ARG:HH22	2.14	0.41
1:J:79:PHE:HB3	1:J:80:ARG:H	1.76	0.41
2:H:95:ILE:HB	3:I:165:VAL:HG21	2.03	0.41
3:L:86:PRO:HG2	3:L:98:TYR:HB2	2.02	0.41
3:L:144:GLY:O	3:L:146:PRO:HD2	2.20	0.41
1:G:29:ARG:HA	1:G:29:ARG:HD3	1.88	0.41
1:G:46:LYS:HZ2	1:G:61:GLY:HA3	1.85	0.41
3:F:145:GLN:HB2	3:F:146:PRO:HD2	2.02	0.41
2:E:17:MET:HG3	2:E:18:TYR:CD1	2.55	0.41
3:F:144:GLY:N	4:F:229:HOH:O	2.46	0.41
1:A:29:ARG:HD3	1:A:29:ARG:HA	1.90	0.41
1:G:10:HIS:C	1:G:12:THR:H	2.24	0.41
1:A:79:PHE:HB3	1:A:80:ARG:H	1.78	0.41
1:J:41:GLU:HG2	1:J:81:ALA:HB2	2.01	0.41
3:I:75:ILE:HG22	3:I:147:ILE:O	2.21	0.41
1:A:4:PHE:H	1:A:67:ALA:CB	2.32	0.41
2:H:64:GLU:CB	4:H:118:HOH:O	2.65	0.41
3:I:145:GLN:CG	4:I:264:HOH:O	2.64	0.41
3:I:145:GLN:HB2	3:I:146:PRO:HD2	2.03	0.41
1:J:22:SER:O	1:J:56:THR:HA	2.20	0.41
3:L:74:VAL:CG1	3:L:75:ILE:N	2.84	0.41
3:I:177:ARG:HH11	3:I:177:ARG:HG2	1.86	0.41
2:E:71:SER:O	2:E:75:MET:HG3	2.21	0.41
3:I:196:LYS:CE	3:I:200:ARG:HH22	2.12	0.41
1:G:24:VAL:HB	1:G:53:ASP:HA	2.03	0.41
1:D:70:GLN:HG3	2:E:79:TYR:HD1	1.85	0.41
3:F:181:VAL:HG12	3:F:182:ARG:N	2.36	0.41
3:C:96:GLN:HA	3:C:97:PRO:HD2	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:64:GLU:OE1	2:H:64:GLU:HA	2.21	0.40
1:A:46:LYS:HZ2	1:A:61:GLY:HA3	1.85	0.40
3:C:177:ARG:HG2	3:C:177:ARG:HH11	1.85	0.40
2:H:103:LEU:HD22	3:I:158:LEU:HD21	2.03	0.40
3:I:68:SER:O	3:I:70:GLU:N	2.54	0.40
3:C:198:LEU:HA	3:C:198:LEU:HD23	1.89	0.40
1:A:4:PHE:N	1:A:67:ALA:HB1	2.33	0.40
2:E:46:LEU:C	2:E:46:LEU:HD12	2.42	0.40
1:A:7:ILE:HD11	1:A:27:LEU:CD2	2.52	0.40
3:C:75:ILE:HG22	3:C:147:ILE:O	2.22	0.40
1:D:4:PHE:N	1:D:67:ALA:HB1	2.34	0.40
1:A:38:PRO:HA	1:A:39:PRO:HD3	1.96	0.40
1:G:41:GLU:HG2	1:G:81:ALA:HB2	2.03	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:70:GLU:OE2	3:F:142:VAL:O[6_565]	2.17	0.03

## 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	96/118 (81%)	85 (88%)	5 (5%)	6 (6%)	2	2
1	D	96/118 (81%)	85 (88%)	5 (5%)	6 (6%)	2	2
1	G	96/118 (81%)	85 (88%)	5 (5%)	6 (6%)	2	2
1	J	96/118 (81%)	85 (88%)	5 (5%)	6 (6%)	2	2
2	B	84/112 (75%)	82 (98%)	2 (2%)	0	100	100
2	E	84/112 (75%)	81 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	84/112 (75%)	81 (96%)	3 (4%)	0	100	100
2	K	84/112 (75%)	81 (96%)	3 (4%)	0	100	100
3	C	140/160 (88%)	127 (91%)	6 (4%)	7 (5%)	3	5
3	F	140/160 (88%)	128 (91%)	5 (4%)	7 (5%)	3	5
3	I	140/160 (88%)	127 (91%)	7 (5%)	6 (4%)	3	7
3	L	140/160 (88%)	126 (90%)	8 (6%)	6 (4%)	3	7
All	All	1280/1560 (82%)	1173 (92%)	57 (4%)	50 (4%)	4	8

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	ALA
3	C	142	VAL
3	C	143	ASP
3	C	145	GLN
1	D	81	ALA
3	F	142	VAL
3	F	143	ASP
3	F	145	GLN
1	G	11	LYS
1	G	81	ALA
3	I	142	VAL
3	I	143	ASP
3	I	145	GLN
1	J	81	ALA
3	L	142	VAL
3	L	143	ASP
3	L	145	GLN
1	A	11	LYS
1	A	84	THR
1	A	97	PRO
3	C	90	ASN
1	D	11	LYS
1	D	84	THR
1	D	97	PRO
3	F	90	ASN
1	G	84	THR
1	G	97	PRO
1	J	11	LYS
1	J	84	THR

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Mol	Chain	Res	Type
1	J	97	PRO
1	D	10	HIS
1	G	10	HIS
1	J	10	HIS
3	L	90	ASN
1	A	10	HIS
1	A	80	ARG
3	C	69	ARG
1	D	80	ARG
3	F	69	ARG
3	F	140	LEU
1	G	80	ARG
3	I	69	ARG
3	I	90	ASN
1	J	80	ARG
3	L	69	ARG
3	C	103	PRO
3	C	140	LEU
3	F	103	PRO
3	I	103	PRO
3	L	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	81/103 (79%)	75 (93%)	6 (7%)	17	39
1	D	81/103 (79%)	74 (91%)	7 (9%)	13	29
1	G	81/103 (79%)	75 (93%)	6 (7%)	17	39
1	J	81/103 (79%)	74 (91%)	7 (9%)	13	29
2	B	76/96 (79%)	72 (95%)	4 (5%)	28	57
2	E	76/96 (79%)	72 (95%)	4 (5%)	28	57
2	H	76/96 (79%)	72 (95%)	4 (5%)	28	57
2	K	76/96 (79%)	72 (95%)	4 (5%)	28	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	130/147 (88%)	125 (96%)	5 (4%)	40	71
3	F	130/147 (88%)	125 (96%)	5 (4%)	40	71
3	I	130/147 (88%)	125 (96%)	5 (4%)	40	71
3	L	130/147 (88%)	125 (96%)	5 (4%)	40	71
All	All	1148/1384 (83%)	1086 (95%)	62 (5%)	27	56

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	13	THR
1	A	27	LEU
1	A	50	LEU
1	A	53	ASP
1	A	70	GLN
2	B	64	GLU
2	B	70	LEU
2	B	103	LEU
2	B	104	LEU
3	C	69	ARG
3	C	77	CYS
3	C	118	LEU
3	C	148	PHE
3	C	186	GLU
1	D	3	VAL
1	D	13	THR
1	D	27	LEU
1	D	39	PRO
1	D	50	LEU
1	D	53	ASP
1	D	70	GLN
2	E	64	GLU
2	E	70	LEU
2	E	103	LEU
2	E	104	LEU
3	F	69	ARG
3	F	77	CYS
3	F	118	LEU
3	F	148	PHE
3	F	186	GLU
1	G	3	VAL

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Mol	Chain	Res	Type
1	G	13	THR
1	G	27	LEU
1	G	50	LEU
1	G	53	ASP
1	G	70	GLN
2	H	64	GLU
2	H	70	LEU
2	H	103	LEU
2	H	104	LEU
3	I	69	ARG
3	I	77	CYS
3	I	118	LEU
3	I	148	PHE
3	I	186	GLU
1	J	3	VAL
1	J	13	THR
1	J	27	LEU
1	J	39	PRO
1	J	50	LEU
1	J	53	ASP
1	J	70	GLN
2	K	64	GLU
2	K	70	LEU
2	K	103	LEU
2	K	104	LEU
3	L	69	ARG
3	L	77	CYS
3	L	118	LEU
3	L	148	PHE
3	L	186	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	GLN
3	C	141	ASN
3	C	174	ASN
1	D	49	GLN
1	D	70	GLN
3	F	132	GLN
3	F	141	ASN
3	F	174	ASN

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Mol	Chain	Res	Type
1	G	70	GLN
2	H	35	HIS
3	I	141	ASN
3	I	174	ASN
1	J	70	GLN
3	L	141	ASN
3	L	174	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.